School of Education

Learning Molecular Structures and Interactions Using Immersive Virtual Reality

Henry Matovu

0000-0003-0503-5416

This thesis is presented for the Degree of

Doctor of Philosophy

of

Curtin University

March 2024

Declaration

To the best of my knowledge and belief, this thesis contains no material previously published by any other person except where due acknowledgement has been made.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Human Ethics The research presented and reported in this thesis was conducted in accordance with the National Health and Medical Research Council National Statement on Ethical Conduct in Human Research (2007) – updated March 2014. The proposed research study received human research ethics approval from the Curtin University Human Research Ethics Committee (EC00262), Approval Number HRE2020-0081.

Signature: ……………………………………….

Date: ………………………………..……..

Acknowledgement

I would like to extend my deepest gratitude to Associate Professor Mihye Won, my principal supervisor, for the opportunity to work with you on this amazing chemistry visualisation project. Your unwavering support, insightful feedback, encouragement, and mentorship have enhanced the quality of my research and shaped my growth as a researcher. I would like to thank Professor David Treagust for your timely feedback and guidance, along with the delightful dinners and trips that kept me sane during the demanding PhD program. I would also like to thank Professor Mauro Mocerino for generously sharing your expertise, experiences, and invaluable insights that have greatly enriched my research project. My sincere appreciation goes to Professor Roy Tasker and Professor Chin-Chung Tsai for your thoughtful feedback and collaboration. It has been a great privilege for me to work with you. I express my gratitude to fellow PhD students on the research team, Dewi and Bruno, for all your support along this journey. A heartfelt thank you also goes to the friends from Curtin Humanities HDR Hub and the Department of Chemistry. The shared experiences and discussions have made my PhD journey both enriching and enjoyable. Special thanks go to my best friend Brendah for your patience, encouragement, and understanding during my absence, and to my family for their unwavering support throughout my personal and academic journeys.

The research in this thesis was funded by the Australian Research Council Discovery Projects, *Drawing science diagrams to enhance students' scientific* creativity (DP180100143) and *Using immersive virtual reality to enhance students' scientific visualisation* (DP190100160).

Abstract

Visualising molecular structures and their interactions is often challenging for students. However, due to its 3D visualisation and motion-tracking capabilities, and opportunities for collaborative learning, immersive Virtual Reality (IVR) technology holds promise to support students' learning of these abstract concepts. This thesis aimed to critically evaluate how undergraduate students learn about molecular structures and interactions using IVR. First, to identify trends and gaps in the use of IVR for science learning, a systematic review of the literature was conducted (study 1). The review identified the need for more pedagogical considerations in IVR design, and comprehensive evaluation of IVR-based learning. Empirical case studies were then conducted to explore the influence of a collaborative IVR activity on students' conceptual understanding of hydrogen bonds in snowflakes (studies 2-3). Analysis of pre-/post- interviews and student-generated diagrams revealed marked improvements in students' conceptual understanding after the collaborative IVR experience. This thesis further investigated how different designs of learning tasks influenced students' interactions to learn hydrogen bonds and enzyme-substrate reactions in collaborative IVR contexts (study 4). Qualitative analysis of students' interactions in different IVR contexts revealed that students engaged in extensive social and conceptual interactions during the tasks that demanded embodied exploration of concepts. Overall, this thesis illustrates significant learning benefits of collaborative IVR and generates insights for innovative and effective utilisation of IVR in science education.

Keywords: Immersive Virtual Reality; Technology-Enhanced Learning; Human-Computer Interaction; Collaborative Learning; Chemistry Education

Table of Contents

Declaration ii
Acknowledgement iii
Abstract iv
Table of Contents v
List of Tables vii
List of Figures viii
List of Publications Comprising This Thesis ix
Statement of Contribution to Co-authored Published Paper 1 x
Statement of Contribution to Co-authored Published Paper 2 xi
Statement of Contribution to Co-authored Published Paper 3 xii
Statement of Contribution to Co-authored Published Paper 4 xiii
Chapter 1. Introduction 1
1.1. The Importance and Challenges of 3D Visualisation in Chemistry 1
1.2. IVR to Support Students' Visualisation of Chemistry Topics 3
1.3. Design, Implementation, and Evaluation of IVR For Chemistry Learning 4
1.4. Collaborative Learning in IVR 6
1.5. Research Aims and Questions 7
1.6. Overview of the Research Methods 8
Chapter 2. Designing and Evaluating Immersive Virtual Reality Learning Environments 11
2.1. Theoretical Backgrounds 11
2.2. Research Methods: The Systematic Literature Review 19
2.3. Research Methods: Empirical Studies for Evaluating Students' Learning in IVR 20
2.4. Ethical Considerations 28
Chapter 3. Immersive Virtual Reality for Science Learning: Design, Implementation, and Evaluation 30
3.1. Abstract 31
3.2. Introduction 31
3.3. Immersive Design Features for Educational IVR Applications 33
3.4. Methods 37
3.5. Results 50
3.6. Discussion 70
3.7. Limitations of the Study 72
3.8. Conclusion 72
Chapter 4. Analysis of Students' Diagrams of Water Molecules in Snowflakes to Reveal Their Conceptual Understanding of Hydrogen Bonds 74
4.1. Abstract 75
4.2. Introduction 75

4.3. Theoretical Framework ... 76
4.4. Methods ... 81
4.5. Findings ... 85
4.6. Discussion ... 97
4.7. Implications ... 101
4.8. Limitations ... 103
4.9. Conclusion ... 104

Chapter 5. Change in Students' Explanation of the Shape of Snowflakes After Collaborative Immersive Virtual Reality ... 105

5.1. Abstract ... 106
5.2. Introduction ... 106
5.3. Materials and Methods ... 110
5.4. Findings ... 120
5.5. Discussion ... 133
5.6. Implications ... 135
5.7. Limitations ... 136
5.8. Conclusions ... 137

Chapter 6. The Perceived Complexity of Learning Tasks Influences Students' Collaborative Interactions in Immersive Virtual Reality ... 138

6.1. Abstract ... 139
6.2. Introduction ... 139
6.3. Collaborative Interactions in Digital Learning Environments ... 141
6.4. Methods ... 143
6.5. Findings ... 146
6.6. Discussion ... 154
6.7. Theoretical Contribution and Limitations of This Study ... 156
6.8. Conclusions ... 158

Chapter 7. Discussion and Conclusion ... 159

7.1. Addressing the Four Research Questions ... 159
7.2. Investigating the Potential of IVR for Enhancing Science Learning ... 166
7.3. Implications of This Research ... 170
7.4. Limitations of This Research ... 173
7.5. Conclusion ... 175

References ... 177

Appendix A: Pre-Interview prompts ... 197

Appendix B: Post-Interview Prompts ... 199

Appendix C: Copyright Approval ... 201

List of Tables

Table 2.1 An Excerpt of a Multimodal Transcript from a Synchronised Video of an IVR Activity 27

Table 3.1 Inclusion and Exclusion Criteria for the Studies 41

Table 3.2 Coding Scheme for Evaluation of the Immersive Design Features in IVR Studies 46

Table 3.3 Average Levels of Integration of the Immersive Design Features Depending on the Rationales for Adopting IVR 60

Table 3.4 Achieved Learning Outcomes in Studies with Different Rationales for Adopting IVR 63

Table 3.5 Reported Learning Experience Evaluations 64

Table 3.6 Average Immersive Design Feature Integration Levels and Achieved Learning Outcomes 68

Table 4.1 Target Concepts and Interview Prompts to Support Students' Drawings in the Drawing Activity 83

Table 4.2 Categories of the Students' Diagrams on Hydrogen Bonds Among Water Molecules in Snowflakes 87

Table 5.1 Categories of Students' Conceptual Understanding of the Nature of Hydrogen Bonds Among Water Molecules in Snowflakes 116

Table 5.2 Categories of Students' Explanations of the Shape of Snowflakes 119

Table 5.3 Changes in Students' Conceptual Understanding of the Nature of Hydrogen Bonds Among Water Molecules in Snowflakes 121

Table 5.4 Retaining Preconceptions After IVR: Diagrams and Explanations Produced by Ross 123

Table 5.5 Recognition of the Role of Lone Pairs of Electrons in the Formation of Hydrogen Bonds After IVR: Diagrams and Explanations Produced by Collin 124

Table 5.6 Recognition of the 3D Nature of Molecular Interactions After IVR: Diagrams and Explanations Produced By Brian 125

Table 5.7 Comparison of the Changes in Students' Conceptual Understanding Made by Individual and Collaborative Students 127

Table 5.8 Changes in Students' Explanations of the Shape of Snowflakes After IVR 129

Table 6.1 An Excerpt of Jesse and Noah's Interaction in Snowflakes IVR 149

Table 6.2 An Excerpt of Noah and Jesse's Interaction in Protein IVR 153

List of Figures

Figure 2.1 Some of the Learning Tasks Completed by Students in Snowflakes IVR 23

Figure 2.2 Some of the Learning Tasks Completed by Students in Protein IVR 24

Figure 3.1 The Literature Selection Chart 38

Figure 3.2 Immersive Design Features Adopted in IVR Studies 55

Figure 4.1 Examples of Students' Diagrams Showing Difficulties in Reasoning About the Structure of Water Molecules and/or the Nature of Intermolecular Interactions 89

Figure 4.2 Examples of Students' Diagrams Illustrating Difficulties in Reasoning About the Directionality of Hydrogen Bonds 90

Figure 4.3 Examples of Students' Diagrams Showing Three Partially Charged Regions in Water Molecules Forming Hydrogen Bonds 92

Figure 4.4 Examples of Students' Diagrams Showing Hydrogen Bond Formation with Individual Nonbonding Electrons 92

Figure 4.5 Examples of Students' Diagrams Showing the Formation of Hydrogen Bonds in 2D 94

Figure 4.6 Examples of Students' Diagrams Showing Water Molecules Forming Multiple Hydrogen Bonds in 2D 95

Figure 4.7 Examples of Students' Diagrams Showing Water Molecules Forming Hydrogen Bonds in 3D 96

Figure 5.1 Some of the IVR Learning tasks on Hydrogen Bonds Among Water Molecules in Snowflakes 110

Figure 5.2 Examples of Images of Snowflakes Used in the Pre-interview..................................... 113

Figure 6.1 Some of the Learning Tasks Completed by Students in Snowflakes and Protein IVR Contexts 145

Figure 6.2. Students' Initial Attempts at Forming a Hydrogen Bond Between Water Molecules.. 147

Figure 6.3 An Example of Students' Illustrations of an Enzyme-Substrate Reaction Before IVR 151

List of Publications Comprising This Thesis

This thesis is presented with a series of publications.

1. Matovu, H., Ungu, D. A. K., Won, M., Tsai, C.-C., Treagust, D. F., Mocerino, M., & Tasker, R. (2023). Immersive virtual reality for science learning: Design, implementation, and evaluation. *Studies in Science Education*, *59*(2), 205-244. https://doi.org/10.1080/03057267.2022.2082680.
2. Matovu, H., Won, M., Treagust, D. F., Mocerino, M., Ungu, D. A. K., Tsai, C.-C., & Tasker, R. (2023). Analysis of students' diagrams of water molecules in snowflakes to reveal their conceptual understanding of hydrogen bonds. *Chemistry Education Research and Practice*, *24*, 437-452. https://doi.org/10.1039/d2rp00175f.
3. Matovu, H., Won, M., Treagust, D. F., Ungu, D. A. K., Mocerino, M., Tsai, C.-C., & Tasker, R. (2023). Change in students' explanation of the shape of snowflakes after collaborative immersive Virtual Reality. *Chemistry Education Research and Practice*, *24*(2), 509-525. https://doi.org/10.1039/D2RP00176D.
4. Matovu, H., Won, M., Hernandez-Alvarado, R. B., Ungu, D. A. K., Treagust, D. F., Tsai, C.-C., Mocerino, M., & Tasker, R. (2024). The perceived complexity of learning tasks influences students' collaborative interactions in immersive Virtual Reality. *Journal of Science Education and Technology*. Onine first. https://doi.org/10.1007/s10956-024-10103-1.

I warrant that I have obtained, where necessary, permission from the copyright owners to use any third-party copyright material reproduced in the thesis, or to use any of my own published work (e.g., journal articles) in which the copyright is held by another party (e.g., publisher; please see Appendix C).

Statement of Contribution to Co-authored Published Paper 1

Chapter Three includes the content of the co-authored paper "Immersive virtual reality for science learning: Design, implementation, and evaluation", published in *Studies in Science Education* in 2023. The bibliographic details of the paper, including all authors are:

Matovu, H., Ungu, D. A. K., Won, M., Tsai, C.-C., Treagust, D. F., Mocerino, M., & Tasker, R. (2023). Immersive virtual reality for science learning: Design, implementation, and evaluation. *Studies in Science Education*, *59*(2), 205-244. https://doi.org/10.1080/03057267.2022.2082680.

I, Henry Matovu, as the primary author, undertook the leading role in data collection, analysis, and manuscript writing. The co-authors contributed to data analysis for inter-rater reliability, reviewed the manuscript, and/or supervised the research.

Henry Matovu ……………………………………………………

I, as a co-author, endorsed that this level of contribution indicated above by the candidate is appropriate.

Dewi A.K. Ungu ……………………………………………………

Mihye Won ……………………………………………………

Chin-Chung Tsai ……………………………………………………

David F. Treagust ……………………………………………………

Mauro Mocerino ……………………………………………………

Roy Tasker ……………………………………………………

Statement of Contribution to Co-authored Published Paper 2

Chapter Four includes the content of the co-authored paper "Analysis of students' diagrams of water molecules in snowflakes to reveal their conceptual understanding of hydrogen bonds", published in *Chemistry Education Research and Practice* in 2023. The bibliographic details of the paper, including all authors are:

Matovu, H., Won, M., Treagust, D. F., Mocerino, M., Ungu, D. A. K., Tsai, C.-C., & Tasker, R. (2023). Analysis of students' diagrams of water molecules in snowflakes to reveal their conceptual understanding of hydrogen bonds. *Chemistry Education Research and Practice*, *24*, 437-452. https://doi.org/10.1039/d2rp00175f.

I, Henry Matovu, as the primary author, undertook the leading role in data collection, analysis, and manuscript writing. The co-authors contributed to data analysis for inter-rater reliability, reviewed the manuscript, and/or supervised the research.

Henry Matovu ……………………………………………………

I, as a co-author, endorsed that this level of contribution indicated above by the candidate is appropriate.

Mihye Won ……………………………………………………

David F. Treagust ……………………………………………………

Mauro Mocerino ……………………………………………………

Dewi A. K. Ungu ……………………………………………………

Chin-Chung Tsai ……………………………………………………

Roy Tasker ……………………………………………………

Statement of Contribution to Co-authored Published Paper 3

Chapter Five includes the content of the co-authored paper "Change in students' explanation of the shape of snowflakes after collaborative immersive Virtual Reality", published in *Chemistry Education Research and Practice* in 2023. The bibliographic details of the paper, including all authors are:

Matovu, H., Won, M., Treagust, D. F., Ungu, D. A. K., Mocerino, M., Tsai, C.-C., & Tasker, R. (2023). Change in students' explanation of the shape of snowflakes after collaborative immersive virtual reality. *Chemistry Education Research and Practice*, *24*(2), 509-525. https://doi.org/10.1039/D2RP00176D.

I, Henry Matovu, as the primary author, undertook the leading role in data collection, analysis, and manuscript writing. The co-authors contributed to data analysis for inter-rater reliability, reviewed the manuscript, and/or supervised the research.

Henry Matovu ………………………………………………………

I, as a co-author, endorsed that this level of contribution indicated above by the candidate is appropriate.

Mihye Won ………………………………………………………

David F. Treagust ………………………………………………………

Dewi A. K. Ungu ………………………………………………………

Mauro Mocerino ………………………………………………………

Chin-Chung Tsai ………………………………………………………

Roy Tasker ………………………………………………………

Statement of Contribution to Co-authored Published Paper 4

Chapter Six includes the content of the co-authored paper "The perceived complexity of learning tasks influences students' collaborative interactions in immersive Virtual Reality", published in the *Journal of Science Education and Technology* in 2024. The bibliographic details of the paper, including all authors are:

Matovu, H., Won, M., Hernandez-Alvarado, R. B., Ungu, D. A. K., Treagust, D. F., Tsai, C.-C., Mocerino, M., & Tasker, R. (2024). The perceived complexity of learning tasks influences students' collaborative interactions in immersive Virtual Reality. *Journal of Science Education and Technology*. Online first. https://doi.org/10.1007/s10956-024-10103-1

I, Henry Matovu, as the primary author, undertook the leading role in data collection, analysis, and manuscript writing. The co-authors contributed to data analysis for inter-rater reliability, reviewed the manuscript, and/or supervised the research.

Henry Matovu ……………………………………………………

I, as a co-author, endorsed that this level of contribution indicated above by the candidate is appropriate.

Mihye Won ……………………………………………………

Ricardo B. Hernandez-Alvarado ……………………………………………………

David F. Treagust ……………………………………………………

Dewi A. K. Ungu ……………………………………………………

Mauro Mocerino ……………………………………………………

Chin-Chung Tsai ……………………………………………………

Roy Tasker ……………………………………………………

Chapter 1. Introduction

Imagine a classroom where students step into a virtual world, navigating through intricate molecular structures, grabbing and connecting molecules, sharing ideas with peers, and intuitively grasping fundamental chemistry concepts. This scenario is the promise of immersive Virtual Reality (IVR) for enhancing teaching and learning chemistry. Once students wear IVR head-mounted display units, their views of the physical world are replaced with stereoscopic displays of computer-generated graphics (Slater & Sanchez-Vives, 2016). IVR hardware also can track students' body movements (Slater & Sanchez-Vives, 2016). When learners rotate their heads around, their views change as naturally as they would in real life. The motion-tracking capability of IVR allows learners to have first-person interactions with virtual objects and exercise power over their learning.

This thesis critically evaluated undergraduate students' learning of challenging chemistry topics, molecular structures and interactions, in IVR. In this first chapter of the thesis, the importance of 3D visualisation in learning chemistry, the difficulties that students face in learning chemistry, and traditional approaches to teaching chemistry are discussed (Section 1.1). The subsequent sections (1.2-1.4) introduce IVR, its implementation and evaluation in chemistry learning, and the importance of investigating collaboration in IVR-based learning. The chapter concludes with an outline of the research aims (Section 1.5), and a summary of the methods used in this research (Section 1.6).

1.1. The Importance and Challenges of 3D Visualisation in Chemistry

Chemistry learning involves understanding how interactions amongst molecules influence the observable behaviour of substances around us (Wu & Shah, 2004). Therefore, the ability to visualise molecular structures and interactions is vital in learning chemistry. However, the invisible nature of molecules poses a significant challenge for students in comprehending these interactions (Cooper et al., 2013). Consequently, students tend to rely on intuitive ideas which are often inconsistent with scientific theories (Roth, 2008; Talanquer, 2006). Such students' scientifically inconsistent ideas of how the world operates are often referred to as *alternative conceptions* (Gilbert & Watts, 1983; Taber, 1998). The existing literature shows that students at all levels of formal education often have alternative conceptions of fundamental chemistry concepts, such as the particulate nature of matter (e.g., Nyachwaya et al., 2011), intermolecular forces (e.g., Cooper et al., 2015; Ungu et al., 2023), or chemical bonding (e.g., Nakhleh, 1992; Othman et al., 2008).

Chemistry learning also demands that students recognise that real molecules are not as flat as they appear on paper. Therefore, when students look at 2D representations of molecules, they need to reason about molecular structures in 3D and recognise relevant spatial features (e.g., bond distances and angles) within the molecules (Wu & Shah, 2004). Proficiency in 3D molecular visualisation often correlates with better performance in chemistry (Carter et al., 1987; Wu & Shah, 2004). However, visualising molecules in 3D is not a trivial task; many high school and university students have difficulties with this skill (Harle & Towns, 2011; Olimpo et al., 2015; Wu & Shah, 2004). To effectively create 3D mental images, a student must discern frames of reference, depth cues, and geometry in molecules (Boukhechem et al., 2011). At times, students also need to be able to mentally deduce how changes in a molecule, such as rotation, influence the spatial positions of different atoms and the distribution of charge within the molecule (Boukhechem et al., 2011; Furió & Calatayud, 1996; Wu et al., 2001; Wu & Shah, 2004).

Visualising molecules in 3D is often further complicated by the requirement for students to interpret and translate across various forms of molecular representations, which demands sufficient background knowledge and spatial reasoning skills (Kozma et al., 2000; Kozma & Russell, 1997; Wu et al., 2001). For instance, chemists may use a formula to convey the atomic composition of a molecule, a 2D structural diagram to depict the arrangement of the atoms and a 3D molecular model to emphasise spatial details like bond angles in the molecule. However, even concepts typically depicted in 2D often contain 3D information which is conveyed through cues like wedge-dash notation, foreshortened lines, and distorted angles, highlighting bonds going in or out of the plane (Harle & Towns, 2011). Consequently, students lacking the necessary background knowledge may struggle to construct useful mental images of the molecules (Wu & Shah, 2004).

The challenges that students face in visualising chemistry concepts underscore the importance of support from educators, such as providing students with relevant visualisation tools. Research indicates that visualisation skills can be improved by training and practice (Harle & Towns, 2011). Conventional tools like physical molecular models, such as ball-and-stick models, aid students in visualising 3D spatial relationships in molecules. The tools translate 2D representations into tangible 3D structures, enabling hands-on manipulation for a better understanding of molecular shapes (Stieff et al., 2016; Stull et al., 2012). Modified physical models, such as magnetic kits, also allow students to feel forces of attraction between molecules (e.g., Ungu et al., 2023). However, physical models fail to simulate the dynamic nature of molecular interactions. In addition, modelling intricate structures with these tools can be time-consuming and expensive (Al-Balushi & Al-Hajri, 2014). Consequently, students may struggle to grasp the true scale and complexity of molecular systems based on these tools (e.g., Ungu et al., 2023).

Computer visualisation tools that represent molecular structures on 2D screens offer ways to overcome the limitations of physical models. Computer tools accurately represent electron density maps, bond angles and distances, and dynamic interactions in molecules, and can enhance students' understanding of molecular shapes (Abraham et al., 2010; Mistry et al., 2020; Stull et al., 2012). However, students must manipulate the molecular representations using a keyboard and mouse. This mode of interaction is non-intuitive and offers poor correspondence between the action performed and the resulting visible movement of the virtual model. Students may also still have difficulty appreciating the scale and depths of complex molecular structures presented on 2D screens (Qin et al., 2021).

Given the benefits and drawbacks of conventional physical models and 2D computer visualisation tools for supporting students' molecular visualisation and learning, a possible way forward is to explore the potential of a learning medium that can leverage the strengths of both.

1.2. IVR to Support Students' Visualisation of Chemistry Topics

IVR shows promise in supporting students' visualisation of key chemistry topics, such as molecular structures and interactions. IVR technology employs high-fidelity 3D graphics presented through head-mounted display units to represent abstract molecular concepts in tangible forms (Dede et al., 2017). These representations can help students develop 3D mental models of these concepts (Chen, 2010). IVR can also simulate the dynamic nature of molecular interactions (Bennie et al., 2019; Gandhi et al., 2020; Zhao et al., 2022) and provide educators with a means to demonstrate the applicability of science concepts in relevant contexts. With its motion-tracking capabilities, IVR enables learners to explore 3D molecules by walking around and changing perspectives (Dede, 2009; Won et al., 2019). Students can also engage with virtual objects in a first-person, non-symbolic way, testing their ideas by rotating and connecting molecules to revise their conceptions of molecular interactions (Chen, 2010; Fombona-Pascual et al., 2022; Johnson-Glenberg, 2018;

Winn, 1993). Moreover, learners can also share virtual environments to exchange ideas and co-construct knowledge (e.g., Won et al., 2019).

While IVR promises these exciting possibilities for chemistry learning, high-quality educational outcomes are not guaranteed by simply asking students to wear IVR headsets (e.g., Makransky, Terkildsen, et al., 2019). Effectively integrating new visualisation technologies, such as IVR, in education is a complex endeavour; it demands careful consideration of the unique capabilities of the technology and a systematic investigation of when and for whom it is most beneficial (Dalgarno & Lee, 2010). This approach resonates with previous calls from educators emphasising the importance of considering educational contexts and pedagogical needs when adopting new technologies (Fowler, 2015; Mikropoulos & Natsis, 2011). Without first considering these issues, implementing the technology may produce mixed outcomes and some educators may be quick to dismiss its value.

1.3. Design, Implementation, and Evaluation of IVR For Chemistry Learning

Significant improvements in computational powers and display graphics, and accessibility to IVR technology have spurred educators to explore IVR's educational benefits in recent years (Won et al., 2023). IVR hardware options vary widely, ranging from phone-based devices like Google Daydream headsets to stand-alone gear such as Meta Quest, and high-end devices like HTC VIVE Pro headsets which rely on computer processing. These hardware options offer varying experiences to learners (Cummings & Bailenson, 2016), and could influence the achieved learning benefits (Qin et al., 2021). For example, phone-based IVR devices typically display lower-quality visuals and less interactive IVR experiences often resulting in passive observation of content (Won et al., 2023). In contrast, higher-end support interactive experiences, enabling highly embodied interactions with objects in virtual environments (Won et al., 2023).

With improvements in IVR technology, Dede and colleagues (2009; 2017) identified a comprehensive framework for exploring the unique technological and pedagogical design features for educational IVR applications: sensory, actional, narrative and social. Sensory features (e.g., 3D visuals) allow students to experience molecular concepts in a concrete and non-symbolic manner (Dede, 2009). Actional features enable students to manipulate virtual objects and observe the consequences of their actions. Narrative features relate to content design and learning tasks to engage learners, while social features facilitate interactions with teachers for guidance or peers for collaborative knowledge-construction (Won et al., 2023). The comprehensive framework by

Dede and colleagues has been expanded to guide educators in systematically designing and evaluating IVR applications (Won et al., 2023).

Although science educators have started designing IVR for learning, it is currently not clear how they are designing IVR applications for learning (Radianti et al., 2020). Which features of IVR do science educators find most compelling for inclusion in their designs and which learning objectives are desired to be achieved? In addition, although IVR is known for its unique 3D visualisation capability, the literature shows that many chemistry educators use IVR to display simple molecular shapes that can also be easily modelled with molecular model kits (e.g., Brown et al., 2021; Edwards et al., 2019; Fujiwara et al., 2020). This trend prompts fundamental questions about the value of investing in IVR when comparable or even superior learning outcomes can be achieved in traditional classroom settings. How does the design of learning tasks influence students' learning interactions in IVR? Do students recognise the value of IVR when it is used to display conceptually familiar objects?

Researchers are also still divided about the conceptual benefits of IVR (Wu, Yu, et al., 2020). In chemistry learning, current literature showed that educators tend to evaluate students' perceptions of the usefulness of IVR (e.g., Elford et al., 2021) or IVR's impact on students' motivation and engagement rather than conceptual understanding (Bennie et al., 2019; Edwards et al., 2019; Qin et al., 2021). In addition, the evaluation was mainly based on one-time learning opportunities offered to students (e.g., Ferrell et al., 2019). These issues raise scepticism regarding whether any achieved learning outcomes are due to the "novelty" effect of the technology that Clark (1983) warned educators about. Moreover, when educators attempted to investigate students' knowledge gains, they predominantly used multiple-choice questions, and researchers did not provide meaningful contexts to help students integrate concepts learned in IVR (e.g., Brown et al., 2021; Ferrell et al., 2019).

Consequently, there also would appear to be insufficient support for IVR's potential to support learning in the long term. The questionable assessment methods also provide limited evidence of IVR's potential to improve conceptual understanding, which demands higher-order skills such as application and evaluation of information (Krathwohl, 2002). A fair evaluation of IVR-based learning calls for documentation of students' interactions in varied learning contexts. Furthermore, the use of robust assessment methods could allow educators to move beyond assessing students' recall of facts. Such methods include student-generated representations (e.g., diagrams and gestures) which encourage deeper reasoning and integration of concepts among students (Ainsworth et al., 2011; Ainsworth & Scheiter, 2021).

In addition, since collaborative learning is a well-regarded approach in learning settings (e.g., Vygotsky, 1978), educators may want to explore the potential of collaborative IVR environments for supporting chemistry learning. In the section that follows, the importance of investigating this approach in IVR-based learning is further discussed.

1.4. Collaborative Learning in IVR

Another exciting possibility of IVR technology is that it allows students to approach and talk to peers in a shared virtual space, and manipulate shared objects (Barreda-Ángeles et al., 2023). When socially interacting in IVR, students' movements or gestures in the real world produce similar movements in the virtual space, making students feel like they are physically interacting with peers as if they are in the real world (Oh et al., 2018). Despite these possibilities, the adoption of collaborative IVR environments in education is still in very early stages (Won et al., 2023). Instead, most IVR applications are being designed and tested for individual learners (e.g., Ferrell et al., 2019; Fujiwara et al., 2020). This focus on individual learners in IVR may not be because educators do not recognise the value of collaborative learning, but because designing and implementing collaborative IVR designs is financially and technically challenging (Won et al., 2023).

Fortunately, recent developments in IVR technologies have increased access to collaborative IVR spaces through open-source applications such as *Mozilla Hubs* or *Engage VR*. Consequently, some science educators have started exploring the potential of "social" IVR environments for learning. However, most of these educators are still using IVR as spaces for students to meet and simply "talk about" concepts (e.g., Ripka et al., 2020). The few researchers who used IVR as spaces where students could meet, manipulate sharable virtual objects, and co-construct knowledge did not extensively document students' interactions within IVR (e.g., Southgate et al., 2019; Won et al., 2019). This omission raises important research questions: How do students interact with peers in this novel environment? How does the learning context or the design of learning tasks influence students' interactions with peers?

Exploring how students interact in collaborative IVR settings is important because students' collaborative interactions are not always productive and researchers need to know why (Barron, 2003; Kreijns et al., 2003). There are several possibilities; for example, students' collaborative interactions are moderated by factors, such as the nature of learning tasks (Cohen, 1994) or the relational history between the interactants (Kreijns et al., 2022). Complex tasks that require students to draw each member's skills tend to encourage extensive collaborative interactions among students compared to tasks that appear individually manageable (Care et al., 2015; Cohen, 1994). Similarly, compared to friends, strangers may hesitate to engage critically with peers (Janssen et al., 2009). Therefore, investigating how students interact in different collaborative IVR contexts can provide a clearer understanding of how different IVR-based learning tasks constrain or facilitate learning. Such knowledge would allow educators to design IVR learning environments that can promote effective collaborative interactions and learning.

In this context, this thesis aimed to explore how students use collaborative IVR environments to learn molecular structures and interactions in different contexts, such as hydrogen bonds in snowflakes, and enzyme-substrate reactions. Based on the literature on IVR design, students' learning, and assessment of learning, this study documents how educators design, implement, and evaluate IVR-based learning. The thesis also systematically explores what students learn about molecular structures and interactions with IVR and their collaborative interactions in different IVR-based learning contexts. By critically investigating collaborative IVR-based learning, this thesis generates insights in terms of designing collaborative learning tasks in IVR and evaluating collaborative IVR-based science learning.

1.5. Research Aims and Questions

The overarching aim of this thesis was to critically evaluate students' learning of molecular structures and interactions using collaborative IVR. To achieve this multi-faceted aim, this thesis was based on four studies which are elaborated in four research papers. Each of the four studies is guided by one of the following general research questions[1].

1. How do researchers design, implement, and evaluate IVR for science learning? (Study 1 in Chapter 3)
2. What is the level of students' conceptual understanding of hydrogen bonds in snowflakes before a collaborative IVR experience? (Study 2 in Chapter 4)

[1] Each of the four general research questions was addressed through a set of sub-questions as discussed later in this thesis (please see Sections 2.2-2.3).

3. How does students' conceptual understanding of hydrogen bonds and the shape of snowflakes change after a collaborative IVR learning experience? (Study 3 in Chapter 5)
4. How do students interact to learn hydrogen bonding and enzyme-substrate reactions in collaborative IVR contexts? (Study 4 in chapter 6)

In answering research question 1, this thesis systematically identified key trends and gaps in the design, implementation, and evaluation of existing IVR applications for chemistry learning. Answering research question 2 helped to evaluate university students' conceptual understanding of molecular structures and interactions (hydrogen bonds) in snowflakes before participating in a collaborative IVR activity on snowflakes. The third research question then investigated how the collaborative IVR experience changed the students' understanding of hydrogen bonds in snowflakes and the shape of snowflakes. Lastly, to answer research question 4, this thesis study investigated students' multimodal interactions to co-construct their understanding of molecular structures and interactions in different collaborative IVR-based learning contexts. One context dealt with conceptually familiar virtual objects (water molecules in snowflakes), and the other with conceptually unfamiliar virtual objects (enzyme and substrate molecules).

1.6. Overview of the Research Methods

Evaluating students' learning of molecular structures and interactions in collaborative IVR environments necessitated using multiple *methods*. First, to gain an understanding of the trends and gaps in the design, implementation, and evaluation of IVR-based learning in science education, a systematic review of the current literature on IVR-based science learning was necessary. Next, to support an in-depth investigation of what and how students learn about molecular structures and interactions in collaborative IVR settings, qualitative case studies (Cohen et al., 2018; Denzin & Lincoln, 2005) were designed. Multimodal qualitative analyses were employed (Bateman et al., 2017; Kress, 2010) following a constructivist/interpretivist epistemology (Krauss, 2005). The applicability of the constructivist learning approach is discussed below.

Epistemology

The case studies used in this research were conceptualised in the realm of qualitative methodology and adopted an interpretivist epistemology, which emphasises understanding localised meanings of human experience (Krauss, 2005). The interest of this thesis was to understand from their perspectives how students interact and learn in collaborative IVR settings. Human actors construct their understandings and meanings based on their experiences, culture, and context (Krauss, 2005; Treagust & Won, 2023). Individual participants in the same situation can construct their reality and knowledge differently; all reality is subjective (Creswell, 2013). Therefore, this study assumed a constructivist ontology that is aligned with the conception of learning in IVR as involving the construction of meanings through interactions with the environment and other social actors (Huang et al., 2010).

In this study, various methods were selected to respond to the different research questions and to collect reliable and valid data appropriate to the specific nature of each research question. The methods included a systematic literature review and case studies.

The Systematic Review

To answer the first research question, a systematic review of the recent literature on the use of IVR in science education was necessary to explore the state of the art and to identify gaps in the existing studies (Xiao & Watson, 2019). The design, implementation, and evaluation of IVR for science learning in recent studies (2016-2020) were analysed. The rationales for adopting IVR, the purpose and methods of evaluating IVR, and the features commonly adopted in IVR designs for different rationales were evaluated. The different features of IVR programs were evaluated using Dede's (2009; 2017) sensory, actional, narrative, and social design considerations for IVR.

The Empirical Case Studies

To address research questions 2, 3, and 4, three case studies were designed to understand students' learning from IVR, and collaborative meaning-making processes in different collaborative IVR contexts. A case study allows a comprehensive and holistic understanding of an educational phenomenon by providing "thick descriptions" of participants' lived experiences in a naturalistic context (Cohen et al., 2018).

The second and third research questions concerned the evaluation of students' conceptual understanding of molecular structures and interactions (hydrogen bonds) in snowflakes before and after IVR. To allow students multiple ways of expressing conceptual understanding, and to delve deeper into their conceptions of hydrogen bonds in snowflakes, student-generated representations (diagrams, verbal explanations, and gestures) were used for assessment (Ainsworth et al., 2011; Treagust et al., 2017). Semi-structured interviews (Denzin & Lincoln, 2005) were further used to gain insights into students' ideas by prompting students to explain as they constructed diagrams to illustrate their conceptual understanding. Semi-structured interviews explore participants' understanding of their experiences and situations through an interactional dialogue between the researcher and the participants in a relatively informal style (Denzin & Lincoln, 2005). In this study, although the interview prompts were initially set, the researcher was open to students' ideas and adapted interview prompts depending on the participants' responses.

Answering research question 4 involved analysing students' physical, social, and conceptual interactions within collaborative IVR environments through video analysis (Jewitt, 2013). These analyses were complemented by student-generated diagrams and responses from pre- and post-interviews. This was done to fully understand students' interactions and experiences as they completed learning tasks in two different collaborative IVR contexts, one with conceptually familiar virtual objects and the other with conceptually unfamiliar objects.

The chapter that follows provides an overview of the theoretical frameworks employed in this thesis. The specific research questions addressed in the literature review and each empirical study, as well as the methods used to answer these questions, are further elaborated.

Chapter 2. Designing and Evaluating Immersive Virtual Reality Learning Environments

In Chapter 1 (Section 1.5), four main research questions were stated to achieve the aim of this thesis – evaluating how students learn molecular structures and interactions using IVR. The data that this thesis builds on comes from four different studies. Each study aimed to answer one main research question through a series of sub-questions. In addition, each study aimed to build on the information before it to generate more insights regarding what and how students learn in IVR.

The research journey in this thesis started with a systematic literature review which explored the current landscape of IVR utilisation (design, implementation, and evaluation) in science learning settings. The rationale for employing IVR, the design features integrated into IVR applications, and the purpose and methods of evaluating IVR studies were investigated. The systematic literature review identified the need for more focus on pedagogical considerations such as task designs, opportunities for collaboration, and comprehensive evaluation of IVR-based learning. To address these concerns, three collaborative IVR-based environments targeting challenging chemistry topics were designed. Three empirical case studies were then conducted to evaluate in-depth the change in students' conceptual understanding of molecular structures and interactions through collaborative IVR, and the nature of students' collaborative interactions while learning in these environments.

The first section of this chapter (section 2.1) discusses the theoretical backgrounds that guided the research in this thesis. The next section (2.2) summarises the rationale for the literature review and steps taken to review the literature while the last section (2.3) discusses the contribution of the three empirical case studies and summarises the methods used to conduct the studies. The last section (2.4) summarises the ethics considerations adopted in this research.

2.1. Theoretical Backgrounds

3D Visualisation for Chemistry Learning

The ability to visualise and mentally manipulate molecular structures and their interactions in 3D is a fundamental aspect of learning chemistry (Oliver-Hoyo & Sloan, 2014; Wu & Shah, 2004). 3D visualisation skills encompass a range of abilities at different levels of complexity (Echeverri-Jimenez & Oliver-Hoyo, 2023; Harle & Towns, 2011; Tuckey, 1993). At the foundational level is *spatial visualisation* which involves creating precise 3D mental images of molecular structures from 2D representations, taking spatial aspects like depth and angles into account (Barnea, 2000). Building on this skill is *spatial orientation* which entails envisioning how the 3D structure created would appear from a different perspective. At the highest level of complexity are *spatial relations* which involve mentally manipulating 3D objects and visualising the consequences of transformations, such as rotation, reflection, or inversion (Barnea, 2000; Harle & Towns, 2011; Tuckey, 1993).

Substantial evidence indicates a correlation between proficiency in 3D visualisation skills and students' ability to learn and solve chemistry problems (Harle & Towns, 2011; Thayban et al., 2021; Wu & Shah, 2004). Building a coherent understanding of fundamental chemistry topics, such as hydrogen bonds or stereochemistry, requires students to apply their visualisation skills accurately (Barnea, 2000). For instance, explaining why snowflakes have a hexagonal shape is only possible when considering the arrangement of many water molecules in a 3D space. Similarly, differentiating between two forms of phenylalanine (D-phenylalanine which is sweet, and L-phenylalanine which is bitter) with identical connectivity of atoms relies on visualising these molecules in a 3D space (Oliver-Hoyo & Sloan, 2014).

However, novice learners often find it challenging to develop and apply these visualisation skills (Echeverri-Jimenez & Oliver-Hoyo, 2023), especially when dealing with complex structures (Qin et al., 2021). Even conventional teaching approaches that employ 2D diagrams or computer-generated animations on 2D screens have limitations in effectively conveying spatial information, such as depth and scale, to students (Cassidy et al., 2020). Consequently, students often have difficulties understanding concepts and hold diverse alternative conceptions regarding spatially demanding chemistry concepts, such as the hydrogen bonds (e.g., Schmidt et al., 2009; Ungu et al., 2023) or stereochemistry (Boukhechem et al., 2011; Duis, 2011; Durmaz, 2018).

The difficulties in visualising molecular structures also hinder students from establishing clear links between various forms of representations (Wu & Shah, 2004). Chemistry representations are classified into observable (macroscopic) level, particulate (sub-microscopic) level, and symbolic level (Johnstone, 1991). Macroscopic representations pertain to observable phenomena, particulate representations involve models of atoms and molecules, and symbolic representations include chemical symbols, equations, graphs, and formulae (Barnea, 2000). While experts seamlessly translate across the different levels, students often struggle to connect different forms of representations (Kozma & Russell, 1997). Particulate representations are particularly challenging to understand and link to the other levels as they involve abstract and unobservable molecules (Barnea, 2000; Harle & Towns, 2011). Numerous studies have reported alternative conceptions among students regarding the particulate nature of matter (Kern et al., 2010; Nyachwaya et al., 2011). When students cannot visualise and comprehend interactions at the particulate level, they tend to rely on surface features and heuristics to explain macroscopic phenomena (Cooper et al., 2013; Talanquer, 2018).

Considering the importance of 3D visualisation in chemistry, innovative approaches are being explored to support students' learning. Strategic interventions in teaching chemistry, such as the use of molecular models that facilitate the identification of depth cues and the transformation between 2D and 3D representations, can improve students' 3D visualisation skills (Merchant et al., 2013; Oliver-Hoyo & Sloan, 2014; Wu et al., 2001). In this context, IVR emerges as a promising approach for aiding students in visualising and learning challenging chemistry concepts that demand spatial skills (Echeverri-Jimenez & Oliver-Hoyo, 2023; Laricheva & Ilikchyan, 2023). IVR presents concepts in 3D, enabling students to observe them and recognise spatial relationships within structures (Dalgarno & Lee, 2010; Di Natale et al., 2020). In addition, IVR addresses the limitations of common visualisation tools because it can represent dynamic molecular interactions, unlike physical models, or offer a sense of scale in molecular structures, unlike computer visualisation tools (Laricheva & Ilikchyan, 2023; Qin et al., 2021). Moreover, when engaged in IVR, students can naturally manipulate molecular structures by grabbing or rotating to observe spatial relations, an approach shown to enhance students' visualisation skills (Boukhechem & Dumon, 2016).

The research in this thesis utilised IVR to enhance students' visualisation and understanding of chemistry topics that require 3D visualisation skills, such as hydrogen bonds, stereochemistry, and enzyme-substrate reactions. However, educators argue that to fully harness the potential of IVR in aiding students' visualisation, it should be designed to leverage its technological and pedagogical capabilities (Dalgarno & Lee, 2010; Mikropoulos & Natsis, 2011). In addition, providing students opportunities to use multiple representations while visualising molecules has been suggested as a means to improve their learning (Wu & Shah, 2004). The subsequent subsections will discuss the design of IVR for effective learning and the benefits of employing multiple representations in learning.

Dede's Educational IVR Design Considerations

Dede and colleagues (2009; 2017) suggested four key technological and pedagogical considerations for designing IVR applications for learning – sensory, actional, narrative, and social. This comprehensive framework provided a starting point for evaluating IVR applications in the literature and designing those applications used in this research. Dede's categories also served as an overarching framework for the theories underpinning the use of IVR for learning in this research.

Sensory design features. Sensory features of IVR capitalise on the potential of head-mounted display units to block out the user's view of the real world and teleport them into a different reality using stereoscopic images (Slater et al., 2022). Unlike watching a 2D screen, IVR gives a sense of being inside a new environment, experiencing it from a first-person perspective, and perceiving it as real (Di Natale et al., 2020). By engaging all their senses, such as visual, auditory, and haptics, in the new reality, learners can feel a sense of "*being there"* with the objects, also known as the *place illusion* (Slater et al., 2022). This possibility opens unprecedented opportunities for learning, such as the simulation of environments that would normally be dangerous or inaccessible in real life. For example, students can walk through a narrow passageway into an enzyme structure to explore its catalytic chamber in 3D (Won et al., 2019). This allows them to learn spatial relationships in such otherwise abstract structures (Dalgarno & Lee, 2010; Dede, 2009; Di Natale et al., 2020). Adding spatial audio to 3D environments in IVR provides a sense of orientation and distance, while the haptic feature could give students a tactile sense of interacting with virtual objects (Dede, 2009; Huang et al., 2010).

In this research, IVR was used to teleport students to different simulated environments, such as a winter forest, or an enzyme environment. In these environments, abstract concepts, such as structures of water molecules or enzyme and substrate molecules, were represented in 3D. Different forms of 3D representations of the molecules, such as ball and stick models or electron-density maps, were also provided. Electron densities were consistently represented as blue and red regions to highlight electron-poor and electron-rich areas in molecules, respectively. It was anticipated that exploring molecular structures in 3D would support students in visualising and learning abstract chemistry topics. In addition, audio instructions were presented to the learners. Students also shared the physical room with their peers and could hear each other to give a sense of direction.

Actional design features. Through its motion-tracking capability, IVR empowers learners to engage in actions and observe the corresponding consequences (Dede, 2009; Dede et al., 2017). In IVR, when a learner uses their avatar (virtual body) to interact with objects and the objects respond realistically, they feel that they are physically manipulating physical objects and that their actions have real consequences. This feeling, often referred to as the *plausibility illusion* (Slater et al., 2022) or *self-presence* (Lee, 2004), promotes a sense of agency and engagement among students learning in IVR (Johnson-Glenberg, 2019; Makransky & Petersen, 2021). The degree of agency depends on several factors such as the responsiveness of the IVR program towards the learner's actions, the feeling of owning a virtual body, and the ability to interact naturally within the virtual environment through bodily movements (Makransky & Petersen, 2021; Slater et al., 2022).

Students' active interactions in IVR align with the principles of the *constructivist* theory of learning (Chen, 2010). According to the theory, students build their understanding through their interactions with objects and other social actors in the environment (Jonassen, 1994; Winn, 1993). Through these experiences, students can integrate new information into already existing knowledge structures to create new meaning (Huang et al., 2010; Jonassen, 1994). Therefore, it is anticipated that, through interactions with objects and peers in IVR, students can actively revise their conceptions (Chen, 2010). Moreover, embodied cognition researchers also argue that learning designs that make use of body movements and gestures which are congruent with the target concepts, such as those supported by IVR, can promote learning (Johnson-Glenberg, 2018, 2019).

In this research, the IVR applications for chemistry learning were designed so that students could interact with virtual molecules as if they were physical objects to observe the effects of their actions. The IVR applications also supported full-body interactions which aligned with the target concepts to optimise the learning (Johnson-Glenberg, 2019). For example, students could manipulate molecules with their hands to explore the strength of chemical bonds by grabbing, rotating, and adjusting them. They could also walk around and lower their bodies to observe spatial relations between molecular structures from different perspectives.

Narrative design features. Narrative features relate to content and learning task design to engage learners in the relevant contexts (Dede, 2009; Won et al., 2023). Csikszentmihalyi's *flow theory* (2014) suggests that the nature of learning tasks and students' experiences, such as prior knowledge, significantly impact student engagement. When learners perceive themselves as capable and learning tasks as appropriately challenging, they are more likely to invest efforts and remain engaged. Conversely, if learners lack the necessary skills or find the task too easy, they may become frustrated or bored, leading to disengagement.

In this research, relevant *contexts* (such as the formation of snowflakes, and enzyme-substrate reactions) were simulated in IVR so students could explore the relevance of molecular structures and interactions. These IVR-based learning contexts featured various virtual objects, some of which were conceptually familiar to students (water molecules), while others were unfamiliar (e.g., complex enzyme and substrate molecules) to promote students' engagement. The learning tasks were also intentionally designed to vary in complexity to maintain learner engagement by presenting challenges that aligned with various levels of abilities.

Social design features. As discussed in Section 1.4, IVR has the potential to support social interactions for knowledge co-construction among learners. For instance, within IVR, students can engage in both verbal and non-verbal communication (e.g., Southgate et al., 2019), creating a sense that students are physically present in the same space (Kreijns et al., 2022; Oh et al., 2018). The use of sharable objects in IVR facilitates turn-taking, enabling students to express and elaborate on their ideas (Zheng et al., 2018). Collaboration in virtual learning environments also increases the students' sense of engagement in the virtual environment and learning tasks (Dalgarno & Lee, 2010; Krämer, 2017).

The *social constructivist* theory of learning (Vygotsky, 1978) maintains that such social interactions with peers are key drivers of learning. For instance, peer-to-peer interactions help students generate varied conceptual perspectives (e.g., Šašinka et al., 2019). Explaining to peers also encourages self-reflection and organisation of one's understanding (Webb, 2009). Considering such benefits of collaboration in learning, the IVR applications employed in this research were designed so that students completed IVR-based learning tasks in pairs. It was anticipated that, by engaging in the co-construction of knowledge with peers, each student would achieve more from IVR than they would if they worked independently (Vygotsky, 1978).

Multiple Representations for Learning and Assessment

Learning complex ideas, such as molecular structures and interactions, can be mediated by different external representations (Ainsworth, 2006), such as formulae, 3D models, diagrams, and audio/verbal explanations (Ainsworth, 2018; Treagust et al., 2017). According to Ainsworth (1999, 2006), these different presentations support learning in three main ways – *complementing*, or *constraining* understanding, or helping students *construct deeper* understanding.

The complementary benefits of multiple representations for learning arise when the information or learning processes (or problem-solving strategies) supported by one representation are enhanced using another form of representation. For instance, in some cases, providing all information about a concept in one form of representation can make it confusing for students (Ainsworth, 1999). Therefore, providing different representations and exploiting the differences between the information provided by each representation can help students learn when they complement information in one representation with another (Ainsworth, 1999, 2006). Constraining understanding relates to using one representation to support the interpretation of another unfamiliar representation. For example, a lattice structure of many water molecules in ice can help students avoid interpreting a snowflake as one involving a few water molecules interacting in a flat plane. Additionally, when learners integrate information from different representations, they can construct a deeper conceptual understanding (Ainsworth, 2006). For example, by looking at a lattice structure of ice, students can extend their knowledge beyond the hexagonal arrangements of water molecules to recognise the many possibilities in expanding the structure to result in variations in the appearance of snowflakes.

In this research, collaborative IVR environments were used to support students' learning of molecular structures and interactions in different contexts, such as the formation of snowflakes or enzyme-substrate reactions. The research leveraged the sensory features of IVR as multiple external representations to facilitate learning by complementing, constraining, or allowing the construction of understanding (Ainsworth, 1999), and shaping conversations for meaning-making (Kozma, 2003). In each IVR context, students explored different visual representations of molecular structures. For example, to learn hydrogen bonds, students interacted with 3D models of water molecules (highlighting the geometry and polarities in the molecules), a lattice structure of ice, and models of macroscopic snowflake shapes. Similarly, when learning about enzyme structures, students could switch between different modal representations of the protein structure, each highlighting different aspects, such as the electron density, atomic composition, secondary and tertiary structures, or the carbon chain. Moreover, in each context, in addition to visual information, students were also provided with audio instructions about the relevant processes (e.g., the growth of snowflakes, or the mechanism of the reaction between the enzyme and its substrate).

Despite the anticipated benefits of multiple representations in learning, previous studies indicated that students do not automatically achieve better learning when they use multiple representations (Kuo et al., 2017; Won et al., 2014). To benefit, learners must fully understand the relation between the different representations and be able to translate freely across different representations (Ainsworth, 2006). Unlike experts who can easily relate different representations and use them in reasoning, many students often find it hard to establish relations between representations (Kozma et al., 2000). Therefore, it is critical to explore how students use different representations in collaborative IVR (sensory features) to learn.

Assessing understanding from multiple representations also demands using approaches that assess students' knowledge structures at a deeper level (Ainsworth, 1999). Indeed, one of the aims of this research was to evaluate students' conceptual understanding of molecular structures and interactions before and after a collaborative IVR. Conceptual understanding encompasses students' knowledge of scientific facts and their ability to apply their knowledge in new situations such as explaining scientific phenomena (Holme et al., 2015). Therefore, it seemed fitting to explore students' understanding using ways in which they could demonstrate what they knew.

In this research, students were asked to draw diagrams to elaborate on their understanding. These student-generated diagrams were triangulated with students' verbal explanations and gestures. These different representations were used because human communication is multimodal in nature (Jewitt, 2013). Previous studies also suggest that students benefit more when they are allowed to construct their representations, rather than interpret already developed ones (Tytler et al., 2013). Drawing diagrams provides students an opportunity to select the most relevant spatial features of phenomena, organise them, and represent them visually (Cooper et al., 2017; Wu & Rau, 2019). In this way, students not only develop a coherent understanding of chemical phenomena but also make their mental models of science concepts visible (Ainsworth et al., 2011; Tippett, 2016). Through diagrams, educators can identify alternative conceptions in students' ideas, and students can illustrate their understanding that may not be explicitly articulated through verbal explanations (Cooper et al., 2017; McLure et al., 2021a). Consequently, student-generated representations can be a useful approach for assessing students' conceptual understanding (Tippett, 2016).

2.2. Research Methods: The Systematic Literature Review

Rationale and Research Questions Addressed

Study 1 (presented in Chapter 3) was conducted to explore the breadth and width of the existing body of work on IVR and identify the current trends and gaps in the design, implementation, and evaluation of IVR in science learning settings. These particular aspects were explored because they influence students' learning experience (Cummings & Bailenson, 2016), and learning outcomes (Clark, 1994). To achieve this aim, a systematic review of the literature was conducted. Dede's (2009; 2017) immersive interface design framework of sensory, actional, narrative, and social design features was adopted and reconceptualised into a set of 10 concrete IVR design features (visual, audio, haptics, interactivity, virtual body, embodied movements, context, storyline, challenge, and social). The reconceptualised framework helped to identify what design features were often employed to achieve learning goals and which features were underutilised in current educational IVR studies. The overarching research question for Study 1 was: "*How do researchers design, implement, and evaluate IVR for science learning?*" To answer this research question, the following specific questions were addressed:

1. What were the rationales for adopting IVR in science education?
2. What learning theories were identified and incorporated in the design, implementation, and evaluation of IVR learning activities?
3. What immersive design features were incorporated in IVR studies?
4. Did the immersive design features incorporated differ for different rationales for adopting IVR?
5. How were IVR learning activities evaluated and what learning outcomes were achieved through IVR learning activities?
6. Did the evaluation of learning activities and achieved learning outcomes differ for different rationales for adopting IVR?
7. Did particular immersive design features lead to more positive learning outcomes?
8. Did learners with particular characteristics report more positive learning outcomes?

Procedure

The guidelines for Preferred Reporting Items for Systematic Reviews and Meta-analyses (PRISMA; Page et al., 2021) were followed. The literature analysed was systematically identified from five scholarly databases (ProQuest, Google Scholar, Springer Link, Web of Science, and Scopus) with a complementary search on two other databases (ERIC and IEEE *Xplore*). A total of 64 articles published from 2016 to 2020 were identified and analysed. The year 2016 was selected as the starting year because high-end IVR headsets, such as HTC's VIVE and Meta's Oculus Rift, became available this year which increased the number of studies exploring the educational potential of IVR in science learning. Detailed information on the search process and literature analysis is presented in Chapter 3.

2.3. Research Methods: Empirical Studies for Evaluating Students' Learning in IVR

Rationales and Research Questions

As discussed in Sections 1.3 and 1.4, there were divided opinions among science educators about the effectiveness of IVR in enhancing conceptual understanding, limited evaluation of learning from IVR, and a limited focus on collaborative learning in IVR. The results from Study 1 also confirmed these trends. Therefore, three empirical studies were designed to evaluate the conceptual benefits of collaborative IVR for learning challenging chemistry topics and to document the process of students' learning in IVR. The empirical studies were based on three IVR activities focusing on hydrogen bonds in snowflakes, stereochemistry in the context of taste receptors, and molecular shape and electron density in enzyme-substrate reactions. These topics require students to visualise molecular structures and their functions in 3D, which can be challenging to many students, as previously discussed in section 2.1. In this research, it was anticipated that, by making use of sensory and actional features, well-designed tasks and a collaborative design, students could benefit from using IVR to visualise and learn these topics.

Studies 2 (Chapter 4) and 3 (Chapter 5) aimed to clarify the conceptual benefits of collaborative IVR. Study 2 aimed to assess students' conceptual understanding of hydrogen bonds in snowflakes before engaging in collaborative IVR-based learning. On the other hand, Study 3 aimed to investigate the change in students' conceptual understanding of the nature of hydrogen bonds in snowflakes and the shape of snowflakes after participating in a collaborative IVR-based learning activity.

The primary research question addressed in Study 2 was: "*What is the level of students' conceptual understanding of hydrogen bonds in snowflakes before a collaborative IVR experience?"* The specific research questions addressed in response to this question were:

1. How do students use diagrams to represent their understanding of the nature of hydrogen bonds among water molecules in snowflakes?
2. What are the common conceptions of the nature of hydrogen bonds among water molecules in snowflakes inferred from these student-generated diagrams?

For Study 3, the overarching research question was: *How does students' conceptual understanding of hydrogen bonds and the shape of snowflakes change after a collaborative IVR learning experience?* To answer this question, the following specific research questions were addressed:

1. How do university students change their conceptions of the nature of hydrogen bonds among water molecules in snowflakes after exploring the concept in collaborative IVR?
2. How do university students change their explanations of the shape of snowflakes after exploring the concept in collaborative IVR?

The fourth and final study (Chapter 6) was conducted to provide insights into students' interactions behind learning in collaborative IVR settings. Study 4 aimed to investigate *how* students interact to learn hydrogen bonds, stereochemistry, and enzyme-substrate reactions in different collaborative IVR learning contexts. Understanding how collaborative interactions vary depending on the nature of learning tasks or virtual objects is crucial for designing effective IVR-based learning experiences. The primary research question addressed by Study 4 was: *"How do students interact to learn hydrogen bonding and enzyme-substrate reactions in collaborative IVR contexts?"* To answer this question, Study 4 was designed to answer the following specific questions:

1. How do students interact with conceptually familiar virtual objects in IVR to collaboratively learn chemistry?
2. How do students interact with conceptually unfamiliar virtual objects in IVR to collaboratively learn chemistry?

Research Design: Qualitative Case Studies

This thesis aimed to critically evaluate what and how students learn molecular structures and interactions through collaborative interactions in IVR. To address these aspects, a qualitative case study design (Denscombe, 2017; Yin, 2009) was employed in three empirical studies (Chapters 4-6). Case studies are well-suited for in-depth investigations of complex interactions to answer "*how*" and "*why*" questions, such as those central to this thesis. Case studies allow for a deep investigation of human interactions, how these events unfold in real contexts, and the various factors influencing them (Cohen et al., 2018; Denscombe, 2017). However, the use of case studies in research is a subject of debate due to the unique and complex nature of each case, which may limit generalisability (Denscombe, 2017). Nevertheless, the uniqueness of each case can generate key insights that may be overlooked by other research methods (Cohen et al., 2018). Another challenge is that defining the boundaries of a case can be challenging (Denscombe, 2017), and the salient factors in interactions often only become evident during the investigation (Yin, 2009). In this research, this flexibility was crucial in understanding students' learning benefits and meaning-making processes in IVR-based learning contexts.

Participants

Participants were 70 undergraduate chemistry students at a large public university in Western Australia. These students were enrolled in two first-semester chemistry units of 2021; CHEM 1002 (Reactions and Function in Chemistry) for the first year, and CHEM 2002 (Chemistry of Biological Processes) for second-year students. The units were designed for students with a strong background in chemistry. Students needed to have passed high school chemistry and at least one university-level chemistry unit. Consequently, participants were students pursuing degrees in chemistry-related, such as chemistry, chemical engineering, biochemistry, food science, nutrition, and biomedical science. The two chemistry units were structured with a combination of lectures, laboratory experiments, and interactive tutorial workshops.

The designed IVR activities were integrated into the lab programs, making participation in these IVR activities mandatory for all enrolled students. However, participation in the research itself was voluntary. Students engaged in the activities in pairs. The pairing of students was not directly controlled by the researcher but was based on students' convenience. Consequently, some students were paired with peers with whom they had worked before (friends), while others were paired with peers whom they were meeting for the first time (strangers). For consistency, once the students were paired, they went through all three learning activities with the same peers.

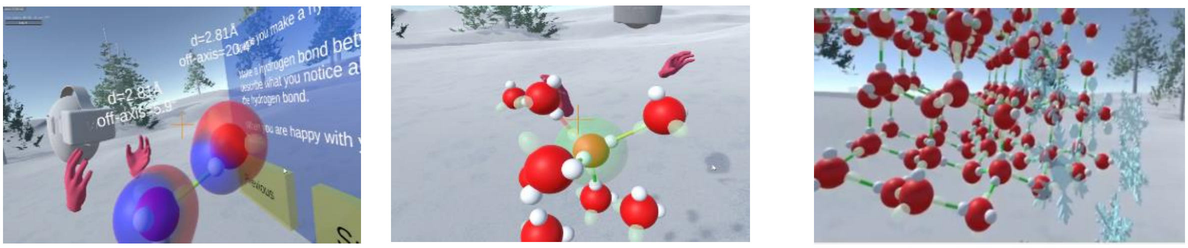
Learning Materials: The IVR Learning Activities.

A multidisciplinary team of researchers developed three IVR activities following the frameworks for IVR design outlined in Section 2.1. First, storyboards were created to identify the key learning tasks in IVR, diagrams and instructions to students. IVR applications were then programmed (primarily using Unity®) and were tested via several testing sessions before data collection. The IVR activities were: Snowflakes IVR targeting the concept of hydrogen bonds in the context of snowflakes; Taste IVR targeting the concept of stereochemistry in the context of taste receptors; and Protein IVR on the reaction between an enzyme (acetylcholinesterase) and its substrate molecule (acetylcholine).

In the first activity, students completed a set of interactive tasks involving water molecules. For example, students explored the nature of a hydrogen bond between two water molecules (Figure 2.1a), the maximum number of water molecules around one central molecule (Figure 2.1b) and later connected many water molecules to form a lattice structure of molecules (Figure 2.1c). The tasks were sequenced from simple to complex, enabling students to progressively apply their understanding in the learning tasks. Similarly, in the last IVR activity (protein IVR), students completed multiple tasks involving an enzyme (acetylcholinesterase) and substrate (acetylcholine) structures, such as those presented in Figure 2.2 (a-c).

Figure 2.1

Some of the Learning Tasks Completed by Students in Snowflakes IVR

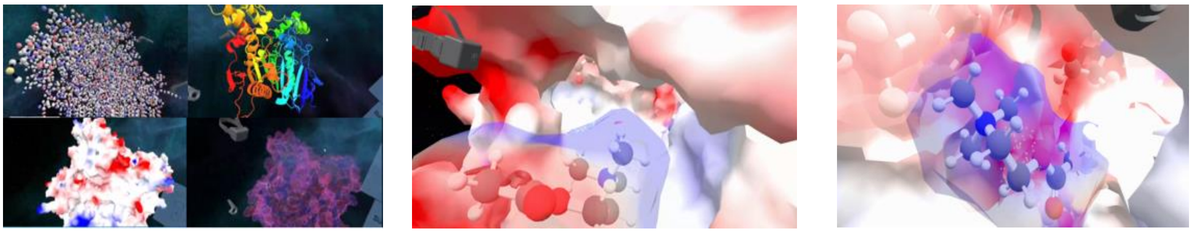


(a) (b) (c)

Note. (a) exploring the nature of a hydrogen bond between two water molecules. (b) connecting many water molecules around one. (c) constructing a lattice structure of ice to explain the shape of snowflakes

Figure 2.2

Some of the Learning Tasks Completed by Students in Protein IVR



(a) (b) (c)

Note. (a) Exploring different modal representations of the protein enzyme (b) Orienting the substrate molecule at the entrance of the enzyme shown. (c) orienting the substrate molecule in the catalytic chamber for the reaction to occur.

At every step in each IVR environment, students received prompts (audio and text instructions) to encourage their exploration of virtual objects and collaborative discussions. For example, to explore the best orientation of the substrate molecule at the entrance of the protein enzyme in the protein IVR environment, a prompt was given "*Decide on the orientation of acetylcholine at the entrance of the enzyme for the reaction to occur. When you are happy with your answer, click the submit button*". Upon clicking the submit button, students were asked to explain their reasoning before proceeding to the next task. In some cases, audio explanations of molecular interactions in each environment were also provided.

Research Procedure

Students completed the three IVR-based learning activities sequentially, with a 2–3-week gap between each pair of activities. Each session involved a semi-structured pre-interview lasting 15-20 minutes, an IVR activity spanning 30-50 minutes, and a semi-structured post-interview taking 20-30 minutes, for each pair of students. The interviews were semi-structured (Brinkmann, 2013; Denzin & Lincoln, 2005) in nature. Semi-structured interviews provide an open framework for two-way communication between the researcher and participants (Brinkmann, 2013).

Pre-interviews aimed to assess students' understanding of the target concepts before engaging in collaborative IVR experiences. For instance, before the snowflakes IVR activity, students were asked to illustrate their ideas of interactions among water molecules in snowflakes and to explain the shape of snowflakes. Similarly, before the protein IVR activity, students were tasked to illustrate their understanding of enzyme-substrate reactions and explain why enzyme reactions were faster than non-enzyme-catalysed reactions. During the interviews, the researcher used verbal prompts to stimulate students' prior knowledge and to allow them to develop their explanations and drawings step-wise. The prompts did not include key concepts, such as hydrogen bonds, as these terms tend to be confused by students (Cooper et al., 2015). For instance, when investigating students' understanding of hydrogen bonds in water molecules, students were simply asked to illustrate how water molecules in snowflakes would interact with each other. The detailed pre-interview prompts are provided in Appendix A.

Following the pre-interviews, students were trained on the use of handheld controllers to interact with virtual objects. They were also briefed on what the IVR environments would look like. Assisted by the researcher, students then donned HTC VIVE Pro Eye headsets with wireless adaptors and handheld controllers to complete the IVR-based learning tasks. HTC VIVE pro eye headsets were chosen for their multi-user interactivity, wide field of view and accurate movement/position tracking. Students were encouraged to discuss their ideas with peers, explore the virtual environment by walking around to change perspectives, and immediately report any form of discomfort with the IVR headsets. Within IVR, students walked around a 4m × 4m physical room to change their perspectives and interacted with the molecular structures by rotating, connecting, and flipping to observe different patterns. The students saw each other's avatars (floating headsets and hands) in a shared virtual space and communicated verbally.

After each IVR session, students' conceptual understanding was re-evaluated. For example, after the snowflakes IVR activity, students were asked to revise their diagrams of water molecule interactions in snowflakes (with reasons) and explanations of the shapes of snowflakes. After the protein IVR activity, students revised their explanations of enzyme-substrate reactions and the difference in rates of enzyme-catalysed reactions and non-enzyme-catalysed reactions. The detailed post-interview prompts are provided in Appendix B.

Qualitative data in the form of audio and videos of learning sessions, screen recordings, pre- and post-interviews, and students' hand-drawn diagrams were collected. All sessions (pre-interview, IVR activity and the post-interviews) were videotaped, each from two different angles. Videos of each student's views of virtual environments during IVR were also recorded using a screen recording application (OBS Studio). Video recording allows researchers to obtain and permanently store details of multimodal interactions that can be revisited for comprehensive analysis (Derry et al., 2010; Norris, 2002).

Data Analysis

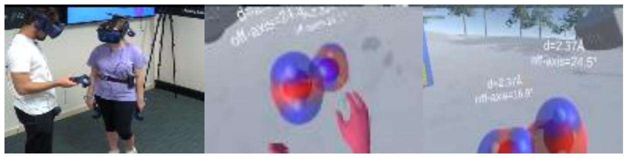
Analysis of students' diagrams of hydrogen bonds in snowflakes. Student-generated diagrams were analysed to explore students' conceptual understanding of hydrogen bonds before and after IVR (Study 2 in Chapter 4, and Study 3 in Chapter 5). This analysis was based on a set of procedures for interpreting student-generated diagrams (McLure et al., 2021b; Tenzin et al., 2022). Student-generated diagrams were first analysed inductively (Merriam & Tisdell, 2015) and then constantly compared to each other to identify categories of students' understanding. To confirm the interpretations of the diagrams, students' verbal explanations and gestures were referred to because the diagram-drawing tasks were embedded in semi-structured interviews. The analyses were also constantly reviewed by other researchers.

Analysis of students' explanations of the shapes of snowflakes. Transcripts of students' explanations (and their gestures) of the shapes of snowflakes before and after IVR were initially analysed inductively (Merriam & Tisdell, 2015). A wide variation in students' ideas and comprehensiveness of the explanations was observed. A combination of both inductive and deductive approaches was then adopted to capture these variations. Common topics in students' explanations were identified: spreading out of molecules, hydrogen bonds, tetrahedral units, 3D lattices, hexagonal shapes among molecules interacting in 2D, hexagonal shapes among molecules interacting in 3D, and variations in patterns of snowflakes. Based on these topics, students' explanations were then coded to identify common patterns or combinations of the key topics. Broader categories were then generated. The detailed categories are further elaborated in Chapter 5.

Analysis of students' interactions in IVR. Before analysis, the videos of students' physical interactions in the iVR room and screen recordings of the students' views in IVR were synchronised. This synchronisation of the records enabled the researcher to review the data multiple times from different perspectives, enhancing the researcher's understanding of the data on a moment-by-moment basis. Multimodal transcripts (Cowan, 2014), such as Table 2.1, were then generated from the synchronised videos. These transcripts facilitated a detailed microanalytic and multimodal interpretation of the events in the interactions. The transcripts also allowed other members of the research team who had access to the data to check and verify patterns in students' behaviour.

Table 2.1

An Excerpt of a Multimodal Transcript from a Synchronised Video of an IVR Activity

Time	Speaker	Room view	Dom's view	Sandra's view
32:22.0 – 32:27.0	Sandra: (Looking at the screen) But it says make a hydrogen bond or …	 (Dom is focused on the numbers; Sandra looks at the instructions on the screen)		
32:27.0 – 32:34.0	Dom: That [d] is the distance between but that's the bond distance, ... What do they mean, by off axis? I think it's not rotated …	 (Dom moves his body to the left to get a clear view of the bond).		

Note. Two students Dom and Sandra are interacting in Snowflakes IVR. Dom (white top) and Sandra (purple top)

Exploring how students interact in collaborative IVR environments (Study 4 in Chapter 6) was a novel endeavour. Initially, the researcher, in collaboration with the IVR research team, watched some of the synchronised videos to identify key aspects of the interactions. Subsequently, the analysis utilised a constant comparison method (Glaser, 1965) to identify any emerging patterns. The focus of the analysis was students' physical interactions (movements, actions, and positions in IVR space), conceptual discussions, and social dynamics (patterns in generating, introducing, and elaborating on ideas, negotiating control of virtual objects, and negotiating consensus).

Validity and reliability. Initially, the researcher had limited experience conducting interview sessions. During the early stages of data collection, interviews were conducted with two or more other IVR team members (including doctoral supervisors) present to observe and offer valuable feedback. As the research progressed, the researcher became more adept at interviewing, but there was always at least one team member (a doctoral researcher) present to provide feedback. When students were hesitant to share their ideas, the researcher assured them that they were not to be directly graded based on their understanding and encouraged them to freely share their ideas. When students' meanings were unclear, the researcher asked for clarification, encouraged students to elaborate on their answers, or repeated what the students had said to check if he had properly interpreted the students' responses.

Another potential source of bias stemmed from the fact that the researcher was a chemistry teacher and a member of the IVR research team with a vested interest in observing positive changes in students' understanding. To address this, the researcher practised reflexivity, continually re-evaluating his own interpretation of the data. The coding schemes were also revised iteratively, and the data interpretation was always discussed with other researchers, including doctoral supervisors, until a consensus was reached. Furthermore, different forms of data (e.g., videos, transcripts, and diagrams) were triangulated to confirm the interpretations and solidify the trustworthiness of the results (Cohen et al., 2018). Moreover, in all empirical studies, the data were mainly analysed using a bottom-up procedure rather than categorising the data in pre-set schemes. This way, the research was inductive, literally allowing the data to speak for itself. The researcher's background as an experienced chemistry teacher and chemistry researcher provided the necessary knowledge to interpret students' conceptual understanding based on their conceptual discussions, actions, and student-generated diagrams.

2.4. Ethical Considerations

Approval to conduct this research was granted by the Human Research Ethics Committee of Curtin University (HRE2020-0081) and the research followed the Australian Code for the Responsible Conduct of Research. Participants were provided with information sheets and the purpose of the research was explained to them. Participation in the research was voluntary and all students signed consent forms before participating. In addition, anonymity was guaranteed to the participants; students' names were replaced with pseudo names and any identifying features were removed from the data during analysis and dissemination. Moreover, access to the data collected was limited to the researcher and members of the research team.

Potential risks, such as cybersickness from the use of IVR headsets, were minimised by testing the programs and resolving technical issues before data collection sessions. Students were also properly trained on using the program and were encouraged to report any form of discomfort during the IVR experience. None of the participants failed to complete the IVR experience due to excessive dizziness. Moreover, since data were collected during the pandemic (classes at Curtin continued except for a few weeks), the face pads in the headsets were always wiped with ethanol and replaced after every session. In addition, the number of people in the data collection room was always kept at a minimum, typically fewer than five individuals.

Chapters 3-6 that follow present the four different studies that comprise the research in this thesis. Each study is presented independently with an abstract, introduction, methods, results, implications and/or conclusion. Together, the four studies helped to address the main research questions of this thesis.

Chapter 3. Immersive Virtual Reality for Science Learning: Design, Implementation, and Evaluation

Before evaluating what and how students learn molecular structures and interactions in IVR, this chapter (Chapter 3) explored the current landscape of IVR utilisation in science education settings through a systematic literature review. This chapter addresses the first research question of this thesis (*How do researchers design, implement, and evaluate IVR for science learning?*[2]; please see Section 1.5).

The content of this chapter has been published in *Studies in Science Education,* a Q1 journal published by Taylor & Francis Group. The content presented here is the version of the submitted article accepted by the journal. The table and figure numbers have been formatted for the chapter. The full citation of the published article is:

Matovu, H., Ungu, D. A. K., Won, M., Tsai, C.-C., Treagust, D. F., Mocerino, M., & Tasker, R. (2023). Immersive virtual reality for science learning: Design, implementation, and evaluation. *Studies in Science Education*, *59*(2), 205-244. https://doi.org/10.1080/03057267.2022.2082680.

[2] Research question 1 was addressed through a series of eight specific sub-questions (please see Section 2.2) and they were included in Section 3.2.

3.1. Abstract

The advanced visualisation and interactive capabilities make immersive virtual reality (IVR) attractive for educators to investigate its educational benefits. This research reviewed 64 studies published in 2016-2020 to understand how science educators designed, implemented, and evaluated IVR-based learning. The immersive design features (sensory, actional, narrative, and social) originally suggested by Dede (2009; 2017) provided the framework for the analysis of IVR designs. Educators commonly adopted IVR to better aid visualisation of abstract concepts and enhance learning experience. IVR applications tended to have sensory and actional features, leaving out narrative and social features. Learning theories did not appear to play a strong role in the design, implementation, and evaluation of IVR-based learning. Participants generally reported their IVR experiences as positive on engagement and motivation, but the learning outcomes were mixed. No particular immersive design features were identified to result in better learning outcomes. Careful consideration of the immersive design features in alignment with the rationales for adopting IVR and evaluation methods may contribute to more productive investigations of the educational benefits of IVR to improve science teaching and learning.

Keywords: Immersive Virtual Reality; Science education; Technology-enhanced learning; Human-computer interaction

3.2. Introduction

The interest in advanced visualisation technologies, such as immersive virtual reality, has increased in recent years (Radianti et al., 2020). In education, researchers have investigated the technologies to enhance engagement and learning experiences (Di Natale et al., 2020; Radianti et al., 2020). Three forms of visualisation technologies, namely, augmented reality (AR), desktop virtual reality (DVR), and immersive virtual reality (IVR) are often discussed together as 'virtual technologies' (e.g., Martín-Gutiérrez et al., 2017) but they have distinct differences. Augmented reality (AR) involves a device with a camera (such as AR goggles or smartphones) to overlay digital content onto the real-world objects so that users can see both the real and virtual environments simultaneously (Garzón, 2021). Desktop virtual reality (DVR) relies on 2D computer screens for display, with a key-board, mouse, or joystick for interactivity (Di Natale et al., 2020). Immersive virtual reality (IVR), on the other hand, involves a headset to block out the view of the real physical environment and instead provides a stereoscopic display of computer-generated 3D graphics to immerse users in the virtual environment. IVR hardware can track users' body movements in real time to allow them to perform actions and experience the consequences, which may be practically impossible in real life (Slater & Sanchez-Vives, 2016). These technical features of IVR allow learners to believe that they are present in the new virtual environment and the virtual events are really happening to enhance their engagement.

The distinct nature of IVR on graphics, interactivity, and embodied movement opens up new opportunities for learning (Slater & Sanchez-Vives, 2016). These capabilities have prompted more researchers to investigate the educational benefits of IVR (Radianti et al., 2020). Science and engineering education, in particular, have been identified as discipline areas heavily investigating the educational benefits of IVR (Hamilton et al., 2021; Radianti et al., 2020; Villena-Taranilla et al., 2022; Wu, Yu, et al., 2020).

With increasing interest in adopting IVR in education, researchers have conducted literature reviews on the effects of IVR for engaging learners and achieving learning outcomes (e.g., Coban et al., 2022; Di Natale et al., 2020; Jensen & Konradsen, 2018; Wu, Yu, et al., 2020). However, despite science education being a major area of educational IVR research, previous reviews have focused on general educational areas without clearly addressing the specific needs of science education. In addition, these reviews tended to overlook the nature of the IVR applications used or the rationales for which educators adopted IVR. Consequently, these reviews did not attempt to explain why some IVR studies resulted in positive learning outcomes while others had mixed or negative outcomes. Other literature reviews identified key design features in educational IVR applications such as perceptual and content stimuli (Suh & Prophet, 2018), fidelity; usability, autonomy, movement, and navigation (Chavez & Bayona, 2018); or realistic surroundings, passive observation, interaction with objects, and immediate feedback (Radianti et al., 2020). Knowing about these design features is helpful in gaining ideas of what is already employed in educational IVR applications but does not provide insight into the levels of the features integrated or their relationship with the rationales for adopting IVR in educational settings.

To design meaningful learning experiences with technological tools, educators need to understand the unique features of the technology that could be used to facilitate learning and offer new educational possibilities (Dalgarno & Lee, 2010; Fowler, 2015; Mikropoulos & Natsis, 2011). The present review was designed to investigate how IVR applications have been designed, implemented, and evaluated in science learning settings and identify what researchers have found in terms of the effectiveness of IVR for achieving different learning outcomes. Based on the available literature of recent years, this review paper investigated the following research questions:

1. What were the rationales for adopting IVR in science education?
2. What learning theories were identified and incorporated in the design, implementation, and evaluation of IVR learning activities?
3. What immersive design features were incorporated in IVR studies?
4. Did the immersive design features incorporated differ for different rationales of adopting IVR?
5. How were IVR learning activities evaluated and what learning outcomes were achieved through IVR learning activities?
6. Did the evaluation of learning activities and achieved learning outcomes differ for different rationales of adopting IVR?
7. Did particular immersive design features lead to more positive learning outcomes?
8. Did learners with particular characteristics report more positive learning outcomes?

By documenting the common immersive design features and learning outcomes in relation to the rationales for adopting IVR, this review aims to establish how and why researchers adopted different combinations of immersive design features to achieve different learning outcomes in science education.

3.3. Immersive Design Features for Educational IVR Applications

Immersive virtual reality (IVR) started to gain public attention around 2016. With major breakthroughs in computational powers and display graphics, coupled with heavy investment on IVR development from major technology companies such as Samsung and Facebook (Meta), the IVR technology has become more affordable with high fidelity graphics (Bower et al., 2020; Wu, Yu, et al., 2020). Educators are now considering IVR in practical terms rather than in hypothetical terms (e.g., Klippel, Zhao, Jackson, et al., 2019).

In designing IVR applications for educational purposes, researchers have focused on the unique technical capabilities of IVR: realistic 3D visualisation and real-time motion tracking give users the feeling of being transported into the virtual environment and interacting with virtual objects (Cummings & Bailenson, 2016; Radianti et al., 2020; Suh & Prophet, 2018). The perception of being immersed in a virtual environment, referred to as presence, often serves as the design goal of the IVR applications (Cummings & Bailenson, 2016). To learn science through IVR, students need more than feeling presence in IVR; they also need to be engaged. Researchers (e.g., Mikropoulos & Natsis, 2011; Winn, 1993) have recommended various ways to take advantage of the technical capabilities of IVR for science education. Examples include offering first-order experiences of being able to move and interact with objects in unfamiliar environments (e.g., Kwon, 2019), embodying a different being or object (e.g., Markowitz et al., 2018), or showing extremely small or large objects that are not easily visible (Slater, 2017). These recommendations highlight the technical capabilities of IVR in the context of science learning. However, these recommendations have the risk of undervaluing the importance of the organisation of the learning content and the benefits of social interactions in IVR studies.

To highlight the key aspects in designing IVR applications for educational purposes, Dede and colleagues identified four immersive design features that educators may consider: sensory, actional, narrative, and social (Dede, 2009; Dede et al., 2017). This consideration provided a useful starting point for identifying key features that researchers may wish to consider when designing IVR applications to engage learners and help them learn science. However, those categories are generally broad (except sensory) and do not state how the suggested features could be implemented or how they would support learning. Therefore, in our earlier work (Won et al., 2023), we adapted the four categories and expanded them to create a set of immersive design features. In the present paper, we used ten immersive design features for analysis: visual, audio, haptics, interactivity, virtual body ownership, embodied movement, character, challenge, storyline, and social interactions. Below, each design feature is described:

Sensory

Compared to other technological tools (such as AR or DVR), IVR has superior sensory appeals, especially the *visuals*, to induce a perception that users are physically in the virtual environments (Dede, 2009; Dede et al., 2017). Through stereoscopic 3D visual representations, IVR displays realistic but simulated environments. For example, when the realistic 3D graphics of a wooden plank at the top of a skyscraper and its surroundings are well delivered in an IVR application, users feel the fear of falling off from the skyscraper as they would in real life (Krupić et al., 2021). The perception of being present in the computer-generated location is referred to as ‘place illusion’

(Slater & Sanchez-Vives, 2016). The 'place illusion' can be induced for both real and imagined virtual environments, such as visiting an old temple to marvel at its architecture and artefacts (real environments e.g., Han et al., 2019) or walking across a narrow passageway to the catalytic chamber of an enzyme (imagined environments, e.g., Won et al., 2019).

The visualisation capabilities of IVR can be advantageous for science education because, instead of dealing with abstract science concepts in symbolic representations such as equations and formulas, learners can explore science concepts in a concrete way. For example, by moving into human cells to look around and observe different organelles in 3D (e.g., Jian Zhao et al., 2020) or scaling down planets in the solar system and observing them from multiple perspectives (Madden et al., 2020). Such 3D visualisation of scientific phenomena supports the development of learners' conceptualisation as well as their spatial knowledge (Bowman & McMahan, 2007; Dalgarno & Lee, 2010).

In addition to the realistic graphics, the *audio* effects through IVR headsets can enhance the place illusion by providing a sense of direction and distance in virtual environments (Slater, 2017). *Haptic* feedback through IVR controllers or gloves can also enhance the feeling of interacting with virtual objects to increase engagement (Dede, 2009), but compared to other sensory appeals of IVR technology, haptics is the least realistic.

Actional

IVR has powerful motion tracking capabilities to map learners' body actions onto the display of the virtual environments to give an illusion that their interactions in virtual environments are real and have real consequences (Slater & Wilbur, 1997). For example, when learners move their heads left and right and arms up and down in the physical environment, they would see a rock from left and right and a virtual ruler moving up and down to measure the dimensions of a rock in the virtual environment (Klippel, Zhao, Jackson, et al., 2019). A responsive IVR system with a high degree of user *interactivity* induces the perception that learners themselves are in the virtual environment, making consequential actions (Dede, 2009; Dede et al., 2017). This perception is called 'plausibility illusion' which can be enhanced by interactive interfaces and real-time tracking of embodied movements (Slater, 2017).

The motion tracking capabilities of IVR for *embodied movement* coupled with an interactive interface can be beneficial for science education not only because this combination allows learners to become familiar with dangerous or ethically restrictive procedures such as handling dangerous chemicals (e.g., Broyer et al., 2020) or operating on ill patients (e.g., Lohre et al., 2020), but also because it encourages learning of abstract concepts by engaging embodied cognition (Johnson-Glenberg, 2018).

Related to IVR's motion tracking capabilities is *virtual body ownership*. When learners interact in virtual environments, they can assume either a bodiless spirit or a virtual persona (avatar) to interact and make changes in the virtual environments (Sanchez-Vives & Slater, 2005). When avatars are well constructed to give personal meaning to users, such as going through a job interview as a person of different gender and ethnicity, the users readily assume the virtual bodies and their roles to experience virtual events as avatars (Slater, 2017).

Narrative

Beyond the technical capabilities of IVR, the content of the IVR applications and how to organise the content are critical for educational designers to consider (Suh & Prophet, 2018; Won et al., 2023). Based on game design, the authors of the current review paper identified three design components, *character*, *storylines*, and *challenge*, to engage learners as the main character (protagonist) of an intriguing story that would challenge and improve their knowledge and skills (Dede, 2009; Dede et al., 2017). For example, in a story, learners can assume the character of a soldier in a white blood cell army who patrols a human body and fights off pathogens in case of an infection (L. Zhang et al., 2019). Learners can identify pathogens, experiment ways to fight off the pathogens without damaging the body and complete the quest of defending the body.

Assigning clear character roles to learners offers an opportunity for learners to execute their roles and become emotionally engaged in the learning tasks (Dede, 2009; Dede et al., 2017; Lee, 2004). Making intriguing storylines and assigning appropriate challenges in IVR applications involves knowing where learners are and what they are willing to do in IVR settings. As Csikszentmihalyi (1990) noted, when the learning tasks are comprehensible and aligned to learners' knowledge and skills, learners immerse themselves to complete the learning tasks, losing sense of themselves and the track of time.

Although those three components of narrative design features are drawn from game design, they have a direct link to general educational principles of learning: having ownership of the task, recognising the relevance and importance of the task, and acquiring the feeling of accomplishment from completing challenging and manageable tasks.

Social

Learning occurs not only through the interactions between a learner and the environment, but also through interactions amongst learners and with knowledgeable others (Dede et al., 2017; Vygotsky, 1978). Learning designers consider learners' interactions with other people (peers and teachers) and animated characters (pedagogical agents) in IVR environments (Dede et al., 2017). Recent developments in IVR technology allow learners to interact with others in virtual environments by sharing a virtual space through a network or other means (e.g., Šašinka et al., 2019). Going through learning tasks together with peers in computer-supported collaborative learning environments tends to increase learner motivation and conceptual understanding (Chen et al., 2018; Krämer, 2017). In addition, being there together in a virtual environment increases the sense of belonging in the virtual environment and thus engages learners (Dalgarno & Lee, 2010). On the other hand, social interactions between learners and pedagogical agents in the virtual learning environments or teachers may provide a constructive way to prompt learners to reflect on their progress in the learning tasks, as well as to provide feedback or guidance on the learners' performance. *Social* is the last design feature the authors of this manuscript identified for IVR applications.

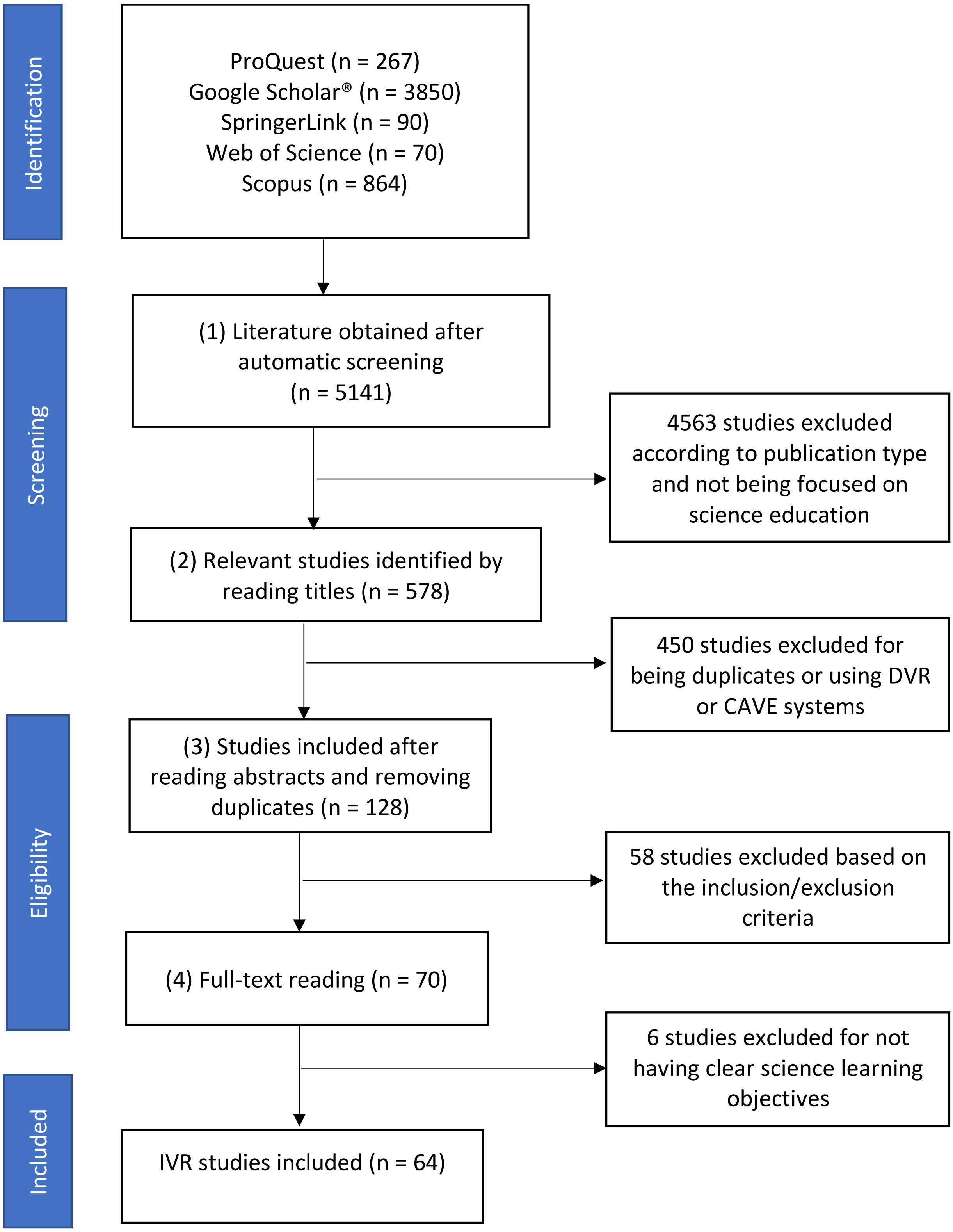
3.4. Methods

Selection of the Literature for Analysis

To retrieve literature on the use of IVR in science education, we surveyed studies published in the period 2016-2020. The year 2016 was chosen as the starting year because HTC's VIVE and Facebook's Oculus Rift headsets then became available to the general public and the number of studies exploring the potential of IVR in science education increased dramatically. The last literature search for this study was conducted on 18 October 2020. Figure 3.1 shows a summary of the literature selection process.

Figure 3.1

The Literature Selection Chart



An electronic literature search was conducted on five scholarly databases (ProQuest, Google Scholar®, Scopus, Web of Science and Springer Link®). ProQuest, Scopus, and Web of Science were chosen because they contain a large collection of journal articles from a wide range of research fields. Google Scholar and Springer Link were included because they are large repositories of book chapters and conference papers from various research domains. Initially, a general search term "virtual reality" was included in the search string. A large number of studies (>30,000) was generated, including those which employed desktop-based applications such as *Second Life*. To limit the search to only studies using head-mounted display (HMD) units in science education fields, we used the search term "immersive virtual reality" instead of "virtual reality". The final search string employed was "immersive virtual reality" AND (education OR teach OR learn) AND (science OR chemistry OR biology OR physics OR astronomy OR earth) AND NOT (medical OR therapy OR rehabilitation). The specific search terms (education OR teach OR learn) AND (science OR chemistry OR biology OR physics OR astronomy OR earth) were included to restrict the search to only those studies using IVR in science learning disciplines.

The initial automatic database search yielded a total of 5,141 documents (ProQuest 267, Google Scholar 3850, Springer Link 90, Web of Science 70, and Scopus 864). We conducted a supplementary literature search on two other databases, ERIC, and IEEE *Xplore.* The search did not yield any new studies which met the inclusion criteria.

Two of the authors of this paper read through the titles of the studies and initially screened the studies according to document type and field of study. Only documents from sources rated in SciMago Journal and Country Rankings were retained for further review. These included peer-reviewed journal articles, book chapters, and conference papers or proceedings from reputable conferences. The field of study was limited to science education fields (chemistry, biology, physics, astronomy, environmental science, integrated science, and earth science/geology). Studies in the fields of entertainment/gaming, safety training, computer science, engineering, cognition, medicine, therapy, and rehabilitation (e.g., Feng et al., 2020; Lee et al., 2020) were excluded. Based on these criteria, 4653 studies were excluded.

The same two authors then read through the abstracts of the remaining 578 documents to screen out duplicates and studies which used DVR and Cave Automatic Virtual Environment (CAVE) systems (450 studies). A total of 128 studies remained. The first round of focused reviews of full text with further inclusion and exclusion criteria was conducted. A particular study was included in the review if the full text was available in English and the study reported use of an IVR headset (HTC VIVE, Oculus Rift or DK, Sony PlayStation VR, or phone-based headset such as Xiaomi Mi VR, Samsung Gear VR or Google Cardboard VR). In addition, only studies reporting empirical evaluations of the students' learning outcomes were included in the review while those only focusing on the design of IVR programs without evaluating learning outcomes (e.g., Salvadori et al., 2018) or those that used secondary data (such as literature reviews) were excluded (e.g., Pellas et al., 2020). The inclusion and exclusion criteria used to screen the studies are outlined in Table 3.1**.** After applying the inclusion and exclusion criteria, 70 studies were retained. Six more studies were further removed for lacking clear science learning objectives (e.g., Filter et al., 2020). A total of 64 studies remained.

Analysis of the Studies

The 64 studies were analysed qualitatively using a content analysis methodology (Krippendorff, 2018). For each study, information relevant to each research question was identified. We created a spreadsheet to summarise the key information including the science discipline (chemistry, biology, geology/geoscience, general science, environmental science, physics, and astronomy), the target learners (elementary school, middle school, high school, university levels, or general public), the learning objectives, and the research objectives for each study. When stating the research objectives of the studies, the terms "effectiveness" and "impact" were consistently used. The former was used when the studies measured science learning outcomes and the latter when the studies evaluated learners' perceptions such as usability or usefulness of IVR.

We then identified the rationales for adopting IVR, the learning theories employed, the integration levels of the immersive design features in IVR studies, the immersive design features for different rationales, the learning outcomes reported, and the methods used to measure the learning outcomes. We also identified the learning outcomes achieved depending on the rationales of adopting IVR, and the design features and learner characteristics that led to positive science learning outcomes. Below we describe the coding process:

Table 3.1

Inclusion and Exclusion Criteria for the Studies

Screening stage	Category	Inclusion Criteria	Exclusion Criteria
1	Search terms	"immersive Virtual Reality" AND (education OR teach OR learn) AND (science OR chemistry OR biology OR physics OR astronomy OR earth) AND NOT (medical OR therapy OR rehabilitation)	
	Publication period	Studies published from January 2016 to October 2020	Studies published before January 2016
	Language of publication	Full-text available in English	Full-text available in other languages
2& 3	Study Materials	Studies reporting use of head mounted displays, HMDs (e.g., HTC VIVE, Oculus Rift, Samsung Gear, Google Cardboard)	Not using HMDs (i.e., those reporting use of AR gears, CAVE, or desktop VR)
	Document Type	Studies published in peer-reviewed journals, books, or conference proceedings rated in Scimago Journal and Country Rankings (SJR)	Studies from sources that are not rated in SJR
	Field of Study	Studies conducted in science education fields	Studies outside science education, such as those in medical, therapy, rehabilitation, or gaming fields
	Type of Study	Studies reporting empirical evaluation of science learning outcomes	Studies focusing on IVR program development without evaluations of learning outcomes; studies using secondary data (e.g., literature reviews, or meta-analyses)
4	Use of IVR in the study	Studies providing enough descriptions of the science learning objectives	Studies without clear science learning objectives

Coding of the rationales for adopting IVR. Based on commonly listed educational benefits of IVR (Freina & Ott, 2015; Slater, 2017), we identified five potential categories as the rationales for adopting IVR in science education: visualization, enhancing learning experience, procedural skills development, field trips, and first-person experience. Researchers tended to explicitly state the rationales for adopting IVR in the introduction or literature review sections of the studies. For instance, Thompson et al. (2020) designed an IVR application to help learners visualise human cells. Cells are practically hard to visualise due to their extremely small sizes. The rationale for adopting in this study was coded as enhancing visualisation of abstract concepts. In another study, Bibic et al. (2019) designed an IVR application with an explicit aim of improving engagement of learners in learning about the biochemistry behind spider venoms. The rationale for adopting IVR here was coded as enhancing learning experience.

In some studies, however, researchers discussed the rationales for adopting IVR in very general terms, citing several advantages of using IVR or simply comparing learning outcome gains for IVR with other media. In such cases, the authors of the present study inferred the rationale for adopting IVR from the nature of the IVR application used, the nature of the learning tasks, and the learning outcomes evaluated. For example, Meyer et al. (2019) compared the effect of pretraining on declarative knowledge acquisition using a 2D video or an IVR simulation. Although the authors did not explicitly state why they adopted IVR in their study, the nature of the IVR simulation (*The Body VR: Journey Inside a Cell)* suggested that it was meant to help learners visualise organelles and their functions, concepts which are not easily perceptible. Besides, the authors evaluated declarative knowledge about the nature and functions of organelles. In this case, the rationale for adopting IVR was coded as enhancing visualisation of abstract concepts.

Coding of the learning theories identified and incorporated in IVR learning activities. The learning theories that researchers identified and used to design or adopt, implement, and evaluate IVR for science teaching and learning varied in depth and details. In coding these, the theories, models, approaches, or principles were first summarised as they were stated in the introduction, the literature review, and the method sections of the studies. We then identified hierarchical relationships of these specific models, principles or approaches to the broader learning theories, such as cognitive theory of multimedia learning, experiential learning theory, motivational theories, embodied cognition, and social constructivist theory (Pritchard, 2017; Schunk, 2012). For example, Andreasen et al. (2019) designed a study to evaluate the effectiveness of enactment as a way of fostering active cognitive processing of science content learned from IVR. The study was designed and evaluated based on the assumption of active processing of the cognitive theory of multimedia learning. Therefore, for this study the theoretical principle for designing, implementing, and evaluating IVR was identified as fostering generative processing; and the broader learning theory was identified as the cognitive theory of multimedia learning (Mayer, 2005).

For each study, information on how the identified learning theory was used to design, implement, or evaluate the IVR application was also extracted from the descriptions provided in the method section of the study. We then referred to the relevant informing literature and compared the descriptions provided in the studies with the principles of the stated theory from literature to confirm if the theory was appropriately employed to design, implement, and evaluate the IVR application.

Coding of the immersive design features in IVR studies. The integration levels of the 10 immersive design features were evaluated for each of the 64 studies. For each study, information about the IVR application used and its design features was obtained from the descriptions and/or screenshots provided in the studies, electronic supplementary materials, or links to promotional YouTube videos of the IVR applications, where available. In some cases, different studies used the same IVR application with very similar hardware. For example, Parong and Mayer (2018), Parong and Mayer (2020), and Jian Zhao et al. (2020) all used the same commercial program *The Body VR: Journey Inside a Cell* with HTC VIVE headsets to conduct their studies. However, because the studies used the IVR application with different groups of learners to obtain different learning outcomes, the IVR studies were coded independently.

For each design feature integration, the authors of the present study devised a 3-level coding scheme – low, medium, or high. Three of the authors initially selected five representative studies and trained on the coding scheme, detailing rules of what constituted each level of integration. The coding of the IVR design features was not a linear process. The three authors went back and forth between the reviewed literature and the coding scheme and held meetings to refine the categories and the descriptors for each immersive design feature until consensus was reached.

For example, the level of integration of visuals depended on the type of environment being simulated (real or imaginary), the type of HMD used (lower-end mobile phone-based HMDs such as Samsung Gear, or the high-end HTC VIVE and Oculus Rift HMDs), and the comprehensiveness or realism of the visual representations. Generally, mobile phone-based IVR devices have low screen resolutions, low refresh rates, and small fields of view, and tend to be less effective in sensory immersion (Cummings & Bailenson, 2016). Therefore, if an IVR application displayed very simplified real environments (such as those generated using Minecraft®) in a mobile phone-based HMD, the view is less immersive, and we coded the study as low on visuals. If high-quality images of a real environment were displayed in a high-end HMD, such as HTC VIVE or Oculus Rift, the IVR application was coded high on visuals. For imaginary environments, if representations of the reified science concepts were displayed on a mobile phone-based headset, the level of visuals was coded as medium. This decision is because learners are still likely to have an immersive experience when they have not had any prior physical experience with these objects in the real-world (Lee, 2004). When scientifically comprehensive representations of reified concepts were displayed using a high-end HMD, the study was rated as high on visual immersion. Scientifically inconsistent visual representations of reified concepts were coded as low level.

For the three actional immersive design features, how well an IVR application represented learners' bodies and made learners' actions feel natural and believable within the virtual environment was considered. For example, in terms of *interactivity*, if the learner had limited control over the content presented (such as in 3D movie-type IVR designs), the level of interactivity was coded as low. On the other hand, if the learner could rotate or flip virtual objects and the IVR system responded realistically, the level of integration was coded as medium. A high level of integration of the interactivity feature was assigned when the IVR application afforded the learner to create new artefacts in the virtual environment.

For narrative immersive design features, the extent to which learners were engaged with the learning content and motivated to exert efforts to accomplish the set tasks was considered. For *character*, for example, if the learner simply completed a learning task without any character role they could identify with, the study was coded as low-level. However, when the IVR application assigned to the learner a character role with which they could identify in first-person but the learners did not execute any consequential actions, the level of integration of *character* was coded as medium; such examples of medium-level character are as a coral being affected by climate change (Markowitz et al., 2018) or as a forensic analyst who simply collected evidence from a crime scene (Kader et al., 2020). An IVR application was rated as high level on *character* if the role assigned to the learners allowed them to make decisions which significantly influenced the unfolding of the storyline.

Regarding the social immersive design feature, we considered whether or not the IVR design encouraged social interactions between learners in IVR and their peers to construct knowledge together, or with teachers or pedagogical agents for guidance or feedback on the learners' progress. If the learners went through the learning tasks individually without any form of social interactions during the IVR session, the level of integration of *social* was coded as low. If the learner in IVR engaged in some form of mediated social interactions with peers or teachers who were outside the IVR space, or received feedback from a pedagogical agent in IVR, the level of integration of *social* was coded as medium. However, if the IVR application allowed learners to share the virtual space and work on the IVR learning tasks collaboratively, the level of integration of *social* was coded as high. Descriptors of each integration level of the different design features are detailed in Table 3.2.

Two of the authors of this paper individually read and coded all the 64 studies using the above criteria. The authors assigned individual scores to the immersive design features in each study and then compared their individual analyses of the studies. To assess the reliability of the coding scheme, Spearman's correlation coefficient (rho) for ordinal data was calculated between the coders. Interrater reliability was 0.863 ($p < 0.01$). Any disagreements in coding were resolved through extensive discussions between the coders.

Table 3.2

Coding Scheme for Evaluation of the Immersive Design Features in IVR Studies

Immersive design features	Level of integration of the immersive design features		
	Low	Medium	High
Visual	Low-fidelity graphics (e.g., low-quality images of real environments rendered in Google Cardboard as in Cheng & Tsai, 2020)	Medium quality graphics (e.g., comprehensive representations of science concepts or realistic graphics of real environments rendered in phone-based headsets as in Makransky, Terkildsen, et al., 2019)	High-quality graphics of real and imagined environments (e.g., comprehensive representations of science concepts rendered in high-end devices such as HTC VIVE as in Jian Zhao et al., 2020)
Audio	No audio effects	Background audio in the form of instructions, narrations, or sound from other social agents (e.g., instructions from a pedagogical agent as in Dunnagan et al., 2020)	Immersive sounds to give a sense of distance and direction in the virtual environment (e.g., immersive ocean sounds as in Lamb et al., 2019)
Haptics	No haptic feedback	Vibration or force feedback from controllers or haptic gloves (e.g., vibrations from controllers as in Lamb et al., 2018)	Haptic feedback to give a realistic sense of interacting with virtual objects (e.g., synchronisation of real and virtual environments as in Ahn et al., 2016)
Interactivity	Minimum or no interaction between the learner and the IVR program content (e.g., watching a 3D movie as in Petersen et al., 2020)	Learner can manipulate objects in the virtual environment to observe effects of their actions (e.g., the learner can rotate, or flip virtual objects as in Parong & Mayer, 2018)	High level of user control (e.g., the learner can create a new artifact in IVR as in Southgate et al., 2019)

Virtual body ownership	The learner’s body is not represented in any form in the virtual environment (e.g., Jong et al., 2020)	The learner’s body is represented partly in the virtual environment (e.g., learner's hands are represented in the form of floating controllers as in Pirker et al., 2017)	Learner assumes a full virtual body (e.g., the learner embodies a coral as in Markowitz et al., 2018)
Embodied movements	Minimum or no embodied movements relevant to the task (e.g., simple head movements while watching a 3D movie as in Fokides & Kefallinou, 2020)	Some embodied movements relevant to the task (e.g., using hand movements to lift and flip objects as in Lui et al., 2020)	Full body engagements relevant to the learning task (e.g., walking and lowering one's body to measure rock dimensions as in Klippel, Zhao, Oprean, et al., 2019)
Character	No clear character role assigned to the learner	The learner assumes some form of character role but does not make consequential decisions (e.g., as a forensic analyst who gathers evidence at a crime scence as in Kader et al., 2020)	The learner is a main protagonist responsible for making consequential decisions (e.g., as a commander of white blood cells to fight pathogens and restore life of a host as in L. Zhang et al., 2019)
Storyline	The storyline is linear without alternative endings	Storyline with some form of alternative endings (e.g.,the learner's actions and decisions determine whether the host lives or dies as in L. Zhang et al., 2019)	The storyline is clear and changes infinitely depending on the decisions made by the learner
Challenge	Learning task does not demand integration of prior knowledge or skills (e.g., learners follow simple instructions as in Ferrell et al., 2019)	Task provides some opportunity for integration of prior knowledge and skills (e.g., learner uses prior understanding to complete learning tasks as in Won et al., 2019)	Task requires integration and application of prior knowledge and/or skills, critical reflection and decision making
Social interactions	Learner individually completes the learning task in IVR	Some form of mediated social interactions with peers, teachers, or pedagogical agents (e.g., one learner in IVR talking to peers outside the virtual environment as in Liu et al., 2020)	Extensive social interactions designed to foster collaborative learning in a shared virtual space (e.g., peer to peer collaboration in a networked environment as in Southgate et al., 2019)

Coding of the evaluation of IVR learning activities. The learning outcomes and experience ratings following instruction in IVR were identified as each was discussed in the 64 studies. In some studies, IVR was compared against an alternative learning mode, such as a 2D learning platform or a lecture type of instruction, while in other studies, learning outcomes or experience ratings after IVR were simply compared to those before the IVR session without a separate comparison group. For each study, the alternative learning mode against which IVR was compared (where applicable), and the methods for evaluating learning outcomes or experience ratings were identified from the methodology and results sections.

Coding of the achieved learning outcomes. Learning outcomes are specifications of the kind of knowledge and understanding, skills and competencies, or values and attitudes that learners are expected to have, demonstrate, or hold at the end of a learning experience (Savickiene, 2010). Learning outcomes were identified directly from the studies and coded as declarative knowledge, procedural knowledge, and attitudinal and behavioural change outcomes. Declarative knowledge dealt with students' understanding of scientific facts and concepts (Anderson & Krathwohl, 2001). Procedural knowledge gains were related to students' understanding of practical techniques, processes, or methods (Adams, 2015; Anderson & Krathwohl, 2001). Learning outcomes coded as attitudinal or behavioural change outcomes dealt with changes in students' perceptions, attitudes, and behavioural intentions towards science and socio-scientific issues.

In addition to learning outcomes, several factors related to the students' learning experience in IVR were identified from the studies. These experience ratings were coded as presence ratings, engagement on learning task, motivation, perceived usefulness, and negative effects (such as dizziness, physical discomfort, or simulator sickness) of IVR.

Learning outcomes and experience ratings for IVR were coded as *better* if they were higher than those evaluated before the IVR session or those reported from use of an alternative learning mode. Similarly, a *worse* code was assigned if the IVR experience was rated negatively or resulted in lower learning outcomes compared to an alternative learning mode or a pre-IVR evaluation. Learning outcomes or experience ratings were coded as *similar* if a study reported no significant differences in learning outcomes or experience ratings between IVR and an alternative learning mode or a pre-evaluation.

Identification of immersive design features incorporated for different rationales of using IVR. After coding the rationales of adopting IVR and the immersive design features incorporated in each study, the 64 studies were categorised based on the rationales for adopting IVR. For each category of studies, the average integration level for each of the 10 design features was calculated. In calculating the average integration levels, we assigned a value of 1 to each low integration level, 2 to a medium integration level, and 3 to a high integration level. The averages were then compared to identify similarities and differences in how IVR studies integrated immersive design features depending on their rationales. Immersive design features which were more commonly adopted had the highest average ratings per category.

Coding of the evaluation of learning activities and achieved learning outcomes for the different rationales of adopting IVR. The 64 studies were categorised depending on the rationale for adopting IVR. For each cluster, the number of studies evaluating the different learning outcomes, the methods used to evaluate the outcomes, and the reported outcomes were identified. The number of the studies reporting *better, similar*, or *worse* learning outcomes for IVR compared to other learning modes or pre-tests were documented for each category.

Identification of the immersive design features that led to positive learning outcomes. The 64 studies were combined and categorised based on whether they reported *better, similar,* or *worse* learning outcomes for IVR compared to other learning modes or pre-tests. Average integration levels of the 10 design features were calculated for each cluster. The averages were then compared to identify the design features that might have caused the differences in the reported outcomes. This approach to identifying the immersive design features that led to positive learning outcomes was adopted because IVR research for science education is an emerging field and therefore, for some categories, the number of studies was very low to allow any advanced statistical analyses. For example, only two studies reported positive procedural knowledge gains while three reported no significant differences for IVR compared to alternative learning modes.

Identification of the learner characteristics that led to positive learning outcomes. Learner characteristics such as demographics (age, gender, prior experience with computer games), cognitive characteristics (class level, prior knowledge), and affective characteristics (such as intrinsic motivation and intrinsic self-efficacy) were summarised as reported in the reviewed literature. The methodology and results sections of each study were analysed for any reported influence of learner characteristics on the achieved learning outcomes. Studies were then grouped depending on how the learner characteristics influenced the learning outcomes and patterns were identified from these clusters.

3.5. Results

Overview

IVR has been adopted and studied across all science education areas, with most studies in biology (24 out of 64), followed by chemistry and physics (13 and 11, respectively), and geology and environmental sciences (5 and 6, respectively), and general science (5). Participants in the studies were university level students (58% of the studies), high school (9%), middle school (10%), elementary school (9%), while the rest of the studies (14%) recruited participants from more than one educational level. The number of participants in each study varied. About one-third of the studies had less than 50 participants, another third had 50-100 participants, and the rest of the studies involved over 100 participants in each study.

In most of the studies (n = 57), the students were given a one-time opportunity to learn with IVR. Two studies (Markowitz et al., 2018; Sun et al., 2017) provided initial IVR experiences to familiarize the learners with the technology before the target content was introduced. Some studies (n = 5) provided multiple IVR sessions with different learning content each time (e.g., Artun et al., 2020; Boda & Brown, 2020b; Fokides & Kefallinou, 2020).

More than two-thirds of the studies (n = 44) compared IVR against an alternative learning mode. Forty studies investigated educational benefits of IVR separate from routine learning activities while the rest of the studies (n = 24) adopted IVR as part of the routine learning activities to supplement or even substitute alternative learning modes (Bennie et al., 2019; Ferrell et al., 2019; Klippel, Zhao, Oprean, et al., 2019; Klippel, Zhao, Jackson, et al., 2019; Kwon, 2019). In some studies (n=11), educators recognised that IVR sessions may need to be supported with other learning activities and, therefore, integrated IVR into broader lessons (e.g., Fokides & Kefallinou, 2020; Jong et al., 2020; Kader et al., 2020; Petersen et al., 2020). The target concepts were first introduced to the students through lecture or self-study materials and then explored further in IVR. When learners completed the IVR learning activities, they were then engaged in reflection activities such as group discussions.

Rationales for Adopting IVR

We identified five different rationales for adopting IVR in science education settings: to improve students' visualisation of abstract concepts; enhance learning experience; provide access to faraway places through virtual field trips; develop practical skills; and to provide first-person learning experiences. Below each rationale is discussed:

Visualisation of abstract concepts. Science content is generally abstract in nature, dominated by unobservable phenomena and extreme sizes which makes it hard to comprehend the content (Mikropoulos & Natsis, 2011). Twenty-two studies used IVR to help students visualise scientific phenomena that are not easily accessible for physical perception. For instance, in biology and chemistry, researchers used IVR to magnify microscopic 3D entities such as organelles and their functions (e.g., Parong & Mayer, 2018, 2020; Jian Zhao et al., 2020) or molecular structures and interactions (Bennie et al., 2019; Ferrell et al., 2019). In physics and astronomy, researchers used IVR to help learners visualise concepts such as electromagnetic field lines (Pirker et al., 2018; Pirker et al., 2017) and to reduce the size of extremely large objects such as planets in the solar system (e.g., Madden et al., 2020; Sun et al., 2017).

Enhancing learning experience. Fourteen studies designed or adopted IVR applications to test the general educational effectiveness of the 'new' IVR technology for science teaching and learning. Researchers used IVR to improve learners' engagement (e.g., Bibic et al., 2019; Lamb et al., 2018) and motivation towards learning science (e.g., Han et al., 2020). In their IVR applications, some educators adopted game-like strategies such as integrating rewards, rules, and immediate feedback to the users to keep the learners engaged in IVR (Edwards et al., 2019; Rychkova et al., 2020).

Practical skills development. Science education requires learners to conduct experiments in laboratories to develop competence in observing, predicting, and making inferences about the physical world. In 13 studies, science educators used IVR applications in the form of virtual laboratories to provide learners with an opportunity to access and practice laboratory procedures with virtual laboratory equipment (e.g., Andreasen et al., 2019; Artun et al., 2020; Dunnagan et al., 2020; Klingenberg et al., 2020; Makransky, Terkildsen, et al., 2019) or dangerous chemicals (e.g., Broyer et al., 2020; Makransky, Wismer, et al., 2019). Engaging with the virtual equipment and chemicals in IVR was anticipated to improve the learners' familiarity with laboratory procedures.

***Virtual field trips*.** Many concepts in science disciplines such as geology and environmental science require learners to visit field sites but organising traditional field trips is costly in terms of time and finances (J. Zhao et al., 2020). To this effect, 11 studies used IVR applications that were specifically designed to teleport learners to the relevant field sites. For example, in geology, Jong et al. (2020) teleported learners to a field site where they explored coastal geological formations. IVR was also used to teleport learners to faraway places to observe environmental issues (e.g., Fokides & Kefallinou, 2020; Petersen et al., 2020; Yu & Lin, 2020). IVR allowed learners to conveniently visit and explore relevant but hard-to-reach sites.

Providing first-person experiential learning opportunities. Some science concepts appear distant to learners making them challenging to teach and learn (Markowitz et al., 2018). For example, it is impossible to experience life as another person, or animal. Four studies used IVR to provide first-person experiential learning opportunities to help learners develop empathy or change attitudes towards community and environmental issues that are normally hard to experience (Ahn et al., 2016; Gochman et al., 2019; Markowitz et al., 2018; Nowak et al., 2020). For instance, instead of simply showing a video of community health problems associated with influenza transmission, Nowak et al. (2020) designed an IVR application which transformed the learner into an unvaccinated person who spreads the flu to vulnerable members of the community. The learner was then shrunk to the size of a cell to experience how one's immune system would be overwhelmed by viruses if they were not vaccinated. In this way, IVR changed the learner's perspective from third-person (as in the case of watching a movie on a 2D screen) to first-person, fostering a psychological illusion of non-mediation of the experience.

Learning Theories Identified and Incorporated in the Design, Implementation, and Evaluation of IVR Learning Activities

About half of the studies (29 out of 64) explicitly stated the learning theories supporting the designs, implementation, or evaluation of IVR applications. In these studies, a wide range of learning theories were identified, and their application varied from being applied in the design of the program to the design of the study itself. For instance, following the social constructivist theory of learning, Won et al. (2019) designed an IVR study in which learners shared the virtual space and negotiated meanings within the virtual learning environment. Two other studies were based on the same theory to engage learners in group discussions after individually watching 3D videos in IVR (e.g., Jong et al., 2020; Sun et al., 2017).

However, slightly more than half of the studies that identified learning theories (17 out of 29) designed, implemented and evaluated their IVR applications in line with the referred to learning theories. Lui et al. (2020) explicitly applied a learning theory in the design of an IVR learning activity and research. Using the theory of embodied cognition, an IVR application was designed for learners to learn biology concepts by engaging their bodies, either partly (in a seated position) or fully (standing position). The authors evaluated the effect of sensory-motor engagements by monitoring real-time physiological responses, eye-tracking, and a post-test. The study reported that learning outcomes were influenced by the physical position in which learners experienced the IVR application and their prior knowledge.

Several researchers designed, implemented, and evaluated their IVR applications following the cognitive theory of multimedia learning. These researchers often evaluated specific principles of the theory such as the segmentation, coherence (Parong & Mayer, 2018, 2020), and redundancy principles (Makransky, Terkildsen, et al., 2019), as well as the effectiveness of strategies aimed at helping students to actively process the target science content. These strategies included pre-training (Meyer et al., 2019; Nie & Wu, 2020) and opportunities for reflection through summarizing the learned content, peer tutoring or enactment of the concepts after IVR (Andreasen et al., 2019; Klingenberg et al., 2020; Parong & Mayer, 2018, 2020). The studies contributed to IVR research by providing useful examples of instructional mechanisms to support learning with IVR.

For most studies (55%), it was difficult to discern whether or not theoretical frameworks guided the design, implementation, or evaluation of IVR because theoretical frameworks were not explicitly stated (e.g., Dunnagan et al., 2020; Lamb et al., 2019; Pirker et al., 2018; Southgate et al., 2019). In addition, although some studies identified the theoretical foundations such as play-based learning (Choi et al., 2018), learning by doing (Bhattacharjee et al., 2018), or social-cognitive theories (Makransky & Lilleholt, 2018), these researchers did not specify how the principles of these theoretical foundations were used in the design, implementation, or evaluation of IVR as a learning intervention.

Immersive Design Features in IVR studies

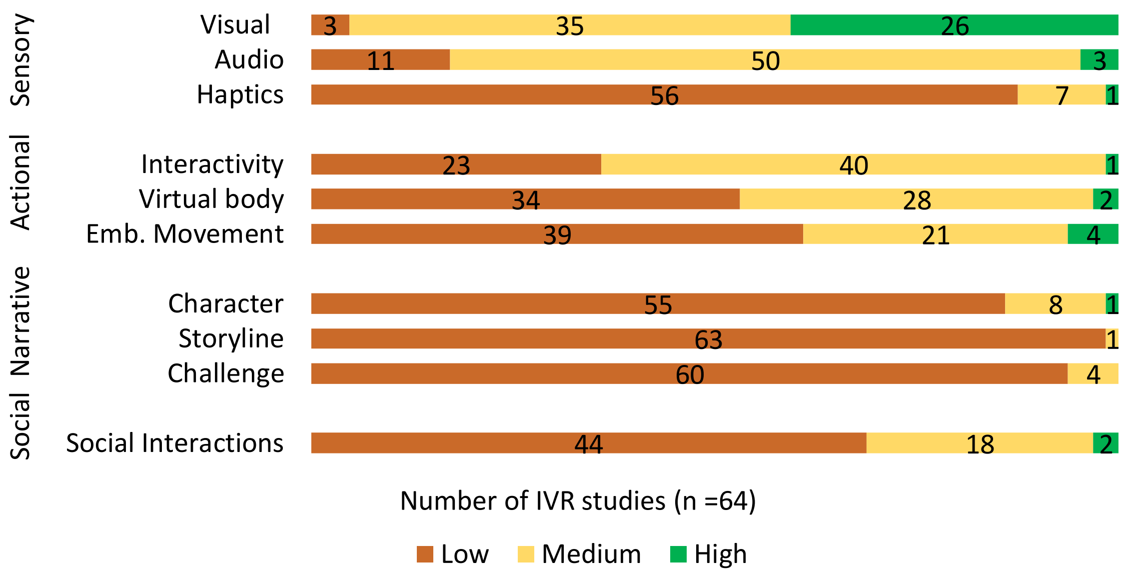
In all the learning settings, the major focus of current IVR studies was the visual and audio design features. Ninety-five percent and 83% of the 64 IVR studies integrated at least medium level visual and audio features, respectively (Figure 3.2). For actional immersive design features, interactivity was the most common design feature with over 60% of the IVR studies employing at least medium-level interactivity in their IVR applications while integration of virtual body ownership and embodied movements was much less. Narrative and social immersive design features were the least integrated in current IVR studies. Over 85% of the studies had low levels of integration of all the narrative immersive design features while over 67% of the studies did not engage learners in any form of social interactions as they completed the learning tasks. Below we further elaborate on these findings:

Sensory—Visual. IVR is a superior 3D visualisation platform which can improve the way we perceive things, and many researchers are utilising this affordance for science education. Twenty-six out of the 64 IVR studies had high level visuals, while 35 studies had medium-level visual representations in their IVR applications. High-level visuals were often integrated in IVR applications to help students recognise spatial relationships in objects that are not easily accessible, such as molecules and planetary systems (e.g., Bennie et al., 2019;

Ferrell et al., 2019; Madden et al., 2020; Parong & Mayer, 2018). For example, in chemistry, Ferrell et al. (2019) used high-quality 3D graphics in IVR to help students explore non-covalent spatial interactions amongst organic molecules. Some researchers used medium quality graphics to recreate laboratory settings in which learners could practice laboratory procedures (e.g., Broyer et al., 2020; Makransky, Terkildsen, et al., 2019).

Figure 3.2

Immersive Design Features Adopted in IVR Studies



Sensory —Audio. Fifty-three out of the 64 IVR studies incorporated audio effects of some form in their IVR applications. The majority of the IVR studies provided background audio instructions or narrations (e.g., Bagher et al., 2020; Jong et al., 2020; Klippel, Zhao, Jackson, et al., 2019; Nowak et al., 2020; Petersen et al., 2020). In some cases, learners could hear sound from peers outside the VR environment but cooperating on the same learning tasks (e.g., Hsu et al., 2018; Uz-Bilgin et al., 2020). Three IVR studies provided learners with immersive sounds to give them a sense of distance and direction in the virtual environment (Lamb et al., 2019; Tsivitanidou et al., 2021; Won et al., 2019). For example, to fully immerse learners in the virtual environment, Lamb et al. (2019) used immersive ocean sounds such as that of flowing water and sounds made by marine animals such as whales.

Sensory—Haptics. Haptic feedback was not a major focus in current IVR studies. The majority of the studies (56 out of 64) did not incorporate any form of haptic feedback in their IVR applications. Seven of the IVR studies integrated vibration feedback from the controllers or gloves to provide users with tactile force feedback when they interacted with virtual objects (Edwards et al., 2019; Hsu et al., 2018; Lamb et al., 2018; Pirker et al., 2017; Won et al., 2019). Only one study (Ahn et al., 2016) had high-level haptics in their design; the floor in contact with the learners' hands and knees in the real-world was made to vibrate and the learners were poked in the back at the same time as a virtual cattle prod hit their virtual bodies. The synchronization of the haptic feedback in the real world with actions in the virtual environment was meant to increase the learners' sense of presence in the virtual world.

Actional—Interactivity. An IVR design that affords a level of high user-control and is responsive to the actions of learners is likely to support experiential knowledge construction by encouraging 'learning by doing' (Slater & Sanchez-Vives, 2016). However, about one-third of the IVR studies provided minimal or no opportunities for the learners to interact with the learning content. These studies generally used IVR applications in the form of 360^{o} videos in which learners simply watched the learning content on their headsets and had limited control over the presentation of the content (e.g., Cheng & Tsai, 2020; Meyer et al., 2019; Petersen et al., 2020).

More than 60% of the studies integrated medium-level interactivity in their IVR applications. Using handheld controllers or gloves, learners could manipulate already existing elements in the virtual environment to observe the consequences of their actions. For example, learners could conduct experiments with science equipment (e.g., Makransky, Wismer, et al., 2019; Pirker et al., 2017), manipulate the structure of DNA (Lamb et al., 2018), or reposition planets in the solar system to observe the moon phases (Madden et al., 2020). A high level of interactivity was provided in only one IVR study (Southgate et al., 2019). The study used Microsoft's Minecraft® in their IVR design which allowed learners to build a model of a plant upon which their discussion of science concepts was based.

Actional—Virtual body. User embodiment using real-time motion capture in IVR encourages transfer of self and the development of soft skills such as empathy through authentic experiences (Slater & Sanchez-Vives, 2016). About one-half of the IVR studies did not represent the learners with any form of virtual body (e.g., Cheng & Tsai, 2020; Fokides & Kefallinou, 2020; Yu & Lin, 2020). Twenty-eight IVR studies represented the learners' bodies in the form of floating controllers or headsets to portray the positions of the learners' hands or heads (Bennie et al., 2019; Broyer et al., 2020; Klippel, Zhao, Jackson, et al., 2019; Lamb et al., 2018; Won et al., 2019).

IVR studies in environmental science employed the user embodiment feature more readily than those in other disciplines. For instance, two IVR studies in the environmental science field allowed the learners to inhabit full virtual bodies. Ahn et al. (2016) embodied learners in virtual bodies of animals to induce feelings of empathy towards the animals while Markowitz et al. (2018) embodied learners in the form of corals being affected by climate change to raise awareness of the effects of climate change on marine environments.

***Actional—Embodied movements*.** For embodied movements, more than half of the IVR studies did not incorporate extensive body movements relevant to the learning tasks. In many of these studies, the only body movement was head rotation to change the view of the learning content in IVR (e.g., Artun et al., 2020; Petersen et al., 2020). Medium-level embodied movements in action-based tasks, such as conducting laboratory experiments (e.g., Broyer et al., 2020) or throwing objects to experience gravity on the surface of the moon (Kwon, 2019), to support procedural and declarative knowledge acquisition were integrated in a third of the studies. Four IVR studies integrated full-body movements to allow learners to explore the learning environments in IVR (Klippel, Zhao, Oprean, et al., 2019; Klippel, Zhao, Jackson, et al., 2019; Won et al., 2019; J. Zhao et al., 2020). In their study, Won and colleagues (2019) allowed learners to explore protein structures by walking into them, and to rotate, drag, and push substrate molecules through the gorge of the enzyme into the catalytic site. These actions were designed to help the learners to understand abstract concepts related to catalytic reactions, such as the effect of shapes of the substrate and enzyme on the reaction.

Narrative—Character, Storyline, and Challenge. Narrative immersive design features were not integrated well in most IVR studies. The majority of the IVR studies (55 out of 64) did not assign any identifiable character roles to the learners, while almost all the IVR studies (63 out of 64) had linear storylines without alternative endings. Nine studies assigned some character roles to the learners, such as being a forensic scientist (Kader et al., 2020), an animal (Ahn et al., 2016), or a space pilot (Rychkova et al., 2020). However, in most cases, the characters had little to no emotions or motivation related to the tasks and their decisions did not significantly influence storylines in the IVR activities. Only one of these studies assigned participants a clear character role to influence the progress of the storyline (L. Zhang et al., 2019). In this study, the learner assumed the role of the commander of an army of white blood cells. The learner made relevant decisions to fight off pathogens and to restore the health of the host without damaging the body cells, and the outcome of the game was different depending on the learner's decisions.

In terms of challenge, most of the studies (60 out of 64) assigned simplistic tasks to the learners which did not support comprehensive integration of prior knowledge, reflection, or decision-making. Only four studies assigned learners tasks that required some integration of prior knowledge and skills – medium level challenge (Kader et al., 2020; Southgate et al., 2019; Won et al., 2019; Zhang et al., 2019). For example, the learners had to use skills as forensic scientists to identify, with reasons, potential criminal evidence from a crime scene (Kader et al., 2020).

Social immersion—Social interactions. Few studies utilised IVR technology to support collaborative learning. Most of the studies (44 out of 64) were designed for individual participants to explore the virtual environments without any mediated social interactions with other learners, teachers, or pedagogical agents. Only two studies allowed extensive social interactions in the virtual space (Southgate et al., 2019; Won et al., 2019). Learners negotiated meanings and collaborated on the learning tasks within the shared virtual environments.

About one third of the IVR studies integrated some form of mediated social interactions in their IVR applications (rated as medium level on the social immersive design feature). In seven studies, one participant was placed in the virtual world and the peers or teachers watched from a 2D screen (e.g., Gochman et al., 2019; L. Zhang et al., 2019). In such an arrangement, the learner exploring the virtual world could interact verbally with peers or teachers in the physical world. Two studies (Hsu et al., 2018; Uz-Bilgin et al., 2020) assigned roles of navigator (inside the virtual space) and co-navigator (watching the virtual environment from a 2D screen) to the learners. The learners were required to cooperate and solve the learning tasks in IVR. In six studies (e.g., Dunnagan et al., 2020; Makransky, Terkildsen, et al., 2019; Makransky, Wismer, et al., 2019), learners followed instructions or received feedback from pedagogical agents to complete the learning tasks in IVR. Overall, the social immersive design feature remains a feature that may require further exploration in future studies.

Immersive Design Features for Different Rationales of Adopting IVR

Depending on the rationale for adopting IVR, researchers adopted different immersive design features as shown in Table 3.3. Below we further elaborate this finding:

Visualisation of abstract concepts. The 22 studies in which IVR was used to aid learners' visualisation of abstract concepts generally integrated high-level visuals in their IVR applications. Medium-level audio effects in the form of background audio instructions were used in the IVR applications and learners had some opportunities to interact with the virtual objects. However, the integration of embodied movements in the learning tasks was slightly less. Also, the integration of haptics, narrative, and social design features was generally low. Visually representing scientific concepts using high-quality graphics in three-dimensional spaces in IVR and allowing the learners to manipulate 3D objects was aimed at improving the learners' awareness of the relevant spatial relationships in the concepts. For example, in chemistry, Bennie et al. (2019) used high-quality graphics delivered in HTC VIVE headsets so that learners could explore molecular interactions in an enzyme reaction. Learners used hand-held controllers to bind and unbind functional groups in the virtual molecules while observing the associated molecular rearrangements.

Table 3.3

Average Levels of Integration of the Immersive Design Features Depending on the Rationales for Adopting IVR

Rationale for adopting IVR	Number of studies (N=64)	Visual	Audio	Haptics	Interactivity	Virtual body	Embodied movements	Character	Storyline	Challenge	Social interactions
Visualisation of abstract concepts	22	2.6	1.8	1.1	1.7	1.6	1.5	1.2	1	1.1	1.3
Enhancing learning experience	14	2.1	1.9	1.3	1.9	1.5	1.5	1.1	1	1.1	1.4
Practical skill development	13	2.1	1.9	1	1.8	1.2	1.2	1.1	1	1.1	1.6
Field trips	11	2.3	2	1	1.3	1.3	1.5	1	1	1	1.2
First-person experience	4	2.8	2	1.5	1.5	2.5	1.5	2	1	1	1.3

Note: 1= low integration; 2= medium integration; 3 = high integration

Enhancing learning experience. On average, the 14 IVR studies in this category integrated medium-level graphics in their IVR applications and the designs were moderately interactive to respond to the learners' actions. The levels of integration of embodiment and embodied movement features were slightly less than that of the interactivity feature, while narrative and social design features were generally not integrated well. For example, citing the poor motivation of students towards learning physics, Han et al. (2020) developed an IVR application which placed learners in a 'moving' virtual car as an alternative way to teach learners about velocity-time graphs. The learners could control the speed of the virtual car by simply clicking controls using a handheld controller to observe real-time changes in the car's velocity-time graph. However, learners did not have any character roles assigned and did not engage in any form of plot or constructive social interactions while completing the learning task.

Practical skills development. The 13 studies adopting IVR for this purpose generally incorporated medium-quality visuals and medium-level interactivity in their IVR applications. Step-by-step audio instructions were also provided by pedagogical agents to guide the learners through the IVR learning tasks. Haptics, user embodiment, and embodied movements, as well as narrative immersive design features were not clearly adopted in IVR applications for this purpose. Moreover, one of the studies (Artun et al., 2020) simply showed 3D videos of laboratory activities in IVR to improve learners' science process skills without engaging learners in any relevant body movements that would normally be involved in conducting laboratory procedures.

Virtual field trips. Overall, the 11 studies in this category integrated the least number of immersive design features in their IVR applications compared to studies using IVR for other purposes. Most of the studies in this category (n = 8) used IVR applications in the form of 3D videos (e.g., Boda & Brown, 2020b; Fokides & Kefallinou, 2020; Jong et al., 2020; Petersen et al., 2020). The applications integrated medium-level visual and audio features while actional, narrative, and social design features were generally not integrated well in these designs. However, some researchers made efforts to integrate more design features (Klippel, Zhao, Oprean, et al., 2019; Klippel, Zhao, Jackson, et al., 2019; J. Zhao et al., 2020). To help university level learners remotely explore regional sedimentary rock formations, the researchers rendered images of geological field sites on high-end HMDs (HTC VIVE). High level actional immersive design features were also integrated in the IVR applications. The students explored the virtual field sites by walking around, lowering their bodies, and taking measurements using a virtual ruler. However, the learners did not have any character roles, or engage in any plots and they did not have opportunities to interact with peers or tutors during learning.

Providing first-person experiential learning opportunities. Unlike studies adopting IVR for other purposes, the four studies in this category generally integrated high-level user embodiment and medium-level character design features in their IVR applications. This was in addition to high-quality graphics and medium-level audio effects. For example, Markowitz et al. (2018) designed an IVR application in which the learner was embodied in the form of a coral in a marine environment. Using high-end (Oculus Rift) HMDs, learners could move their heads around to observe long-term effects of ocean acidification in the marine environment and on their 'own' bodies as corals to appreciate the effect of climate change.

Evaluation of IVR Learning Activities and Achieved Learning Outcomes

As illustrated in Table 3.4, declarative knowledge was the most commonly evaluated learning outcome (43 studies), followed by attitudes and behavioural change outcomes (10 studies), while procedural knowledge was the least evaluated (5 studies). Declarative knowledge was evaluated using pre-and post-tests or interviews (40 studies). Multiple-choice and short-answer questions testing the students' abilities to recall science content presented in IVR were the most common test items. Few studies (n = 3) used relatively more elaborate methods such as argumentative writing (Lamb et al., 2019), or drawing tasks (Bagher et al., 2020; Thompson et al., 2020) to evaluate students' knowledge gains. In addition, in most of the studies, evaluation was conducted before and after the IVR session and there was no significant analysis of the learning process or how learning behaviour in IVR influenced the learning outcomes. Procedural knowledge was evaluated using written post-tests only (Artun et al., 2020; Dunnagan et al., 2020) or in combination with behavioural transfer tests (Andreasen et al., 2019; Makransky, Borre-Gude, et al., 2019; Nie & Wu, 2020), while attitudes and behavioural change outcomes were often evaluated using surveys and interviews.

Table 3.4

Achieved Learning Outcomes in Studies with Different Rationales for Adopting IVR

Rationale for adopting IVR	Learning outcomes	Learning outcomes of IVR vs. other modes				Learning outcomes of IVR vs. pre-test			
		N	Better	Similar	Worse	N	Better	Similar	Worse
Visualization	Declarative	12	6	3	3	5	3	2	0
Learning experience	Declarative	8	7	1	0	1	1	0	0
Practical skills	Declarative	6	7	1	0	1	0	0	0
	Procedural	5	1	4	1	1	0	0	0
Fieldtrip	Declarative	7	4	3	0	1	1	0	0
	Attitudes	4	4	0	0	1	1	0	0
First-person	Declarative	0	0	0	0	2	2	0	0
	Attitudes	2	2	0	0	1	1	0	0

Note: N = number of studies; Declarative = declarative knowledge; Procedural = procedural knowledge; Attitudes = Attitudes and behavioural change outcomes

In terms of learning experience ratings, motivation to use IVR to learn, presence, perceived usefulness, and engagement on the learning task were the most widely evaluated outcomes (Table 3.5). These outcomes were evaluated using surveys and interviews. Some studies (n=4) also used real-time measurements of students' physiological responses to IVR (such as brain activity and skin responses) to track students' cognitive and emotional engagement (e.g., Lamb et al., 2018; Lui et al., 2020).

Table 3.5

Reported Learning Experience Evaluations

Learning experiences	IVR vs. other modes				IVR vs. pre-test			
	N	Better	Similar	Worse	N	Better	Similar	Worse
Motivation	24	24	0	0	10	10	0	0
Presence	20	20	0	0	11	11	0	0
Perceived usefulness	20	16	4	0	10	10	0	0
Engagement	10	8	0	2	8	8	0	0

Note. N = number of studies

In comparison to alternative learning modes, such as 2D computer displays or lecture-type approaches, IVR was more effective in only 55% of the studies on declarative knowledge gains and less effective in 12% of the studies. However, IVR was more effective than alternative learning modes on attitudes and behavioural change outcomes (100%) and received overwhelmingly positive ratings on motivation (100%), presence (100%), perceived usefulness (80%) and engagement (80%) compared to alternative modes. On the other hand, when compared to pre-test scores without comparison groups, studies found that IVR was effective for learning outcomes (83%) and provided a positive learning experience (100%).

In a small number of studies (n=6), negative effects of IVR on students' learning experience were reported such as: dizziness (Broyer et al., 2020; Rychkova et al., 2020; Sun et al., 2017), higher levels of simulator sickness (Rupp et al., 2019; J. Zhao et al., 2020), and physical discomfort (Meyer et al., 2019). Surprisingly, the participants in these studies still rated IVR highly on motivation, presence, or perceived usefulness (Broyer et al., 2020;

Meyer et al., 2019; Rychkova et al., 2020; Sun et al., 2017; J. Zhao et al., 2020). However, in some of these studies (n=4), when IVR was compared against other learning modes on declarative knowledge gains, no significant differences in learning gains were found (Broyer et al., 2020; Meyer et al., 2019; Rupp et al., 2019; Rychkova et al., 2020; J. Zhao et al., 2020).

Evaluation of IVR Learning Activities and Achieved Learning Outcomes for Different Rationales of Adopting IVR

Science educators often evaluated declarative knowledge irrespective of the rationale for adopting IVR and reported mixed outcomes. In addition, in some cases, there was a misalignment between the evaluated outcomes and the rationale for adopting IVR. Below we further elaborate on these findings:

Visualisation of abstract concepts. Evaluation of learning outcomes in the studies in this category generally matched the purpose of adopting IVR as most of the studies (17 out of 22) evaluated declarative knowledge gains (Table 3.5). However, the evaluation focused on low-level cognitive processes. For instance, in most studies (12 out of 17) educators used pre- and post-tests with similar questions before and after the IVR experience to test the students' ability to recall information presented in IVR.

When IVR was compared to alternative learning modes, half of the studies (6 out of 12) reported positive learning gains for IVR (e.g., Bagher et al., 2020; Ferrell et al., 2019) while the other half reported no significant difference or lower learning gains (e.g., Madden et al., 2020; Parong & Mayer, 2018; Jian Zhao et al., 2020) compared to alternative learning modes. Similarly, when IVR was compared to pre-evaluation without a comparison group, three out of five studies reported positive learning gains (Southgate et al., 2019; Won et al., 2019; L. Zhang et al., 2019) and the rest comparable knowledge gains (Papachristos et al., 2017; Thompson et al., 2020).

Enhancing learning experience. Nine of the 14 studies in this category evaluated declarative knowledge gains. All the studies in this category, except one, reported positive knowledge gains for IVR compared to alternative learning modes (e.g., Bibic et al., 2019; Han et al., 2020; Lamb et al., 2018; Webster, 2016). Rychkova et al. (2020) reported comparable learning gains between IVR and a pen and paper condition for learning about electronic configurations in chemistry.

In terms of learning experience, the studies in this category evaluated motivation (n=10) and engagement (n=8), but other aspects of learning experience such as presence, perceived mental effort invested in learning and negative effects of IVR were rarely evaluated. IVR was always rated positively in terms of engagement and motivation.

The studies in this category seemed to suggest that IVR induces positive emotions during learning which may also improve the learning outcome gains. However, the positive results reported in these studies need to be interpreted with caution because researchers mainly relied on pre-and post-tests with multiple-choice type of questions. Therefore, the studies targeted only lower-level cognitive outcomes such as simple recall of some scientific facts. In addition, the evaluation of the learning experience was not comprehensive. In most cases, researchers sought simple responses regarding the students' learning experience by asking questions such as 'How much did you enjoy the learning experience?' or 'On a scale of 1-5, how engaging was learning the content in IVR?'. Consequently, learners reported that they felt engaged and that learning in IVR was 'fun' and 'interesting' but did not highlight the reasons that led to the positive learning experience.

Practical skills development. Most of the studies in this category evaluated declarative knowledge (8 studies) and learning experience in the form of presence (5 studies), motivation (6 studies), perceived usefulness (7 studies), rather than procedural knowledge (5 studies). Regarding declarative knowledge gains, only two studies (Bhattacharjee et al., 2018; Makransky, Wismer, et al., 2019) reported positive learning gains while five reported either lower or comparable learning gains for IVR in comparison with alternative learning modes (e.g., Andreasen et al., 2019; Klingenberg et al., 2020; Nie & Wu, 2020). The fact that more studies reported lower or comparable declarative knowledge gains than positive gains may partly be attributed to the misalignment between the rationale for adopting IVR and the learning outcome evaluated.

In terms of procedural knowledge gains, IVR did not always yield higher learning gains compared to alternative learning modes. Out of the five studies reporting procedural knowledge gains, only two reported better learning gains (e.g., Nie & Wu, 2020), while the rest reported no significant differences in learning gains for IVR compared to alternative 2D modes (Andreasen et al., 2019; Artun et al., 2020; Dunnagan et al., 2020). Despite the mixed outcomes on knowledge gains, participants in the studies often rated IVR positively on learning experience.

Field trips. The studies in this category evaluated attitudes and behavioural change outcomes and declarative knowledge. For attitudes and behavioural change outcomes, the studies reported positive outcomes for IVR regardless of whether IVR was compared to other learning modes (n = 4; e.g., Boda & Brown, 2020b; Yu & Lin, 2020) or to a pre-test (n = 1; Petersen et al., 2020). Regarding declarative knowledge, about half of the studies (n=4) reported better knowledge gains (e.g., Fokides & Kefallinou, 2020; Jong et al., 2020) while the rest (n = 3; e.g., Rupp et al., 2019; J. Zhao et al., 2020) reported no significant differences in knowledge gains for IVR compared to alternative learning modes.

Providing first-person experiential learning opportunities. Three studies in this category evaluated attitudes and behavioural change outcomes while two studies evaluated declarative knowledge gains. The studies reported better learning outcomes for IVR when compared to alternative learning modes (Ahn et al., 2016; Nowak et al., 2020) or to a pre-test without a comparison group (Markowitz et al., 2018) on attitudes and behavioural change outcomes. Similarly, in comparison with pre-tests, the two IVR studies reported better learning gains on declarative knowledge (Gochman et al., 2019; Markowitz et al., 2018). In addition, students in all four studies in this category rated IVR positively on presence in the learning environments.

Immersive Design Features and the Achieved Learning Outcomes

No clear patterns could be identified in immersive design features for studies reporting positive learning outcomes and those reporting lower learning outcomes for IVR. For instance, as shown in Table 3.6, studies reporting different declarative knowledge outcomes in IVR did not differ much in the nature and levels of IVR design features integrated. In addition, for procedural knowledge, the number of studies was very small to allow conclusions to be made.

Table 3.6

Average Immersive Design Feature Integration Levels and Achieved Learning Outcomes

Learning outcome evaluation	IVR vs. other modes or pre-test	Average immersive design feature integration level										
		N	Visual	Audio	Haptics	Interactivity	Virtual body	Embodied movements	Character	Storyline	Challenge	Social interactions
Declarative knowledge	better	26	2.5	1.7	1.2	1.7	1.5	1.5	1.2	1	1.1	1.3
	similar	13	2.5	1.9	1	1.7	1.5	1.5	1.2	1	1	1.4
	worse	4	2.5	2	1	1.8	1.5	1	1	1	1	1.3
Procedural knowledge	better	2	2.5	2	1	2	1.5	1.5	1	1	1	1.5
	similar	3	2	2	1	1.7	1	1	1	1	1	1.7
Attitudes	better	10	2.2	2.1	1.3	1.3	1.6	1.3	1.3	1	1	1.3

Note. N = number of studies; Attitudes = attitudes and behavioural change outcomes; Level of design feature integration: 1 = low; 2=medium; 3 = high

The findings suggested that the relationship between the design features and learning outcomes was much more complicated than expected. For instance, the relationship could be affected by a mismatch between the rationales for adopting IVR applications and the learning outcomes evaluated. In such a case, positive learning outcomes may not be obtained even when many desirable immersive design features are incorporated in the IVR applications. Moreover, each of the IVR studies that evaluated attitudes and behavioural change outcomes tended to report positive learning outcomes; consequently, it was difficult to identify which of the combinations of immersive design features were responsible for the positive outcomes.

Learner Characteristics and Achieved Learning Outcomes

Most of the studies reported the demographic information of the participants but did not explicitly explore how these characteristics influenced learning in IVR. Only four studies explored the influence of students' intrinsic interest, motivational beliefs, and science self-efficacy on their learning (Boda & Brown, 2020a, 2020b; Cheng & Tsai, 2020; Huang, 2019). In addition, only five studies evaluated the effect of prior knowledge, and the results were mixed. Two studies (Jong et al., 2020; Zinchenko et al., 2020) reported that learners with low prior knowledge learn better with IVR than learners with higher prior knowledge but other studies reported otherwise (Lui et al., 2020; Rodrigues & Prada, 2018; Uz-Bilgin et al., 2020).

Three out of 64 studies explored the effect of gender on learning with IVR simulations and the results were contradicting. Makransky et al. (2020) reported that female students learned better than male students while Madden et al. (2020) reported the opposite. In addition, a study suggested that the choice of the appearance of an on-screen pedagogical agent in IVR influenced the learning gains and the effect was moderated by gender (Makransky, Wismer, et al., 2019). In this study, female students recalled more information when they completed tasks under the instruction of a female on-screen agent while boys learned more from a drone.

Overall, although these studies showed that learner characteristics may significantly influence the learning experience and outcomes in IVR, the studies are very limited in number to draw generalisable conclusions regarding the relationship between learner characteristics and the science learning outcomes in IVR.

3.6. Discussion

Science education researchers adopted different design features depending on their focus of investigation, but often inconsistently. For example, when the rationale for adopting IVR was to help students visualise abstract science concepts, researchers highlighted the 3D visualisation capabilities of IVR showing reified objects to great amazement of students, but, in some cases, the main mode of learning was receiving information, with limited opportunities to interact with virtual objects or peers. Consequently, students were not engaged in collaborative knowledge construction processes to interrogate their own ideas and build more scientific understanding from the experience. On the other hand, when IVR activities were developed for practicing laboratory procedures, more interactive features were integrated such as selecting apparatus or the next procedural step to build procedural knowledge, but the IVR studies did not necessarily offer haptic feedback or encourage embodied movements to practice the procedures and help build muscle memory of the actions. When the primary goal was for students to experience someone else's life for implicit learning, the virtual body representation was highlighted in the IVR studies, but without intriguing storylines and challenges to emotionally engage learners to trigger behavioural change.

The reasons for inconsistent design implementation may be varied. Instead of making harsh judgments, we need to acknowledge the fact that integrating more design features takes more resources, in terms of equipment, human resources, time, and effort. Not many educators can afford all these resources; for example, high-end IVR equipment is still expensive and requires a special setup that may be out of reach based on the budgets of many researchers. Due to the limited accessibility of high-end IVR equipment, science educators may have opted for lower-end IVR equipment that are more affordable and easier to set up, but would allow very limited interactivity and embodied movement, let alone synchronised networking across multiple students.

In addition, limited technical and human resources may hinder science educators from designing and developing customised IVR activities to suit their educational and research needs. Some researchers adopted readily available off-the-shelf IVR designs such as Google Expeditions and Body VR or created low-budget IVR designs with limited actional and narrative design features. When the design of IVR programs is not fully controlled by the researchers, it is unlikely that the IVR learning activities would align well with the research goals or research designs.

Although in some studies there were some efforts to increase the alignment by adding pre and post activities, a misalignment between the designers' and the researchers' goals could have negatively impacted the evaluation of the educational benefits of IVR.

No particular combinations of immersive design features were identified to result in positive learning outcomes, partly because researchers designed, implemented, and evaluated the IVR applications inconsistently. For example, this review found misalignment between the rationale for adopting IVR and the evaluation of learning outcomes in IVR studies targeting practical skills development. The studies often evaluated declarative knowledge and learning experience rather than procedural knowledge gains. Such a misalignment might have complicated the relationship between the design features and the learning outcomes. Considering the rationale of using IVR in the design as well as the evaluation of IVR learning activities may contribute to more productive investigations of the educational benefits of IVR in future studies.

This review also found that irrespective of which design features were implemented or the rationales for adopting IVR, students' evaluation of IVR experience was generally positive in terms of presence, motivation, and engagement. Positive ratings of IVR learning experience were also reported by Checa and Bustillo (2020) in their review of 135 studies on IVR games for education and training. These positive ratings can be explained partly by the fact that, in most of the studies reviewed in the present study, learners were given only a single opportunity to learn with IVR. Therefore, the novelty effect might have enhanced the students' perceptions of learning experience (Clark, 1983). Investigating the effect of novelty in future studies is important because novelty may not only enhance learning experience but also pose challenges in students' learning with new technologies such as IVR. For example, students using IVR for the first time may feel uncomfortable or distracted which may increase extraneous processing and negatively impact on the cognitive outcomes (Hamilton et al., 2021).

Regardless of the dilemmas and limitations, science education researchers are making efforts to investigate the educational benefits of IVR technology. However, the conclusions drawn from current IVR studies in terms of the benefit of using IVR in science learning need to be investigated further because of several reasons such as: the researchers' overreliance on test instruments targeting recall knowledge, or the limited investigation of the students' prior experiences in relation to their learning processes in IVR. Another issue of potential concern is the overreliance on self-report measures for evaluation of learning experience. The outcomes may be prone to social desirability bias (Grimm, 2010). As found in some of the studies, students tended to report their learning experience in IVR positively even when they had difficulties in learning with IVR.

In addition, the majority of the studies investigated the benefits of IVR activities outside the normal school curricula. Like earlier investigations on ‘new’ educational tools such as computers and mobile phones, research studies need to move beyond highlighting IVR’s unique technological capabilities on their own but focus on designing and evaluating learning activities with IVR to enhance students’ learning in real educational contexts. Focused research questions could be: What concepts would students learn better from the IVR experience?; How well would IVR support collaborative learning amongst students?; and Why would IVR encourage students to achieve the expected learning outcomes? In designing IVR studies to answer such questions, the immersive design features along with the target learning outcomes could serve as a useful reference point.

3.7. Limitations of the Study

With a fast-evolving technology such as IVR, it is difficult to capture the ‘current’ status of educational adoption of the technology. The high-end computer-supported IVR equipment such as Oculus Rift and HTC VIVE in 2016 were eclipsed by higher resolution IVR models such as Oculus Rift S, HTC VIVE Pro, and Valve Index by 2018/2019, and these models are now competing for the market share with emerging stand-alone IVR headsets such as Oculus Quest 2 in 2020. As content development and the investigation of educational benefits take considerable time, the empirical studies reported in this manuscript may not reflect the most up-to-date IVR technology and educational applications for science teaching and learning. In addition, despite our best efforts to include as many empirical studies as possible, our database search may have unintentionally left out some important educational studies. Researchers may want to conduct periodic literature review studies to see the trends in IVR research for science learning.

3.8. Conclusion

This study investigated why science educators adopted IVR, what design features were integrated into their IVR studies to investigate its educational benefits, and what researchers found to be the impact of IVR on learning outcomes. This study aimed to open up the scholarly discussion of identifying, utilising, and evaluating various design features when investigating the educational benefits of IVR for different reasons. Generally, science educators focused their attention on the sensory aspects of IVR technology, especially on the 3D visualisation capacity for inducing immersive experiences, across diverse learning objectives to obtain mixed learning outcomes. As science educators investigate the educational benefits of IVR, they may wish to consider how various design features would enhance students' learning experiences and their learning of science through IVR.

Chapter 4. Analysis of Students' Diagrams of Water Molecules in Snowflakes to Reveal Their Conceptual Understanding of Hydrogen Bonds

Study 1, presented in Chapter 3, established the rationale for the subsequent studies (Chapters 4-6). Following on from the lack of conclusive evidence about the conceptual benefits of IVR identified from study 1, Chapters 4 and 5 explored the level of students' conceptual understanding of a challenging chemistry concept (hydrogen bonds) before and after a collaborative IVR experience. Chapter 4 presents the process and results of a fine-grained analysis of student-generated representations (diagrams, verbal explanations, and gestures) regarding the concept of hydrogen bonds in snowflakes before IVR. This chapter addresses the second research question of this thesis (*What is the level of students' conceptual understanding of hydrogen bonds in snowflakes before a collaborative IVR experience?*[3]; please see section 1.5).

The content of this chapter has been published in *Chemistry Education Research and Practice,* a Q1 journal published by the Royal Society of Chemistry. The content presented here is the version of the submitted article accepted by the journal. The table and figure numbers have been formatted for the chapter. The full citation of the published article is:

Matovu, H., Won, M., Treagust, D. F., Mocerino, M., Ungu, D. A. K., Tsai, C.-C., & Tasker, R. (2023). Analysis of students' diagrams of water molecules in snowflakes to reveal their conceptual understanding of hydrogen bonds. *Chemistry Education Research and Practice*, *24*, 437-452. https://doi.org/10.1039/d2rp00175f.

[3] The second research question was addressed through two specific sub-questions (please see Section 2.3) and they were included in Section 4.3.

4.1. Abstract

Recent studies have reported a growing trend of using student-generated diagrams for assessment in science teaching and research. However, many educators tend to use diagrams to explore students' perceptions of scientists and their work rather than explore conceptual understanding of abstract concepts. In this study, we used diagrams to investigate students' conceptual understanding of the nature of hydrogen bonds among water molecules in snowflakes. Participants were 70 first- and second-year university students. Following a sequence of interview prompts, the students drew diagrams to illustrate the interactions amongst water molecules in snowflakes. Sixty students' diagrams were analyzed inductively using a constant comparison method. Most diagrams showed that the students did not have major challenges drawing the water molecule structure, recognizing polarity of a water molecule, or recognizing the intermolecular nature of hydrogen bonds. However, the diagrams revealed varied ways in which students conceptualized the formation of hydrogen bonds. A third of the diagrams revealed students' alternative conceptions about the role of lone pairs of electrons in the formation of hydrogen bonds. Most diagrams which showed a good understanding of the nature of a hydrogen bond revealed students' difficulties in recognizing molecular interactions in a 3D space. Our findings suggest that student-generated diagrams can provide a powerful way to understand students' conceptions of abstract science concepts.

Keywords: Chemistry education; Undergraduate; Intermolecular forces; Student-generated diagrams; Conceptual understanding

4.2. Introduction

The use of diagrams is a common practice in many science classrooms (Cheng & Gilbert, 2009; Tippett, 2016). In some science classes, educators provide preconstructed diagrams and ask students to interpret the diagrams without engaging students in creating their own diagrams. For example, in biology, educators may provide students with preconstructed and labelled diagrams of biological systems and processes as a means of mediating classroom discussions (Liu et al., 2014; Quillin & Thomas, 2015). In chemistry, educators commonly provide learners with diagrams of science equipment as pre-lab activities (e.g., Chittleborough & Treagust, 2008), or diagrams of molecular structures to help students link the visible (macroscopic) to the invisible (submicroscopic) entities. In other cases, educators ask learners to construct diagrams to develop observational skills (Ainsworth & Scheiter, 2021; Quillin & Thomas, 2015), increase learners' engagement (e.g., Ainsworth et al., 2011), promote reasoning (Tippett, 2016), and for assessment (Chang et al., 2020). The present study builds on earlier literature on multiple representation research and the use student-generated diagrams for assessment to investigate students' understanding of the nature of hydrogen bonds among water molecules in snowflakes; this literature provides the theoretical framework for this research.

4.3. Theoretical Framework

Diagrams as Forms of Multiple Representations for Learning and Assessment

Multiple representations refer to using more than one way to represent the same or similar concept. Chemistry concepts are often explained in several ways such as by means of analogies, graphs, models, formulae, or diagrams (Treagust et al., 2017). For example, structures of molecules can be described using physical ball-and-stick models, space-filling models, formulae, or 2D structural drawings. Researchers concur that using multiple representations can support students' learning more than using a single representation (Gilbert & Treagust, 2009). Because each form of representation has different characteristics and may convey different but complementary information about a concept, Ainsworth (1999; 2006) proposed several functions of multiple representations in learning – supporting students to use multiple problem-solving strategies, augmenting information in one form of representation by another, and helping students construct a deeper understanding of science concepts. However, because novice students have difficulty translating freely from one form of representation to another (Allred & Bretz, 2019; Kozma, 2003; Kozma & Russell, 1997), the effectiveness of using multiple representations for these students may be limited.

Another line of multiple representation research argues that, rather than interpret externally provided science representations, students learn better when they are given an opportunity to construct and interpret their own representations, such as through drawings (Ainsworth et al., 2011; Van Meter & Garner, 2005). Indeed, a recent review of the use of diagrams in science learning settings has reported a shift from learning science *from* diagrams (interpreting preconstructed diagrams) to learning science *with* diagrams (reasoning while constructing diagrams) in recent years (Tippett, 2016). Constructing diagrams allows students to actively reason and develop mental models of science phenomena by selecting the most relevant spatial features and representing them visually (Wu & Rau, 2019). Moreover, through diagrams, students can flexibly construct, organise, represent, evaluate, and communicate their understanding of science concepts (Treagust et al., 2017). This action helps learners navigate the challenge of accumulating fragmented knowledge (Gilbert, 2006). Students can then build connections amongst concepts, and achieve meaningful learning by incorporating new learning content into already existing knowledge structures to build coherent scientific understanding (Wu & Rau, 2019). There is now a growing body of evidence that learning with drawings promotes deeper processing and integrated understanding of science concepts (e.g., Andrade et al., 2021; Tytler et al., 2020). In chemistry, for example, integrating the drawing of chemical species at the submicroscopic level in teaching and learning sessions improved students' reasoning about chemical equations and stoichiometry (Davidowitz et al., 2010) and the particulate nature of matter (e.g., Andrade et al., 2021; Derman & Ebenezer, 2020).

In addition to promoting students' reasoning and conceptual understanding, research also suggests that engaging students in drawing diagrams of science phenomena can act as a window into students' mental models of spatial and dynamic aspects of the phenomena (Tippett, 2016). Different from other ways of assessing conceptual understanding which restrict students' responses to the lists provided, the process of drawing diagrams allows students freedom to flexibly express their ideas and engage in 'sense-making' rather than 'selecting options' (Nyachwaya et al., 2011). As an exploratory research tool, students' diagrams may reveal students' alternative conceptions that existing diagnostic tests or other modes of assessment may miss (Ainsworth et al., 2011). Diagrams are especially useful when the students lack sufficient competency in the use of the relevant scientific terminologies (McLure et al., 2021b). For example, a multimodal study by Cooper *et al.* (2015) reported that students' diagrams provided a better representation of students' understanding of the nature of intermolecular forces compared to the students' written text.

A recent literature review by Chang et al. (2020) found that, in science learning settings, there is a growing trend of using student-generated diagrams for assessment purposes. However, when educators use students' diagrams for this purpose, many tend to evaluate students' perceptions of scientists through a 'Draw-A-Scientist-Test' or its modified versions (Farland-Smith, 2012; Finson, 2002; Miller et al., 2018; Reinisch et al., 2017). Other studies evaluated students' perceptions of science learning and teaching (e.g., Markic & Eilks, 2015) or students' modelling abilities (Chang et al., 2020).

In chemistry education, few studies have used student-generated diagrams to investigate students' understanding of key chemistry concepts; exceptions are the particulate nature of matter (e.g., Kelly et al., 2010; Kern et al., 2010; McLure et al., 2021a; Nyachwaya et al., 2011), atomic structure (e.g., Derman et al., 2019), and intermolecular forces (e.g., Noyes & Cooper, 2019; Williams et al., 2015). Using an open-ended drawing approach, Nyachwaya *et al.* (2011) tasked college students to balance chemical equations and illustrate the nature of particles involved in the reactions. Some students did not show the distinction between covalent and ionic bonds in chemical species, while other students exhibited difficulties interpreting symbolic language or depicting reasonable molecular geometry, relative atomic and ionic sizes, and oxidation states of the species involved in chemical reactions (Nyachwaya et al., 2011). Derman et al. (2019) reported that, when asked to illustrate their mental models of the structure of an atom, many pre-service teachers drew an atom as a central nucleus surrounded by shells (or orbits). In addition, most participants represented electrons as negatively charged particles on the shells/orbits, but did not represent the charges of protons, the space-filling character of atoms, or the quantum-mechanical theory of atomic structure (Derman et al., 2019). Related to the concept of intermolecular forces, learners used an online drawing tool to illustrate their understanding of the concepts of hydrogen bonds, dipole-dipole interactions, and London dispersion forces (Becker et al., 2016; Cooper et al., 2015; Noyes & Cooper, 2019; Williams et al., 2015). By analysing the students' diagrams, the researchers uncovered several students' alternative conceptions about intermolecular forces, such as hydrogen bonds in ethanol being intramolecular covalent bonds, or students' difficulties in recognising the role of charges in London dispersion forces.

Taken together, previous studies have provided a useful starting point in terms of demonstrating the power of using diagrams to assess students' conceptual understanding in chemistry. Previous studies mainly focused on students representing the nature and number of individual chemical species (e.g., atoms, ions, or molecules) participating in molecular reactions (e.g., Kelly et al., 2010; Kern et al., 2010). When researchers used diagrams to investigate students' understanding of the nature of interactions among particles (e.g., Noyes & Cooper, 2019; Williams et al., 2015), the students' diagrams were based on a small number of particles (two to three) and students were not tasked to reason about how the particles would interact in a context containing many particles. The position taken in our research is that by asking students to consider multiple molecules interacting with each other in a relevant context, they are engaged in thinking beyond individual particles. This action not only helps students appreciate the relevance of their chemistry knowledge but also overtly displays students' thinking about the nature of the interactions.

Students' Difficulties in Learning the Concept of Hydrogen Bonds

The concept of hydrogen bonds is one of the many abstract, yet fundamental, chemistry concepts related to molecular interactions which many students find challenging to grasp. Achieving a coherent understanding of the nature of hydrogen bonds is not a trivial task as students require a good understanding of shapes of molecules, electronegativity effects, and how these relate to the distribution of electrons in the molecules (Henderleiter et al., 2001). Without a coherent understanding of the concept of hydrogen bonds, students may rely on rote memorisation of facts to predict or explain properties of substances (Cooper et al., 2013).

Studies have reported students' difficulties in understanding the concept of hydrogen bonds and its importance in explaining many macroscopic properties of substances, such as boiling and melting points (Henderleiter et al., 2001; Schmidt et al., 2009). Using a two-tier diagnostic test, Schmidt et al. (2009) provided lists of compounds and asked students to identify with reasons which of the compounds would form hydrogen bonds. The authors reported that some senior high school students had difficulties identifying compounds that could form hydrogen bonds. Using interviews and lists of individual structural formulae already constructed by the researchers, Henderleiter *et al.*(2001) tasked undergraduate organic chemistry students to identify the situations in which hydrogen bonds can form among molecules, and to apply their understanding of the concept of hydrogen bonds to explain trends in boiling points of substances. Henderleiter et al. (2001) reported that some students had difficulties in predicting the formation of hydrogen bonds in molecules; for instance, some students explained that water molecules could form hydrogen bonds with methane molecules by polarizing the hydrogen atoms in the methane molecules. Students also tended to confuse the term hydrogen bond with covalent bonds that involve hydrogen atoms (Williams et al., 2015). For example, when tasked to illustrate their understanding of hydrogen bonds through diagrams, the majority (about 60%) of first-year university students enrolled in a general chemistry course illustrated hydrogen bonds in ethanol molecules as bonds occurring "within" the molecules rather than as intermolecular forces (Cooper et al., 2015).

Overall, previous studies employed a range of strategies and prompts to uncover students' understanding of the concept of hydrogen bonds. Some of the studies provided contexts for students to demonstrate their understanding (Henderleiter *et al.*, 2001; Schmidt *et al.*, 2009). However, researchers argued that students could easily rely on their rote memorization of the concept of hydrogen bonds in these contexts by choosing from the lists of options provided (e.g., Schmidt et al., 2009), or invoke key words in their explanations of macroscopic properties without a clear understanding of how hydrogen bonds are formed (Cooper et al., 2013). For example, to predict the occurrence of hydrogen bonds, some students simply focused on identifying the presence of oxygen and hydrogen atoms in molecules or applying periodic trends in electronegativity without considering when such trends fail to apply (Schmidt et al., 2009). In addition, none of the previous studies on students' conceptions of hydrogen bonds investigated in-depth how students conceptualised the formation of hydrogen bonds. Although recognising that hydrogen bonds are intermolecular in nature is important, this is only the first step to understand the nature of these intermolecular interactions. Yet, earlier studies did not go deeper to investigate students' understanding of the reason why a hydrogen bond forms and the role of lone pairs of electrons. Moreover, by using key chemistry terms, such as hydrogen bonds or dipole-dipole interactions in their prompts, previous studies may have limited the students' freedom to express their understanding of molecular interactions (e.g., Cooper et al., 2015). Also, previous studies did not provide prompts for students to coherently reason and demonstrate their understanding of the concept of hydrogen bonds through diagrams.

In this research, we employed student-generated diagrams to investigate students' conceptual understanding of the nature of hydrogen bonds among many water molecules in snowflakes and to identify the difficulties that students may face as they link different chemistry concepts to illustrate the nature of these molecular interactions. Understanding students' ideas and learning difficulties can be used to inform design interventions for addressing students' learning difficulties and alternative conceptions in a more systematic way (Nyachwaya et al., 2011). To effectively engage with drawing activities, students require opportunities to discuss their ideas with peers and knowledgeable others (McLure et al., 2021b), and the drawing activities need to be scaffolded appropriately through training or prompts (Ainsworth & Scheiter, 2021; Van Meter & Garner, 2005). Therefore, in this research, the students were asked to explain their drawings to the researchers. The researchers also provided prompts for students to progressively build on their prior understanding of structure and polarity of water molecules while reasoning about the interactions among water molecules in the context of snowflakes. The present study was designed to answer the following research questions:

1. How do students use diagrams to represent their understanding of the nature of hydrogen bonds among water molecules in snowflakes?
2. What are the common conceptions of the nature of hydrogen bonds among water molecules in snowflakes inferred from these student-generated diagrams?

4.4. Methods

Research Context

A total of 70 first-and second-year undergraduate chemistry students enrolled in two chemistry units (Reactivity and Function in Chemistry for first-year students, and Chemistry of Biological Processes for second-year students) at a large public university in Australia participated in the study. The two chemistry units include a focus on the concepts of intermolecular forces and molecular shape and how these factors influence the chemistry of substances. Each unit is taught in the form of 1-2-hour lectures, 3-4-hour hands-on lab sessions, and 1-2-hour tutorial workshops led by tutors per week. During the tutorial workshops, students work in teams of 3-5 to complete learning tasks following a Process-Oriented Guided Inquiry Learning (POGIL) approach. In some activities, students manipulate ball-and-stick models to explore different forms of molecules such as conformations and enantiomers. Students also often draw diagrams of molecular structures while completing the tasks. However, the emphasis is placed on the symbolic representations but not on the submicroscopic interactions, and no specific emphasis is placed on representing molecules in 3D. In addition, reading materials such as Blackman et al. (2019) are recommended although they are not mandatory. This textbook is recommended for use in over 15 universities across Australia and New Zealand.

Students enrolled in the two units were those taking chemistry-related degree programs such as Chemistry, Chemical Engineering, Food science, and Nutrition. The enrolled students were considered to have an adequate understanding of the basic chemistry concepts related to water molecules as all these students had completed and passed high school chemistry and at least one university level chemistry unit as a prerequisite to be in these two chemistry units. The participation of these students in the interviews and subsequent learning activities was seen as beneficial for the students in the two units, and the lecturers encouraged all students to participate in them.

The interviews and drawing activities were conducted outside the normal course timetables and students were free to choose the most convenient time for them to participate. Scheduling of the sessions was done using an online meeting scheduling tool (doodle.com). Students logged into the online system via a link that was provided by the researchers. The students were informed that they would complete the learning tasks in pairs, therefore, each slot could be occupied by two students. Since the students randomly selected slots, some students were paired with their friends while others with peers with whom they had not worked with prior to this activity.

Data Collection

Before collecting data, ethics approval was obtained from the institutional Human Research Ethics Committee (HRE2020-0081). In addition, before participating in the study, students gave consent to use their diagrams and interview data for this study.

In this study, the students were paired so that they could explain their ideas to each other and were given an opportunity to collaborate on the drawing task to produce a shared diagram if they wished. Each student was given a pen and paper and tasked to draw a diagram to illustrate their understanding of the nature of hydrogen bonds among water molecules in snowflakes. Because explaining the nature of hydrogen bonds requires students to integrate their knowledge of the bonding, structure, and polarity in water molecules, the researchers provided students with a series of verbal prompts so that the students could complete the drawing activity stepwise. The prompts were not intended to guide learners to the correct answers or lead them to a better understanding but to elicit students' ideas about the concepts underlying the interactions amongst water molecules illustrated in their drawings. Also, because it is common for students to confuse the term 'hydrogen bonds' with intramolecular covalent bonds involving hydrogen atoms (e.g., Cooper et al., 2015), or to simply reproduce textbook definitions of the concept, in this study, we did not directly use the term hydrogen bonds in the interview prompts. Instead, we asked the students to illustrate how they imagined the water molecules interacting with one another in the context of snowflakes.

The verbal prompts used in this study were developed in meetings among three authors (HM, MW, and DU), and were checked by the other authors, two of whom had more than twenty-five years' experience in teaching first- and second-year university chemistry units. The final verbal prompts employed by the researchers are provided in Table 4.1.

Table 4.1

Target Concepts and Interview Prompts to Support Students' Drawings in the Drawing Activity

Target concept	Verbal prompt
Structure of a water molecule	Here we have some magnified images of snowflakes (the researcher shows some of the shapes of snowflakes). a) What do you notice about the shapes of snowflakes? b) Snowflakes are made from water molecules. Imagine I am a year 11 (high school) student, what can you tell me about a water molecule? c) Please draw the water molecule you have described at the centre of the piece of paper. d) Why is the water molecule shaped like that?
Polarity and nature of hydrogen bonds among water molecules	Let's imagine that this water molecule is at a very low temperature, say close to its freezing point, and we have another water molecule coming close enough to the first one to interact with it, e) How would you draw the interaction between those two water molecules? f) Why would the molecules interact like that? g) If we have another molecule coming close to the first one, is it still possible for it to interact with the first one? How would you draw the interaction between the third water molecule and the first one? Please explain why the molecules would interact like this. [This prompt was repeated until the student said that no more water molecules would interact with the first one, with reasons]

Students' diagrams in response to the verbal prompts were collected. In addition, all the students' interactions were audio and video recorded. For each pair of students, the interview and drawing activity lasted 15-25 minutes.

As mentioned above, in the present study, students were given opportunities to discuss their ideas with one another and to collaborate while constructing the diagrams. However, most students preferred to construct individual diagrams and to provide individual explanations, irrespective of whether the students were friends prior to the activity or not, or whether the students' ideas were similar or not. Therefore, after a few sessions, the authors dropped the prompts asking the students to discuss with each other every time. Instead, the authors asked each student to draw a diagram to represent their own understanding and to explain their diagram verbally (Table 4.1). After drawing, the individual students were asked to confirm if they were happy with their diagrams.

Students in four of the pairs collaborated during the drawing task, taking turns at drawing to create shared diagrams, and explaining to each other as they drew the diagrams. When students collaborate to construct a shared diagram, it is hard to discern which idea belongs to which student and, by working on the same diagram, students may be forced to change their ideas in the process. Therefore, the authors decided to exclude shared students' diagrams from the analysis. For a given student-generated diagram to be included in the analysis, the student needed to have been enrolled in the two target chemistry units and the student must have constructed the diagram individually to illustrate their understanding of water molecule interactions. A student who did not draw a diagram was not considered for analysis.

Analysis

Of the 70 student participants, data from 60 students was used for analysis. One student was not enrolled in the target chemistry units while one student did not draw a diagram and, therefore, had incomplete data. Diagrams created by eight of the students (4 pairs) were also excluded because the students collaborated to construct shared diagrams (one diagram from each pair). The remaining 60 students' diagrams were analysed qualitatively. In our earlier work (e.g., McLure et al., 2021b; Tenzin et al., 2022), we identified a set of procedures to interpret students' diagrams in relation to their conceptual understanding without extensively relying on students' verbal explanations. We adopted similar procedures to analyse students' diagrams in the present study.

First, inductive analysis (Merriam & Tisdell, 2015) of the diagrams was conducted to identify categories related to the students' conceptions of the nature of hydrogen bonds among water molecules in snowflakes. Two of the authors of this paper (HM & MW) carefully examined each student's diagram to identify the students' conceptions of the structure and polarity of a water molecule and the nature of hydrogen bonds among water molecules in snowflakes. A constant comparison method (Merriam & Tisdell, 2015) was then adopted to identify categories related to students' conceptions of the nature of hydrogen bonds among water molecules in snowflakes.

Although the focus of this study was understanding students' conceptions of the nature of hydrogen bonds as represented in their diagrams, the drawing activity was multimodal in nature (Jewitt, 2013) since students were tasked to draw diagrams as well as verbally explain their understanding. In such a case, students may choose to illustrate some ideas in their diagrams and represent other ideas using other modes (verbal explanations and gestures). Therefore, in analysing the students' diagrams, the first two authors (HM & MW) constantly referred to the transcripts and videos of the interactions the students engaged in during the drawing activities to confirm the authors' interpretations of the nature of students' conceptions represented in the diagrams. For example, when students expressed difficulty in representing the 3D nature of molecular interactions on a piece of paper, the two authors supplemented the students' diagrams with their verbal explanations and gestures to accurately represent the students' understanding. The data and the coding scheme were constantly revisited in meetings between the two authors to refine the categories until a consensus was reached that all the data was correctly represented and that no more categories were emerging out of the data. Once the two authors agreed upon the categorisation of students' understanding, the coding scheme was further checked against the data and refined by a second pair of authors (MM & RT). Amendments in the categorisation of the students' diagrams were discussed with the first two authors until a consensus was reached. The final categories of students' diagrams were discussed and confirmed by four authors (HM, MW, DT, and MM).

4.5. Findings

Analysis of the diagrams in relation to the students' conceptions of the nature of hydrogen bonds among water molecules in snowflakes generated four conceptual categories, A-D. Category A diagrams showed students' difficulties in drawing the structure of a water molecule and/or reasoning about polarity in water molecules and the nature of intermolecular interactions.

Category B diagrams revealed students' difficulties in recognizing the role of lone pairs of electrons in the formation of hydrogen bonds. Both Categories C and D diagrams indicated hydrogen bonds as directional intermolecular forces between lone pairs of electrons on oxygen atoms and hydrogen atoms of neighbouring water molecules; Category C diagrams showed the molecular interactions in 2D space whilst Category D diagrams represented interactions in 3D space. The descriptors of the conceptual categories and the number of diagrams in each category are shown in Table 4.2.

The conceptual categories A-D are further discussed below:

Category A: Uncertain of the Structure of Water Molecules and/or the Nature of Intermolecular Interactions

The diagrams in this category (n = 10) showed that the students had difficulties recognising the difference between the nature of intermolecular and intramolecular interactions. Diagrams in category A did not indicate the existence of polarity in water molecules and its role in the formation of hydrogen bonds. These students' diagrams showed hydrogen bonds as covalent interactions between molecules rather than as electrostatic interactions. Some diagrams in this category (n=3) also showed that the students struggled with drawing the structure of a water molecule. These students had difficulties in reasoning about the number of bonds that individual atoms can form. For example, Craig's diagram (Figure 4.1a) indicated that the student knew that each water molecule consisted of a central oxygen atom which was bonded to two hydrogen atoms. However, the oxygen atom formed double bonds with hydrogen atoms to complete an octet, just like a carbon atom in a carbon dioxide (CO_2) molecule would. The diagram shows that Craig did not realise that the hydrogen atom could not form more than one covalent bond. Craig also had difficulties in recognising the non-covalent nature of intermolecular interactions. Although Craig had heard about hydrogen bonds, the student imagined that these were covalent bonds involving hydrogen atoms of different molecules. To represent a 'hydrogen bond', the student drew a solid line between hydrogen atoms in different water molecules. While drawing, Craig explained that "*it must be hydrogen to hydrogen … because it is a hydrogen bond… it wouldn't be oxygen to oxygen… because oxygen already has a full octet*".

Table 4.2

Categories of the Students' Diagrams on Hydrogen Bonds Among Water Molecules in Snowflakes

Categories	Number of diagrams	Descriptors
A: Uncertain of the structure of water molecules and/or the nature of intermolecular interactions	10	Diagrams show linear water molecules and multiple covalent bonds to hydrogen atoms; no indication of polarity in water molecules; intermolecular interactions are represented as covalent bonds between molecules rather than as electrostatic interactions; hydrogen bonds are formed between hydrogen and hydrogen atoms, or oxygen and oxygen atoms.
B: Uncertain of the role of lone pairs of electrons in forming hydrogen bonds	20	Diagrams show bent structures and polarity in water molecules; hydrogen bonds are not covalent in nature – they are electrostatic interactions between molecules but the role of lone pairs of electrons in forming a hydrogen bond is unclear. The lone pairs form an electron dense region around the oxygen atom to form one or numerous hydrogen bonds, or individual electrons form hydrogen bonds.
C: Molecules form hydrogen bonds in 2D space	25	Diagrams indicate bent structures and polarity in water molecules; hydrogen bonds are electrostatic interactions between oxygen and hydrogen atoms of different molecules; the role of lone pairs in forming hydrogen bonds is clear; water molecules form multiple hydrogen bonds but the interactions among water molecules are represented in 2D space.
D: Molecules form hydrogen bonds in 3D space	5	Diagrams indicate hydrogen bonds as electrostatic interactions between lone pairs of electrons and hydrogen atoms in different molecules; each water molecule forms a tetrahedral structure (four hydrogen bonds) in 3D space.

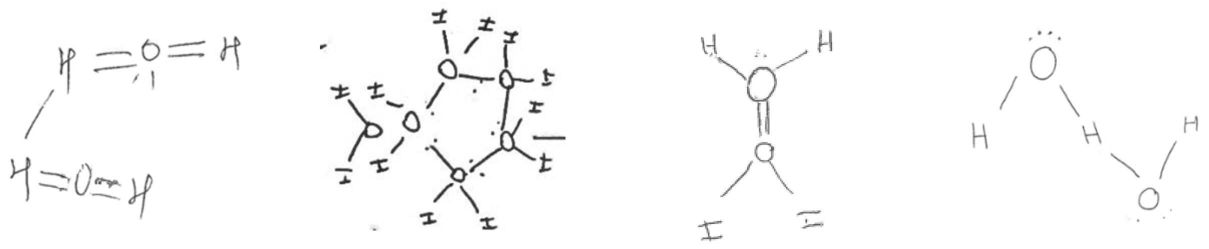
The rest of the diagrams in this category (n = 7), such as those of Ross (Figure 4.1b), Andrea (Figure 4.1c), and Anita (Figure 1d), showed a reasonable understanding of the structure of a water molecule. The students drew a bent structure for a water molecule with two or four dots around the oxygen atom, suggesting lone pairs of electrons. However, the students had difficulty explaining why the molecule was bent in shape and did not recognize polarity in water molecules and its role in intermolecular interactions. When asked to illustrate how the water molecules in snowflakes interacted, the students made attempts to connect different water molecules, but they had difficulty in recognizing that a hydrogen bond was a non-covalent interaction between an oxygen atom in one molecule and a hydrogen atom in another molecule. For example, in his diagram, Ross indicated dots to represent the nonbonding electrons on oxygen atoms but was not entirely sure of why a water molecule was bent. When asked about the shape of the molecule, he explained that "*isn't it the orbital?... it is supposed to actually repel each other depending on its electronegativity…*". In terms of molecular interactions, Ross connected oxygen atoms in two neighbouring water molecules with a solid line coming off the nonbonding electrons. Ross' diagram suggested that the oxygen atoms in water molecules would use the lone pairs of electrons to bond covalently with neighbouring water molecules. The student had difficulties distinguishing interactions between atoms to form molecules and interactions among molecules (such as hydrogen bonds). Ross verbally explained that *"...the oxygen [atom] is just craving for more bonds because it has the two valence electrons."*

Andrea drew a bent structure of a water molecule (Figure 4.1c) and explained that "*the water molecule has a bond angle of 120 … I am not sure if it's because these two hydrogen bonds [the O-H bonds in a water molecule] repel each other*". Andrea also connected the oxygen atoms of neighbouring water molecules, but with a double bond. The oxygen atom in a water molecule looked like a carbon atom in an ethene molecule. While drawing her diagram, Andrea explained that "*the oxygen molecules will attach to each other … because of the lone pairs*." Like Ross, Andrea had difficulty recognising the difference between intermolecular and intermolecular interactions. Both Ross and Andrea reasoned that the water molecules could interact covalently, and this was clearly represented in their diagrams.

Anita's diagram (Figure 4.1d) showed that, the student knew about the composition and bent structure of a water molecule. Anita also knew that a hydrogen bond involved hydrogen and oxygen atoms. However, the student reasoned that a hydrogen bond resulted in a common hydrogen atom being covalently shared between two oxygen atoms. While drawing, Anita commented that, *"I think it [the second molecule] will attach to the hydrogen, because it is hydrogen bonding … two water molecules share a hydrogen atom".*

Figure 4.1

Examples of Students' Diagrams Showing Difficulties in Reasoning About the Structure of Water Molecules and/or the Nature of Intermolecular Interactions



(a) Craig's diagram (b) Ross' diagram (c) Andrea's diagram (d) Anita's diagram

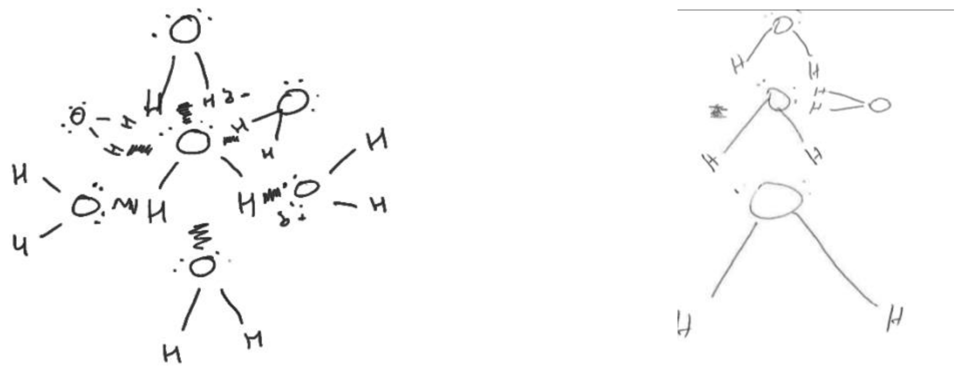
Category B: Uncertain of the Role of Lone Pairs of Electrons in Forming Hydrogen Bonds

The diagrams in this category (n = 20) showed the bent shape of each water molecule. Most of the diagrams in this category indicated dots on the oxygen atoms to illustrate the presence of nonbonding electrons. Most diagrams in category B also showed that students recognised the presence of partial charges in water molecules. In addition, all the diagrams in category B showed that hydrogen bonds were intermolecular in nature and different from intramolecular bonds. For this purpose, the students connected molecules with dashed or zigzag lines, or simply showed water molecules close to one another to show that hydrogen bonds were not covalent bonds but simply electrostatic forces of attraction between oxygen and hydrogen atoms in different molecules. However, the diagrams in category B showed students' difficulties in reasoning about the role of lone pairs of electrons in the formation of hydrogen bonds.

Four of the diagrams in this category, such as those of Harrold (Figure 4.2a) and Jasper (Figure 4.2b), showed that a water molecule has two charged regions, a partially positive (δ+) and a partially negative (δ-) region. The hydrogen atoms of each water molecule collectively formed a partially positively charged region while the nonbonding electrons on the oxygen atom also collectively created a single partially negatively charged region. Water molecules in snowflakes interacted through electrostatic attraction between these oppositely charged regions without any directionality. Neighbouring water molecules were stacked around the central one. For example, Harrold's diagram showed that a water molecule was bent in shape and that the oxygen atom had two lone pairs of electrons. The student explained that these electron pairs repel each other, and the position of the hydrogen atoms result in the bent shape of a water molecule, and that "*the water molecule is polar, one side is slightly negative, the other side is positive (draws partial charges*)". To represent the interactions among molecules, Harrold illustrated that the hydrogen end of each incoming water molecule approached the region of lone pairs of electrons on the central molecule and vice versa. The student used zigzag lines to represent the interactions between the oppositely charged ends of different water molecules, suggesting that the hydrogen bonds were not covalent in nature. While constructing his diagram, Harrold explained that *"opposites attract… so slightly negative will go to the slightly positive side of the other water molecule"* without mentioning the role of lone pairs of electrons or individual hydrogen atoms. Harrold's explanation confirmed our interpretation of his diagram that the student recognized polarity in water molecules but had difficulties in recognizing the role of individual lone pairs of electrons and the individual hydrogen atoms in the formation of hydrogen bonds. A similar explanation of molecular interactions was provided by Jasper.

Figure 4.2

Examples of Students' Diagrams Illustrating Difficulties in Reasoning About the Directionality of Hydrogen Bonds



(a) Harrold's diagram (b) Jasper's diagram

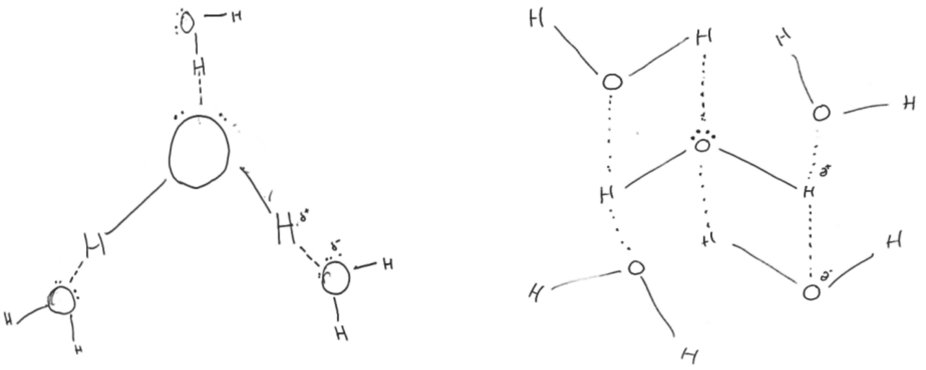
About half of the diagrams in category B (n= 8) also showed that the oxygen atom in a water molecule is partially negatively charged (δ-) and that each hydrogen atom was a partially positively charged (δ+) region. Like the diagrams in Figure 4.2, these diagrams (Figure 4.3) showed that the two lone pairs of electrons in a water molecule collectively formed a single partially negative (δ-) region. However, different from the diagrams in Figure 4.2, each hydrogen atom was a separate partially positively charged region. Therefore, each water molecule had three partially charged regions. Oppositely charged regions in neighbouring water molecules would attract each other in a flat plane.

For example, Gina's diagram showed that, to form hydrogen bonds among water molecules, the partially negative region around the oxygen atom of the central water molecule attracted a single hydrogen atom of a neighbouring water molecule (Figure 4.3a), and each hydrogen atom of the central molecule attracted an oxygen atom of a neighbouring molecule. To support her diagram, Gina first explained that a water molecule was bent because "*based on the electron repulsion theory, the nonbonding electrons force the hydrogen atoms closer together (gestures the bent shape with both hands*)". While drawing the interactions between molecules, Gina first connected water molecules to the hydrogen atoms of the central molecule reasoning that "*there is a hydrogen bond… an intermolecular force between the positive end of this [central] water molecule and the negative end of this [attaching] water molecule, they attract each other*". According to Gina, the oxygen and hydrogen ends of a water molecule created a dipole. However, the two lone pairs of electrons collectively formed a single hydrogen bond. Gina's verbal explanations were aligned with her diagram representing bent shapes of water molecules, partial charges on the atoms, and a single dotted line from each oxygen atom to represent intermolecular hydrogen bonds.

On the other hand, Tobby's diagram (Figure 4.3b) also clearly showed the bent shape and polarity in water molecules, but the oxygen atom of the central molecule had a negative charge all around it that would attract hydrogen atoms of neighbouring molecules from different directions. According to Tobby, *"… there's more electrons present on the central oxygen compared to the hydrogen, which means that this [hydrogen atom] becomes … slightly delta positive and this [oxygen atom] … slightly negative, and … opposites attract*." Just like his diagram, Tobby's verbal explanation did not emphasise the role of lone pairs of electrons. The diagram also indicated that the student had difficulties in recognising how many hydrogen bonds each hydrogen atom could form. From his diagram, each hydrogen atom of a central molecule appeared to have enough positive charge to attract more than one oxygen atom from neighbouring water molecules (Figure 4.3b).

Figure 4.3

Examples of Students' Diagrams Showing Three Partially Charged Regions in Water Molecules Forming Hydrogen Bonds

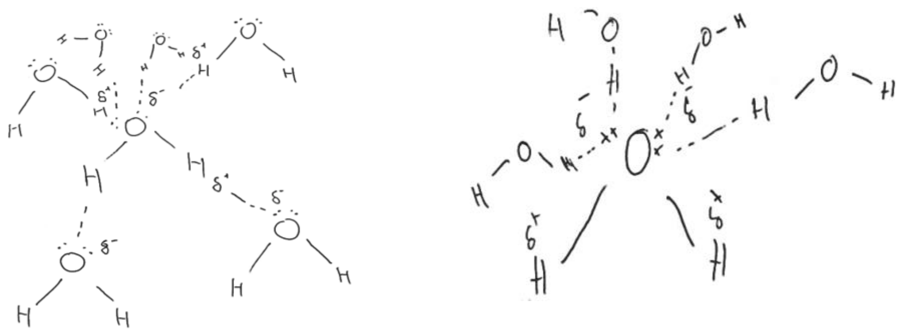


(a) Gina's diagram (b) Tobby's diagram

The rest of the diagrams in category B (n=8) also showed that each hydrogen atom in a water molecule is a separate partially positive (δ+) region, and that hydrogen bonds were electrostatic interactions amongst molecules. However, different from the diagrams in Figure 4.2 and Figure 4.3, these eight diagrams (such as those in Figure 4.4) showed that each of the four nonbonding electrons on the oxygen atom in a water molecule can individually form a hydrogen bond with a hydrogen atom in a neighbouring water molecule. For example, diagrams by Morris (Figure 4.4a) and Aaron (Figure 4.4b) showed that, being negatively charged, each individual nonbonding electron on the oxygen atom can attract a partially positively charged hydrogen atom from a neighbouring molecule.

Figure 4.4

Examples of Students' Diagrams Showing Hydrogen Bond Formation with Individual Nonbonding Electrons



(a) Morris' diagram (b) Aaron's diagram

When asked to provide his reasoning, Morris explained that *"I have attached one of the lone electrons to the positive hydrogen, that's how they bond… the hydrogen only takes one electron … two hydrogens for each pair"*. Although the student talked about the hydrogen atoms 'bonding' to the individual electrons, he indicated these intermolecular hydrogen bonds as dotted lines to distinguish them from the intramolecular covalent bonds. A similar line of reasoning was evident in Aaron's diagram and verbal explanation, except that Aaron did not draw hydrogen bonds from the hydrogen atoms of the central water molecule.

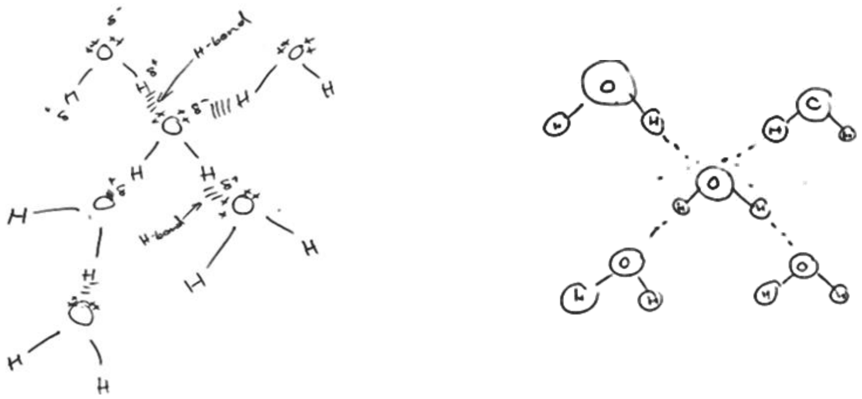
Category C: Molecules Form Hydrogen Bonds in 2D Space

The diagrams in this category (n=25) showed the bent shape of a water molecule. The diagrams also showed that the students recognised that each water molecule is polar in nature and has two pairs of nonbonding electrons on the oxygen atom. Similar to category B, the diagrams in category C also showed a hydrogen bond as an electrostatic force of attraction between different water molecules. Unlike diagrams in category B, the role of lone pairs of electrons in forming hydrogen bonds was clearly shown in the diagrams in category C. Diagrams in category C showed that a hydrogen bond formed between a lone pair of electrons on an oxygen atom in one molecule and a partially positive hydrogen atom of a neighbouring water molecule. Since a water molecule has multiple sites (individual hydrogen atoms and lone pairs of electrons) for forming hydrogen bonds, each water molecule can form multiple hydrogen bonds with other molecules.

Most diagrams in this category (n = 20), such as those of Monica (Figure 4.5a) and Carlos (Figure 4.5b), showed that each water molecule in a snowflake formed a maximum of four hydrogen bonds with neighbouring water molecules using two lone pairs of electrons on the oxygen atom and two hydrogen atoms. In her diagram, Monica illustrated partial charges on the different atoms and labelled the hydrogen bond as the force of attraction between a lone pair and a partially positive hydrogen atom. Monica explained that "*oxygen and hydrogen have different electronegativities which allow molecules to interact via hydrogen bonds … the lone pairs of electrons help the hydrogen atoms to be attracted to the oxygen*". Similarly, after drawing the first four water molecules attached to a central molecule, Carlos explained that any more water molecules would be attached *"not to the first one [central molecule] but on those outside*" suggesting that the student recognized that each molecule had only four opportunities for forming hydrogen bonds. However, these students' diagrams, did not indicate the positioning of water molecules in 3D space, implying that the water molecules were interacting in a flat plane. For example, the drawings by Monica and Carlos showed a square planar arrangement created by water molecules interacting with the central molecule in 2D. Also, the students did not mention molecules interacting in 3D.

Figure 4.5

Examples of Students' Diagrams Showing the Formation of Hydrogen Bonds in 2D



(a) Monica's diagram (b) Carlos' diagram

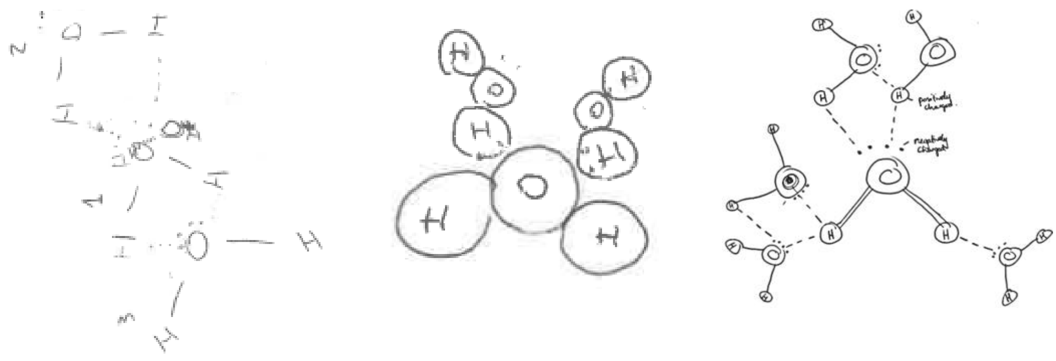
The remaining five diagrams in this category not only showed that molecules interacted in 2D but also that the students did not recognize that, in snowflakes, each water molecule interacted with four other water molecules through hydrogen bonds. For example, Calvin's diagram (Figure 4.6a) indicated that each water molecule had two lone pairs of electrons and two hydrogen atoms, and that each hydrogen atom was attracted to a lone pair of electrons. Both hydrogen atoms and lone pairs of electrons participated in the formation of hydrogen bonds and each water molecule formed four hydrogen bonds. In his explanation, Calvin elaborated that "*the hydrogen and oxygen ends of water molecules differ in polarity… they attract … hydrogen to lone pair*". However, Calvin's diagram showed that he was uncertain of the orientation of the water molecules around the central one – water molecules arranged themselves in a 2D plane.

Miriam's diagram (Figure 4.6b) showed that the student recognised a hydrogen bond as an intermolecular force rather than a covalent bonding interaction; by drawing the attached water molecules in those positions on the central one, the diagram showed that the student recognised the role of lone pairs. After connecting a hydrogen atom to the central water molecule, the student also verbally explained that "*there will be a lone pair here [on the oxygen], and another lone pair here*". However, Miriam's diagram also showed that only the lone pairs of electrons on the central molecule would participate in forming hydrogen bonds. As a result, one water molecule in a snowflake could form a maximum of two hydrogen bonds with neighbouring molecules in 2D. This interpretation was further confirmed when the student explained that it was not possible for more water molecules to interact with the first molecule because “*there were no more lone pairs*”.

Albert’s diagram (Figure 4.6c) showed that both hydrogen atoms and lone pairs of electrons in a water molecule could participate in forming hydrogen bonds. Albert’s representation of the first water molecule was different from the rest. It appeared that the student was trying to produce a realistic diagram of the molecular models he was familiar with. When asked about his representation, the student explained that “*[the double lines] are meant to be like a ball-and-stick model.*" Albert completed the diagram by adopting a simpler convention of representing water molecules using a single line to show the covalent bond between oxygen and hydrogen atoms. The student verbally explained that *“[a hydrogen atom is] slightly more positively charged, which is attracting the negative charge of the oxygen free electrons, lone pairs”*. Despite this understanding, Albert visualised the molecular interactions in 2D. As a result, in his diagram, the student misjudged the distances between atoms in different molecules – water molecules could approach each other so closely that a hydrogen atom in one water molecule could form more than one hydrogen bond and a water molecule could form more than four hydrogen bonds with neighbouring molecules.

Figure 4.6

Examples of Students’ Diagrams Showing Water Molecules Forming Multiple Hydrogen Bonds in 2D



(a) Calvin’s diagram (b) Miriam’s diagram (c) Albert’s diagram

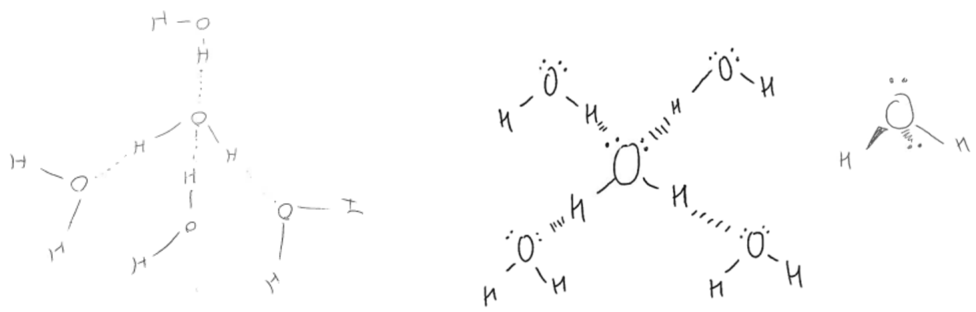
Category D: Molecules Form Hydrogen Bonds in 3D Space

Like most diagrams in category C, the diagrams in category D (n=5) showed a reasonable understanding of the nature of hydrogen bonds among water molecules in snowflakes in that hydrogen bonds were electrostatic in nature and were formed between hydrogen atoms and lone pairs of electrons in different molecules. Using both hydrogen atoms and both lone pairs of electrons on the oxygen atom, each water molecule in a snowflake formed a maximum of four hydrogen bonds with other water molecules. Unlike category C, the diagrams in category D also emphasized that the water molecules interacted in a three-dimensional space rather than in a two-dimensional plane.

For example, the diagram by Matt (Figure 4.7a) showed that the nonbonding electron pairs on the centre oxygen atom in a water molecule were in different planes. Therefore, through hydrogen bonds, water molecules formed a 3D tetrahedral structure. When drawing, Matt explained that "*it [the arrangement of molecules] will be a bit more 3D than that but, yeah, that would be a tetrahedral form*". Similarly, although the first diagram by Timothy (Figure 4.7b) appeared like those in category C, Timothy drew a second diagram to emphasize that the four electron domains in a water molecule were in 3D space. Therefore, water molecules would form 3D structures by interacting with other water molecules through hydrogen bonds. In fact, after drawing the four water molecules around one, Timothy explained that "… *a better way to draw it would be in 3D like (draws the water molecule with electron domains on different sides), you know how we draw 3D? … is that 3D?*".

Figure 4.7

Examples of Students' Diagrams Showing Water Molecules Forming Hydrogen Bonds in 3D



(a) Matt's diagram (b) Timothy's diagram

Some students (n=3) acknowledged that water molecules would interact in 3D, but they could not effectively represent such interactions with their diagrams on a piece of paper. Instead, they used gestures and verbal explanations to express their ideas. For example, after drawing four water molecules connected to a central one with hydrogen bonds, one of the students explained that "*… these four water molecules could in turn bond onto other three individual molecules (uses gestures to show interactions from different angles) … it would create a shape that is 3D lattice.*"

Summary of Analyses

Overall, the analysis of the student-generated diagrams in this study showed that most students (50 out of 60) had a good understanding of the structure and polarity of a water molecule. However, the nature of hydrogen bonds among water molecules in snowflakes was conceptualised in a wide range of ways. While half (n=30) of the student-generated diagrams showed a hydrogen bond as being intermolecular, electrostatic, and directional in nature (categories C and D), the other half of diagrams revealed students' difficulties or alternative conceptions about the structure of a water molecule and/or the nature of intermolecular interactions (category A), or the role of lone pairs of electrons in the formation of hydrogen bonds (category B). Also, the number of students who visualised hydrogen bonds among water molecules in 3D space (5 out of 60) was very small considering that the participants in this study were those majoring in chemistry and chemistry-related degree programs and had experienced teaching with molecular models.

4.6. Discussion

Using student-generated diagrams, this study investigated university chemistry students' conceptual understanding of the nature of hydrogen bonds among water molecules in snowflakes. Irrespective of the students' conceptions of the nature of hydrogen bonds, most of the diagrams showed the bent structure of water molecules and showed the nature of intramolecular bonds in water molecules to be covalent. While constructing the diagrams, many students explained that drawing was not an easy task for them because they had never considered representing molecular interactions when many molecules are involved. The relatively novel approach of visually illustrating their understanding through diagrams challenged students to integrate their prior understanding in a way that they may not have been used to before. Studies also have reported that even though students may be able to express their understanding in symbolic forms, they may have difficulties to visually represent chemical processes at the submicroscopic level (Dickson et al., 2016; Nyachwaya et al., 2011).

Despite the difficulties these students may have faced in representing the molecular interactions among water molecules in snowflakes, with appropriate prompts, these first-and second-year undergraduate students made efforts to illustrate how they visualised the interactions. Many students represented hydrogen bonds as dashed (or dotted) lines. Other students simply positioned hydrogen atoms close to or touching the lone pairs of electrons on oxygen atoms. These representations were efforts by the students to illustrate that a hydrogen bond was a force of attraction between molecules, different from intramolecular bonds. Many students also recognised that water molecules were polar in nature, and some included partial charges on the oxygen and hydrogen atoms in their diagrams. Our findings suggest that, when prompted appropriately, students can engage in drawing diagrams that illustrate their conceptual understanding.

This study found that the students had varied ways of conceptualizing the exact nature of hydrogen bonds among water molecules, even though most recognised the hydrogen bonds as intermolecular forces. Half of the diagrams (30 out of 60) showed a reasonable scientific understanding of the nature of hydrogen bonds among water molecules in snowflakes. The diagrams showed a hydrogen bond as an electrostatic attraction between a hydrogen atom of one water molecule and a lone pair of electrons on the oxygen atom in a neighbouring water molecule. Some diagrams revealed students' difficulties in conceptualising the nature of hydrogen bonds among water molecules in snowflakes, including difficulties in distinguishing hydrogen bonds from covalent bonds (n=10), recognising the role of lone pairs of electrons in the formation of hydrogen bonds (n=20), and recognising molecular interactions in 3D space (n=25).

Previous studies (e.g., Cooper et al., 2015; Henderleiter et al., 2001; Schmidt et al., 2009) have reported a range of students' alternative conceptions and learning difficulties related to the concept of a hydrogen bond including: students recognising hydrogen bonds as bonds "within" rather than as forces "between" ethanol molecules (Cooper et al., 2015; Williams et al., 2015), difficulties in identifying molecules in which hydrogen bonds form (Schmidt et al., 2009), or difficulties in using the concept of hydrogen bonds to explain macroscopic properties of substances (Henderleiter et al., 2001). In the present study, challenging students to construct their own representations of molecular interactions uncovered more students' alternative conceptions of the structure and polarity of a water molecule and the nature of hydrogen bonds. The alternative conceptions about the structure of water molecules included: water molecules forming linear structures like CO_2, hydrogen atoms in water molecules forming multiple covalent bonds with one oxygen atom, and two oxygen atoms in different water molecules covalently sharing a common hydrogen atom between them. Alternative conceptions related to the nature of hydrogen bonds in water molecules included: hydrogen bonds as covalent bonds formed when oxygen atoms in water molecules use their nonbonding electrons to bond to other oxygen atoms in other molecules, individual nonbonding electrons on oxygen atoms forming hydrogen bonds, hydrogen atoms on a water molecule forming a single partially positively charged region which can form hydrogen bonds without directionality, lone pairs of electrons collectively forming a single partially negative region that can form one or multiple hydrogen bonds without directionality, and hydrogen bonds as molecular interactions in 2D space. These alternative conceptions have not been reported in previous studies.

The differences in research designs can be used to explain the differences in students' alternative conceptions of the nature of hydrogen bonds revealed in this study and those reported in earlier studies. Unlike most studies that explicitly ask students to discuss their understanding of key terminologies such as intermolecular forces or hydrogen bonds (e.g., Cooper et al., 2015; Henderleiter et al., 2001; Schmidt et al., 2009), in the present study, we did not directly use the term 'hydrogen bond' in our interview prompts. Instead, we asked students to illustrate how a central water molecule in a snowflake would interact with other molecules in its vicinity. By avoiding key chemistry terms such as 'hydrogen bonds', the students were free to illustrate their true understanding, imaginations, or predictions of the nature of molecular interactions in snowflakes rather than reproduce textbook definitions of the concept. Researchers (e.g., Cooper et al., 2015) have suggested that the term 'hydrogen bond' may be confused by students as any bond that involves a hydrogen atom, such as an intramolecular oxygen-hydrogen bond in water or in alcohol molecules. By asking students to draw diagrams of molecular interactions, they made efforts to imagine and represent their conceptions.

It is often difficult to pin-point the sources of students' learning difficulties and alternative conceptions (Taber, 2019). However, in this study, some of the alternative conceptions exhibited in students' diagrams (for example, a hydrogen atom with more than one covalent bond) may stem from incomplete understanding of basic concepts such as atomic structure and bonding, concepts which are taught at lower levels of formal education. Studies have also reported that students' alternative concepts can be retained over long periods of time (Dickson et al., 2016) and can be retained even after explicit instruction (e.g., Rushton et al., 2008). Drawing flat diagrams without any indication of the 3D nature of molecular interactions may be a result of students' familiarity with 2D drawings without explicit emphasis on the limitations of these models or connections to what the drawings actually represent in 3D (e.g., Nicoll, 2003). Students' difficulties in visualising 3D interactions based on 2D diagrams have also been widely recognised in the literature (Wu & Shah, 2004). In the present study, difficulties with conceptualizing basic concepts such as bonding in water molecules were evident in category A diagrams. In addition, although students used ball-and-stick molecular models in the chemistry units from which we recruited the participants, drawing diagrams to represent molecules and their interactions in 3D was hardly emphasized by the instructors and tutors. When discussing the concept of hydrogen bonds, the recommended textbook materials (e.g., Blackman et al., 2019) did not emphasise the 3D nature of interactions between water molecules either. By providing opportunities for students to interact with 3D molecular model kits, the instructors and tutors may have assumed that the students would intuitively recognise that molecules interact in 3D. However, this was not case as most students drew flat diagrams and did not mention molecules interacting in 3D.

Other learning difficulties may result from the way in which the concept of the nature of a hydrogen bond is taught and assessed. For example, when educators teach, they often emphasise that a hydrogen bond is an electrostatic attraction between a hydrogen atom in one molecule and a highly electronegative atom bearing lone pairs of electrons from a different molecule (Henderleiter et al., 2001). However, such a definition does not emphasise the location of the hydrogen bond. In addition, when discussing molecules that can form hydrogen bonds such as alcohols and carboxylic acids, some chemistry textbooks illustrate a dotted line connecting one oxygen atom in one molecule and a hydrogen atom in another molecule without showing the role of lone pairs of electrons (e.g., Blackman et al., 2019; Brady & Senese, 2004; Brown et al., 2013). Although not a compulsory resource, Blackman *et al.* (2019) was one of the recommended texts in the teaching of the chemistry units we recruited the participants from. Therefore, some of these textbook illustrations may have been partly responsible for students considering both lone pairs of electrons on an oxygen atom as a single negatively charged region. Moreover, the nature of assessment also normally does not go beyond one molecule connecting to one other molecule through hydrogen bonds. By asking students to connect only two molecules, it is easy for the students to attain a full score even though they may have alternative conceptions if tasked to connect multiple molecules. Therefore, in this study, when the students were tasked to connect multiple water molecules, they felt challenged and had to think about what happens amongst many water molecules.

Overall, the wide range of students' conceptions of the nature of hydrogen bonds among water molecules identified in the present study highlights the benefits of using student-generated diagrams to investigate the level of students' conceptual understanding of science concepts. The drawing tasks challenged students to link together their prior knowledge of the nature of bonding, structure, and polarity in a water molecule, and hydrogen bonds amongst water molecules in the context of snowflakes. The students made genuine efforts to express their understanding. The study, therefore, also lends support to previous studies that advocate for the inclusion of drawing tasks in science learning sessions to improve student engagement (Ainsworth et al., 2011) and reasoning (Andrade et al., 2021; McLure et al., 2021b; Tytler et al., 2020).

4.7. Implications

Understanding students' conceptions of a science concept is a key step in identifying students' difficulties and designing teaching interventions to address them. In this study, we used the context of snowflakes and student-generated diagrams to investigate students' conceptual understanding of the nature of hydrogen bonds among many water molecules. The drawing activity provided students with an opportunity to retrieve, organize, and link their knowledge of chemistry concepts to communicate their understanding of hydrogen bonds among water molecules in snowflakes. By analysing the students' diagrams, we were able to identify a range of students' difficulties and alternative conceptions of the nature of hydrogen bonds rather than their recalled knowledge of key chemistry terms.

In terms of assessment, educators may want to employ drawing activities to investigate students' understanding of abstract science concepts. It is worth noting that the use of diagrams as an assessment tool of students' conceptions has garnered some debate over the past 20 years. Some researchers (e.g., Ehrlén, 2009) suggest that drawings may not be a good way to accurately understand students' conceptions because students may inconsistently rely on social-cultural resources to represent their ideas in drawings. Consequently, researchers such as Becker *et al.* (2016) argue that students' diagrams can only be understood when analysed in combination with other modes such as interviews (verbal) or written explanations. Indeed, making sense of students' diagrams on their own is a challenging task because it requires content knowledge, representational skills, and experience in interpreting students' diagrams.

However, previous research has developed a set of procedures that researchers can use to make sense of student-generated diagrams without extensively referring to their verbal explanations (McLure et al., 2021b; Tenzin et al., 2022). In addition, although drawing 2D diagrams may not afford students an opportunity to conveniently represent molecular interactions in 3D space, spatial aspects are even harder to discern in many of the alternative representation modes such as verbal and written explanations. Compared to other conventional representation methods, we believe drawing diagrams is at least as effective in evaluating how students visualise spatial relations among molecules. Moreover, triangulation of the data indicated that students' diagrams were well aligned with their verbal explanations, except for three students who relied on words and gestures to communicate their understanding of 3D interactions of molecules. In future, in addition to diagrams, alternative ways of representing spatial relations (e.g., gestures) could be explored further.

Different from other studies investigating students' conceptions with diagrams (e.g., Cooper et al., 2015; Nyachwaya et al., 2011), this study offered staged prompts to accompany drawing tasks and it might have contributed to increasing the value of the drawings as a conceptual assessment tool. In the present study, the staged prompts engaged the students in imagining and reasoning about molecular interactions and, even though they were not used to the task, the students drew diagrams that reflected their conceptions of science concepts. Research reported that providing students with scaffolding prompts while drawing increases the degree of correlation between the student-generated diagrams and their written explanations (Noyes & Cooper, 2019). When designing diagram-based conceptual assessments, future researchers may wish to provide staged prompts to accompany drawing tasks. The prompts should be designed carefully to make visible the nature of students' conceptual understanding rather than recall of science terminologies. In addition, future researchers may also wish to experiment with different ways of administering the staged prompts to large groups of students at once (e.g., in written form). This is because conducting interviews (as we did) in large classes is very time-consuming and impractical on a regular basis.

For students to represent their ideas in diagrams, the present study used the easy-to-use pen and paper. We made this choice to avoid the additional difficulty that some students may encounter in using technology to represent their ideas. However, digital drawing is becoming more popular in teaching and learning settings (Ainsworth & Scheiter, 2021). In future studies, educators may want to consider using different tools for drawing or to investigate the role of technology in using student-generated diagrams for assessment purposes.

The findings of the present study also have implications on the level of knowledge targeted by drawing assessments, as well as the teaching of chemistry. Assessing students' conceptual understanding at a deeper level, for example by asking students to connect multiple water molecules rather than just two water molecules, can be beneficial in understanding students' learning difficulties and alternative conceptions. In terms of teaching practice, since many students visualized the molecular interactions in 2D, the present study highlights a need for educators to emphasise the 3D nature of molecular interactions in their teaching and the limitations of the different modal representations (such as 2D drawings). It is also important for educators to explicitly guide students in ways of representing molecular interactions at the submicroscopic level. In addition, educators need to design learning interventions to support students' 3D visualisation of molecular concepts. Educators may want to investigate the potential of 3D visualisation technologies such as immersive virtual reality in supporting students' visualisation of molecular concepts.

4.8. Limitations

The limitations of the study were two-fold. First, the study was conducted at a single university in Australia. Therefore, it is not clear whether the findings of this study in relation to the students' conceptions of the nature of hydrogen bonds between water molecules would be evident in other universities. Future studies may benefit from involving participants from multiple institutions to derive more generalisable findings. Secondly, participants in this study were those majoring in chemistry and related courses. Therefore, the findings may not be generalisable to all student populations. Applying a similar assessment protocol to students in a different setting, for example, in high school, would help researchers explore how students develop these ideas across populations. Nevertheless, the present study has identified several alternative conceptions of the nature of hydrogen bonds that have not been reported earlier. These alternative conceptions include; a hydrogen bond resulting in two oxygen atoms of different molecules sharing a common hydrogen atom between them, hydrogen bonds being covalent bonds formed when oxygen atoms in water molecules use their nonbonding electrons to bond to other oxygen atoms, individual nonbonding electrons on the oxygen atoms forming hydrogen bonds, hydrogen atoms on a water molecule forming a single partially positive region which can form hydrogen bonds without directionality, lone pairs of electrons collectively forming a single partially negative region that can form one or multiple hydrogen bonds without directionality, and hydrogen bonds as molecular interactions in a 2D space.

4.9. Conclusion

This study revealed a wide range of alternative conceptions of the nature of hydrogen bonds amongst many water molecules in snowflakes, including the shape of water molecule, the role of lone pairs in forming hydrogen bonds, and the molecular interactions in a 2D plane. These alternative conceptions were uncovered largely due to the unique question prompt (interactions amongst many water molecules) and the distinctive mode of representation (diagrams). Different from the routine written test items, the drawing task demanded that students go beyond repeating scientific vocabulary or applying test-taking skills. The students made genuine efforts to imagine, visualise, and illustrate the interactions amongst many water molecules in snowflakes to demonstrate their understanding of the nature of hydrogen bonds. Considering the powerful insights we gained from the analysis of student-drawn diagrams, chemistry educators may wish to adopt similar strategies to examine and support students' conceptual understanding.

Chapter 5. Change in Students' Explanation of the Shape of Snowflakes After Collaborative Immersive Virtual Reality

This chapter builds on the insights about undergraduate students' conceptions of hydrogen bonds in snowflakes before collaborative IVR established in Chapter 4. The study presented in Chapter 5 is in response to the third research question (*How does students' conceptual understanding of hydrogen bonds and the shape of snowflakes change after a collaborative IVR learning experience?*[4]; please see Section 1.5).

The content of this chapter has been published in *Chemistry Education Research and Practice,* a Q1 journal published by the Royal Society of Chemistry. The content presented here is the version of the submitted article accepted by the journal. The table and figure numbers have been formatted for the chapter. The full citation of the published article is:

Matovu, H., Won, M., Treagust, D. F., Ungu, D. A. K., Mocerino, M., Tsai, C.-C., & Tasker, R. (2023). Change in students' explanation of the shape of snowflakes after collaborative immersive virtual reality. *Chemistry Education Research and Practice*, *24*(2), 509-525. https://doi.org/10.1039/D2RP00176D.

[4] The third research question was addressed through two specific sub-questions (please see Section 2.3) and they are included in Section 5.2.

5.1. Abstract

In recent years, chemistry educators are increasingly adopting immersive Virtual Reality (IVR) technology to help learners visualise molecular interactions. However, educational studies on IVR mostly investigated its usability and user perceptions leaving out its impact on improving conceptual understanding. If they evaluated students' knowledge gains, they tended to use information recall tests to assess knowledge gains. Employing interviews and diagram-drawing tasks, this study explored how students' conceptual understanding of the nature of hydrogen bonds and the shape of snowflakes changed through a collaborative IVR experience on snowflakes. Participants were 68 undergraduate chemistry students. Videos of pre-/post-interviews and student-generated diagrams were analysed. The results indicated a marked improvement in students' conceptual understanding of the nature of hydrogen bonds among water molecules in snowflakes. After IVR, 57 students provided scientifically acceptable explanations of the nature of hydrogen bonds. Improvements in students' understanding were related to the intermolecular nature of hydrogen bonds, the role of lone pairs of electrons in forming hydrogen bonds, and molecular interactions in 3D space. This study suggests that collaborative IVR could be a powerful way for students to visualise molecular interactions, examine their alternative conceptions, and build more coherent understanding. Implications for the design and implementation of IVR activities for science learning are discussed.

Keywords: Immersive Virtual Reality; Chemistry education; Undergraduate; Intermolecular forces; Hydrogen bonding

5.2. Introduction

In recent years, science educators are increasingly adopting immersive Virtual Reality (IVR) as an advanced visualization technology to help students visualize and learn abstract science concepts (Bennie et al., 2019; Ferrell et al., 2019). Immersive Virtual Reality makes use of a head-mounted display unit to shut out the view of the physical world and 'immerse' the learner in an interactive three-dimensional (3D) computer-generated environment (Fombona-Pascual et al., 2022). For example, using handheld controllers in IVR, learners can manipulate 3D virtual molecules by dragging, pulling, or rotating the structures to improve their understanding of spatial relationships in simple and complex molecules (e.g., Seritan et al., 2021; Won et al., 2019). Engaging learners' bodies in IVR can reinforce learning of abstract concepts by activating memory traces through embodied cognition (Johnson-Glenberg, 2018). Moreover, learners can also have opportunities to share IVR learning environments to negotiate meanings and build conceptual understanding together (Won et al., 2019).

Despite the promising benefits of IVR for science teaching and learning, researchers and educators are still divided on whether investment in IVR for science learning is justified (Radianti et al., 2020). For instance, some studies have found IVR to be more motivating, but also more distracting compared to alternative learning modes (e.g., Parong & Mayer, 2020). In several other studies, learners using IVR did not have better science knowledge gains compared to those who used alternative learning modes such as 2D computer platforms or physical models. These observations span across different science education fields such as physics, biology, and chemistry (Coban et al., 2022; Hamilton et al., 2021; Wu, Yu, et al., 2020).

In chemistry learning, the reasons for the lack of conclusive evidence for the conceptual benefits of IVR may be varied. One reason is that many chemistry educators focus on investigating usability of IVR and learners' affective outcomes (such as motivation and engagement) but not conceptual understanding (e.g., Edwards et al., 2019; Elford et al., 2021; Reeves et al., 2021; Rychkova et al., 2020; Zhao et al., 2022). Conceptual understanding involves the knowledge of basic concepts and the ability to use this knowledge in different contexts to solve problems, translate freely across different levels of scale, and to predict and explain observable phenomena (Holme et al., 2015). Yet, most studies that have attempted to investigate knowledge gains in IVR for chemistry learning rely on multiple-choice and short-answer pre- and post-tests (e.g., Ferrell et al., 2019; Webster, 2016). Such multiple-choice questions have limitations on assessing the level of conceptual understanding as they tend to assess the ability for information recall (Martinez, 1999; Treagust, 1988).

Many science educators and researchers contend that IVR learning environments provide opportunities for constructivist science learning (Dede et al., 2017; Winn, 1993). According to constructivism, learning involves construction of knowledge through active interactions with material resources in the learning environment and with peers or knowledgeable others (Vygotsky, 1978). Through these interactions, students continuously integrate new experiences with already assimilated knowledge (Jonassen, 1994). During learning, students gradually restructure disjointed, intuitive conceptions to build more coherent and scientific ideas (Duit & Treagust, 2003). In this view, researchers (Dede, 2009; Dede et al., 2017; Matovu, Ungu, et al., 2023; Won et al., 2019) have suggested various ways of taking advantage of the technical and pedagogical features of IVR through sensory, actional, narrative and social considerations to promote science learning in constructivist ways.

Sensory considerations using IVR to reify abstract science concepts in the form of high-quality 3D displays allow the students to explore these concepts in concrete forms (Matovu, Ungu, et al., 2023; Won et al., 2019). Actional considerations with the smooth interactivity and motion-tracking features of IVR allow learners to interact with virtual objects in embodied ways (Johnson-Glenberg, 2018) and observe the consequences of their actions (Dede et al., 2017). For instance, in IVR, students can interact with molecules, apply their prior knowledge, and test their ideas to reach new understanding (Fombona-Pascual et al., 2022; L. Zhang et al., 2019). Narrative considerations describe how engaging students in challenging but manageable tasks in IVR can increase the learners' engagement and motivation to complete the learning tasks (Matovu, Ungu, et al., 2023). Moreover, social considerations provide opportunities for students to complete learning tasks with their peers in IVR and can increase the students' sense of belonging in IVR and engagement on the learning tasks (Krämer, 2017). Therefore, based on the existing literature on IVR for science learning, the position that the present research is taking is that, when students are provided with clear goals to achieve, interactive and collaborative IVR may help students to explore chemistry concepts in more engaging and productive ways. However, due to the unique nature of the students' roles in learning while in IVR, assessment of learning using traditional information-recall questions provides limited evidence of how IVR benefits students' conceptual understanding (Hamilton et al., 2021).

An alternative way to investigate students' conceptual benefits from IVR is to analyse student-generated diagrams which can act as a 'window' into students' conceptions of science phenomena (Ainsworth et al., 2011; Chang et al., 2020; Tippett, 2016). For example, through drawings, students can elaborate and clarify ideas that they would otherwise not be able to communicate explicitly (Ainsworth et al., 2011). Drawing activities also provide opportunities for students to develop an integrated understanding of science by representing, linking, and communicating ideas coherently (Gobert & Clement, 1999; Treagust et al., 2017). By analysing students' diagrams, educators can identify patterns in students' conceptions of science phenomena and their learning difficulties (McLure et al., 2021b). Moreover, learner's prior knowledge greatly influences their subsequent learning (Taber, 2017). Therefore, analysing patterns of conceptual understanding in student-generated diagrams before and after IVR may provide insights into how students of differing preconceptions benefit from IVR.

In chemistry education, several studies have used student-generated diagrams to assess the level of students' conceptual understanding of key chemistry concepts. The concepts investigated included the particle theory of matter (e.g., Andrade et al., 2021; McLure et al., 2021a), atomic structure (e.g., Derman et al., 2019), and intermolecular forces (e.g., Cooper et al., 2015; Matovu, Won, Treagust, Mocerino, et al., 2023; Noyes & Cooper, 2019). In IVR research, however, few studies have used drawing tasks to assess students' science conceptual understanding. Thompson et al. (2020) reported that student-generated diagrams of human cells after IVR were more complex and depicted a higher density of organelles compared to pre-IVR diagrams, suggesting an improvement in students' conceptions of cells. However, the study provided no context for students to integrate and apply their improved understanding to explain science phenomena. Therefore, it remains unclear whether IVR would help students to build coherent understanding of abstract science concepts.

In the present study, we investigated how IVR would change university students' conceptual understanding of the nature of hydrogen bonds among water molecules and the shape of snowflakes. For this purpose, we analysed diagrams and verbal explanations created by students before and after experiencing an interactive and collaborative IVR program on snowflakes. The nature of hydrogen bonds, the target concept in this study, is a fundamental concept in chemistry. The concept can be used to explain a wide range of macroscopic properties in substances, such as phase changes, boiling points, and solubilities. Yet, previous studies have identified a wide range of students' alternative conceptions about the nature of hydrogen bonds (e.g., Cooper et al., 2015; Henderleiter et al., 2001; Schmidt et al., 2009). Therefore, investigating the benefits of IVR has the potential to provide information on whether the medium can help science educators to confidently deal with this abstract yet important chemistry concept.

This study was designed to answer the following research questions:

1. How do university students change their conceptions of the nature of hydrogen bonds among water molecules in snowflakes after exploring the concept in collaborative IVR?
2. How do university students change their explanations of the shape of snowflakes after exploring the concept in collaborative IVR?

5.3. Materials and Methods

The Collaborative Snowflakes IVR Program

The IVR program was designed to help students build a coherent understanding of the nature of hydrogen bonds among water molecules in snowflakes by integrating their prior knowledge of structure and polarity, hydrogen bonds, and scale of water molecules. The IVR program was developed primarily with Unity®. While in IVR, learners' bodies were represented as generic 'avatars' in the form of floating heads and hands (e.g., Figure 5.1a). In each session, two students in the same physical room also shared the virtual space in IVR through a network. Since the students were in the same physical and virtual spaces, they could observe each other's avatars, communicate in real-time, and collaboratively manipulate the virtual objects. During the IVR learning activity, learners could also walk around the physical space in the room (approximately 4 m × 4 m of virtual space) to change their perspectives of the molecular structures and use their handheld controllers to move and connect virtual molecules. In addition, the students would receive haptic feedback in the form of vibrations from their IVR controllers when the molecular structures connected in the right orientations.

Figure 5.1

Some of the IVR Learning tasks on Hydrogen Bonds Among Water Molecules in Snowflakes

(a) (b)

Note. Two IVR-based learning tasks are shown. (a) Explore how a hydrogen bond forms between two water molecules. (b) Construct a lattice structure to explain the shape of snowflakes

Students completed multiple learning tasks involving water molecule structures in IVR. At every step in IVR, the students were prompted to manipulate the structures to explore molecular interactions. Students were also explicitly prompted to discuss ideas with one another to reach consensus before moving on to the next task. Instructions were provided to the students in the form of audio and text. The students had the freedom to experiment with their ideas and the time the students spent on each IVR task depended on the pace of each pair of students. The IVR learning tasks were presented in the order of increasing complexity and an increasing number of water molecule structures was provided as the students progressed through the learning tasks.

At the initial stage of the IVR activity, students were provided with two water molecules. Each molecule had the electron density regions highlighted – blue for electron poor and red for electron rich regions (Figure 5.1a). A prompt was given to the students – "*What are the features of water molecules? Discuss the features of the water molecules in front of you. When you are happy with your answer click the Submit button*". When the students pressed the *submit* button, a new prompt would appear – "*How do you make a hydrogen bond? Make a hydrogen bond between two water molecules and discuss what you notice about the colour and thickness of the hydrogen bond. When you are happy with your answer, click the submit button."* The students manipulated the molecules to create a hydrogen bond and discussed their observations in terms of the angle and distance between the molecules.

After exploring the interaction between two water molecules, the students were provided with more water molecules. The students were prompted to predict, and then explore by connecting multiple water molecules to a single molecule, the maximum number of hydrogen bonds a central water molecule could form and to explain why this would be the maximum number. By connecting many clusters of water molecules through hydrogen bonds, the students subsequently constructed layers of water molecules, and finally a lattice structure of molecules (Figure 5.1b). Constructing the layers of molecules and the lattice structure required the students to apply their knowledge of hydrogen bonds, and different problem-solving and pattern recognition skills. The students were also prompted to use the lattice structure of water molecules to explain the macroscopic features of snowflakes. The collaborative IVR experience concluded with a short video explaining how variations in environmental conditions can influence the way in which snowflakes crystals grow. Short videos of some of the IVR learning tasks can be accessed online (https://tinyurl.com/je52p6pm).

Participants and Study Design

The study adopted a design-based research approach (Anderson & Shattuck, 2012). The approach follows an iterative cycle of designing and implementing a learning intervention and using mixed research methods to evaluate learning. Design-based research is useful in building a theory of how an intervention, such as IVR, works in the intended context, and to improve the design and implementation of the intervention (Wang & Hannafin, 2005). In the present study, we explored how a collaborative IVR experience would change students' conceptions of the nature of hydrogen bonds among water molecules and the shape of snowflakes. The IVR program used in this study was first developed in 2020 and was refined iteratively following several testing sessions. The present study reports findings from the iteration of our IVR program in 2021. The findings from this study will be used to inform future design and implementation of our IVR programs.

A total of 70 first- and second-year undergraduate chemistry students participated in the collaborative IVR learning activity. The students were those majoring in chemistry or chemistry related courses such as Chemical Engineering, Food science, and Nutrition at a large public university in Australia. The students had passed high school chemistry and at least one university level chemistry unit. The learning activity was integrated into two of the undergraduate chemistry units offered in the first half of the year 2021. The two chemistry units included a focus on the concept of intermolecular forces. The activity was, therefore, mandatory for all the students enrolled in the chemistry units. However, participation in the research study was voluntary. Approval to conduct the study was granted by the institutional Human Research Ethics Committee (HRE2020-0081) and all the students signed consent forms for their data to be used in the study.

The study involved a pre-interview, a collaborative IVR session, and a post-interview. The participating students were requested to complete the series of IVR learning tasks in pairs. The pairing of the students was managed using an online meeting scheduling tool (doodle.com) with time slots from which students could choose. The students were provided with a link where they could log in and select the most convenient time for them to participate in the IVR learning activities. Each slot could be selected by only two students. Because the students selected the time slots based on convenience, some students were paired with their friends while others were not.

The purpose and design of this study were discussed over several meetings among all the authors. Based on these initial discussions, two authors (HM and DU) developed the potential interview prompts. Three authors (HM, DU, and MW) then met to compare, discuss, and refine the interview prompts until consensus was reached amongst these authors. The prompts agreed upon by these three authors were further checked for validity and confirmed by all the authors. The interview prompts employed in this study are provided in the Appendix A.

Pre-interview prompts were designed to elicit the students' ideas about the nature of hydrogen bonds among water molecules in snowflakes before the IVR session. However, to avoid the students reproducing textbook definitions of a hydrogen bond, the interview prompts did not include the term 'hydrogen bond'. Instead, the participants were asked to describe their understanding of the features of a water molecule and water molecule interactions in snowflakes, and to use a pen and paper to draw diagrams to illustrate their ideas. After illustrating the molecular interactions, the students were shown magnified images of snowflakes (such as those in Figure 5.2) and were asked to use the concept of the molecular interactions among water molecules to explain the shape of snowflakes. Each pre-interview lasted 15-25 minutes.

Figure 5.2

Examples of Images of Snowflakes Used in the Pre-interview

Note. Source: Adobe Creative Cloud (Adobe Inc., 2021).

After the pre-interview, the researchers trained the participants on the use of the IVR headsets and controllers. Participants were also encouraged to talk to their partners while completing the IVR learning tasks, and to immediately inform the researchers in case they felt dizziness or any form of discomfort with the IVR headsets. Each student donned an HTC VIVE pro Eye headset and two handheld controllers for interacting with the virtual molecules. The IVR session lasted 40 minutes on average for each pair of learners. During this time, the students collaborated with their peers to complete the IVR learning tasks and did not receive any guidance or feedback from the researchers.

In the post-interview (20-30 minutes), learners were assessed again. The learners were prompted to improve their drawings illustrating the nature of molecular interactions in snowflakes and to provide reasons for any changes in their diagrams. Students were also asked to revise their explanations of the six-fold symmetry in snowflakes and to draw diagrams to show their improved understanding.

Like the IVR learning tasks, the interview tasks were initially designed to be collaborative in nature. Students were paired and asked to discuss their ideas with peers to create shared diagrams illustrating the nature of hydrogen bonds among water molecules in snowflakes. Unfortunately, in many cases, students preferred to provide individual responses and draw individual diagrams. When the students showed reluctance to collaborate with peers in the interviews, the interviewer did not insist that they create shared diagrams and explanations. Instead, he asked the students to confirm whether they were happy with their individual diagrams. For the explanation of the nature of hydrogen bonds among water molecules, students generally worked individually (n=60) in the pre-interview, but a small number of students switched to respond to interview prompts collaboratively in the post-interview (n=12). For the explanations of the shape of snowflakes, the students preferred to provide individual explanations in both the pre- and post-interviews; the exceptions were two students in two pairs who stated that they were each happy with their peers' explanations in the pre-interview. Data in the form of audios, videos, and students' diagrams was collected. Audio and video data were transcribed before analysis.

Analysis

Out of the 70 students recruited, two students' data were excluded on the bases of insufficient information (a student not completing the diagrams) and eligibility (another student not being in the target chemistry class). Therefore, audios, videos, and diagrams of the remaining 68 students were analysed. All student-generated diagrams (pre and post) and accompanying verbal explanations were analysed inductively using a constant comparison method (Merriam & Tisdell, 2015). This was done to generate categories relating to the students' conceptual understanding of the nature of hydrogen bonds among water molecules and the shape of snowflakes.

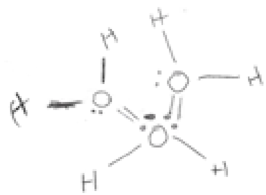
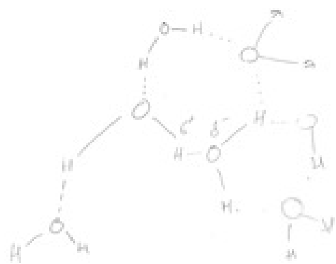
Analysis of students' conceptions of the nature of hydrogen bonds among molecules in snowflakes. The first author analysed each student's pre- and post-diagrams and explanations and documented ideas related to the students' conceptual understanding, including their alternative conceptions about the nature of hydrogen bonds among water molecules in snowflakes. Based on this initial analysis, two authors (HM and MW) combined all the data and identified the initial categories for the students' levels of conceptual understanding of the nature of hydrogen bonds. The first author (HM) then coded all the data (diagrams and accompanying explanations) to identify any emerging categories. Because communication can be multimodal in nature (Jewitt, 2013), the two authors also constantly referred to the videos of the students' interactions during the interviews and supplemented the diagrams and transcripts with descriptions of students' gestures where available. The categories of students' conceptions of the nature of hydrogen bonds that were identified from the data were constantly refined in meetings between the two authors until consensus was reached that no more categories were emerging from the data. The coding schemes for the student-generated diagrams and transcripts were also checked against the data and refined by a second pair of authors (MM and RT). Changes to the categorisation of the students' diagrams and the accompanying explanations were discussed amongst the authors (HM, MW, MM, and RT) until consensus was reached. The final conceptual categories were further discussed and confirmed by four authors (HM, MW, DT, and MM).

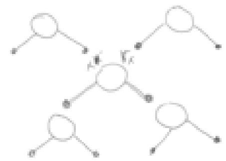
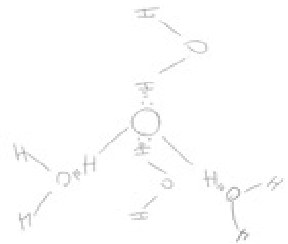
Analysis of the students' diagrams and verbal explanations generated four conceptual categories (A-D) related to the students' conceptual understanding of the nature of hydrogen bonds among water molecules in snowflakes. Category A related to students' difficulties in drawing the structure of a water molecule, recognising polarity in water molecules, and distinguishing the nature of hydrogen bonds as intermolecular interactions from intramolecular interactions. Category B related to students' difficulties in recognising the role of lone pairs of electrons in water molecules in the formation of hydrogen bonds. For categories C and D, the students recognised hydrogen bonds among water molecules as electrostatic interactions between hydrogen atoms and lone pairs of electrons in different molecules. For category C, hydrogen bonds were discussed as interactions in 2D space, while for category D, the students recognised hydrogen bonds as molecular interactions in 3D space. The descriptors of the conceptual categories, together with exemplar verbal explanations are summarised in Table 5.1. The detailed analysis of the student-generated diagrams has been discussed in Study 2 (Matovu, Won, Treagust, Mocerino, et al., 2023).

As mentioned earlier, some students collaborated with their peers in the interviews to construct shared diagrams illustrating the nature of hydrogen bonds among water molecules in snowflakes. Therefore, after coding the combined data, the first two authors (HM and MW) separated the diagrams and transcripts for the students who worked individually from the diagrams and transcripts of the students who collaborated with their peers. This was done to investigate whether the students' ideas or depth of the discussions were different between the two groups of students. Students' collaboration did not appear to have much influence on the depth of the conceptual discussions or to generate any new conceptual categories. Therefore, the authors of this research applied the same analysis scheme to all the data.

Table 5.1

Categories of Students' Conceptual Understanding of the Nature of Hydrogen Bonds Among Water Molecules in Snowflakes

Conceptual Category	Description	Example Explanation	Example Diagram
A: Uncertain of the structure of water molecules and/or the nature of intermolecular interactions	Students have difficulty in drawing a water molecule structure; polarity in water molecules is not represented; students represent intermolecular interactions as covalent bonds between molecules. Hydrogen bonds are shown as interactions between oxygen and oxygen atoms, or hydrogen and hydrogen atoms.	"… oxygen atoms [in neighbouring water molecules] have extra electrons, so they would form bonds [with each other]"	
B: Uncertain of the role of lone pairs in forming hydrogen bonds	Students draw bent structures and discuss polarity in water molecules. Hydrogen bonds are represented as electrostatic interactions between oxygen and hydrogen atoms of different molecules, but students are uncertain of the role of lone pairs of electrons in forming hydrogen bonds. The lone pairs of electrons form an electron-rich region on the oxygen atom which can form one or multiple hydrogen bonds without directionality, or the individual nonbonding electrons can form hydrogen bonds.	"The oxygen is significantly more electronegative than the hydrogen due to the electron density effect … it [the oxygen] has just got more electrons, making it more attracted towards positive charges … and hydrogen is the opposite … the negative of this oxygen … (*draws the partial charges*) and then positive there."	

C: Molecules form hydrogen bonds in 2D space	Students discuss hydrogen bonds as intermolecular, electrostatic, and directional interactions between hydrogen atoms and lone pairs of electrons in different molecules, but the molecules form hydrogen bonds in a 2D plane.	"The hydrogen and oxygen interact through that lone pair of electrons on oxygen… O and H interact because of the electronegativity differences…the maximum number around one molecule would be four"	
D: Molecules form hydrogen bonds in 3D space	Students discuss and/or illustrate each water molecule interacting with four other molecules to form a tetrahedral structure (four hydrogen bonds) in 3D space.	"With these lone pairs and hydrogen atoms, each water molecule interacts with four other water molecules. This leads to a 3D lattice *(uses gestures to illustrate the 3D shape)*"	

Note. The conceptual categories were identified based on both the students' diagrams and supporting verbal explanations

Analysis of students' explanations of the shape of snowflakes. In the pre-interview, the explanations of the shape of snowflakes were in response to the prompt: "How can the intermolecular interactions in water molecules illustrated in the diagrams be used to explain the shape of snowflakes?". At the post-interview, the modified version of the prompt was used: "Imagine that I am a Year 11 student who knows about the structure and polarity of a water molecule. Starting with the structure and polarity of a water molecule, how would you explain to me why snowflakes are shaped the way they are? You may also use a diagram, if you can, to explain to me." All the students provided individual responses to the prompt, except in two pairs where one of the students in each pair simply agreed with the peer's response. For purposes of analysis, these two students were placed in the respective categories of their peers. Also, most of the students explained that they had difficulty drawing the lattice structure of snowflakes on paper. Therefore, the main data used to answer the second research question were the transcripts of the students' verbal explanations of the shape of snowflakes, as well as gestures, before and after the IVR session.

The transcripts of the students' explanations (supplemented with the gestures the students used while explaining their understanding) were first coded inductively. Before and after IVR, there were wide variations in students' explanations both in terms of the ideas the students presented and the comprehensiveness of the explanations. To reflect the differences in the students' explanations, the authors (HM and MW) adopted a combination of both inductive and deductive approaches and identified seven key topics that students would incorporate in their explanations. These topics were: molecules spread out, hydrogen bonds among molecules, tetrahedral units of molecules, 3D lattice structures, hexagonal shapes among molecules interacting in 2D, hexagonal shapes among molecules in 3D, and variations in snowflakes patterns. The authors then coded each student's explanation based on the key topics identified in their explanation to identify common patterns. From these patterns, broader categories were then generated. In each category of explanations, there were variations in the level of complexity or sophistication in the students' explanations. The categories of the students' explanations and their descriptors are shown in Table 5.2.

Table 5.2

Categories of Students' Explanations of the Shape of Snowflakes

Category	Subcategory	Descriptor
Not sure		Student makes no attempt to explain the shape of snowflakes
Incoherent or hard to categorise		It is not clear what feature of snowflakes' shape the student is explaining, or the student's explanation includes contradicting ideas
Focus only on the appearance	flat structure	Student's focus is on explaining why snowflakes appear flat
	variation in patterns	Student focuses on environmental factors or randomness in molecular interactions to explain why there are different patterns of snowflakes but does not explain the hexagonal symmetry
Explain molecular interactions in 3D	In terms of hydrogen bonds	Student recognises that molecules in snowflakes interact in 3D but does not explain other features of snowflakes shapes
	+ 3D lattices and the variations in patterns	Student recognises that molecules in snowflakes interact in 3D and attempts to explain the different variations in snowflakes patterns
Explain hexagonal symmetry	In terms of hydrogen bonds	Students' explanation focuses on the hexagonal symmetry in snowflakes only but there is no mention of tetrahedral units as the building blocks of the structure
	+ the variation in patterns	Student explains the hexagonal symmetry and variations in snowflakes patterns but there is no mention of tetrahedral units as the building blocks of the structure
Recognise tetrahedral unit as the building block of snowflakes	In terms of hydrogen bonds or 3D lattice	Student recognises that molecules in snowflakes interact in 3D to form tetrahedral units but does not explain the hexagonal symmetry or variations in patterns
	+ the hexagonal symmetry	Student recognises that molecules in snowflakes interact in 3D and form tetrahedral units which result in hexagonal patterns amongst water molecules to explain the hexagonal symmetry in snowflakes
	+ the variation in patterns	Student recognises that molecules in snowflakes form tetrahedral units and explains variations in snowflakes shapes but not the hexagonal symmetry
	+ the hexagonal symmetry and the variation in patterns	Student recognises that molecules in snowflakes interact in 3D and form tetrahedral units, explains the hexagonal symmetry, as well as variations of patterns in snowflakes

After coding the students' pre-and post-responses and diagrams, changes in students' conceptual understanding of the nature of hydrogen bonds among water molecules in snowflakes were illustrated using Sankey diagrams (Schmidt, 2008). A Sankey diagram is a flow diagram showing changes in quantities undergoing a given process or transformation. In this study, Sankey diagrams were used to illustrate the number of students with each category of preconceptions of the nature of hydrogen bonds among water molecules before IVR and how many of these students changed to different conceptual categories after IVR (Table 5.3). The width of each band (flow) is proportional to the number of students changing from one conceptual category to another. Sankey diagrams have been used in previous science education research (e.g., Williams et al., 2015) for purposes similar to the present study. In this study, the students approached the task differently (most worked individually while some collaborated to draw diagrams in one or both interview sessions). Therefore, we created different Sankey diagrams depending on whether the students worked individually or collaborated on the tasks. However, the changes in students' explanations of the shape of snowflakes could not be illustrated using a Sankey diagram because of the big number of categories.

5.4. Findings

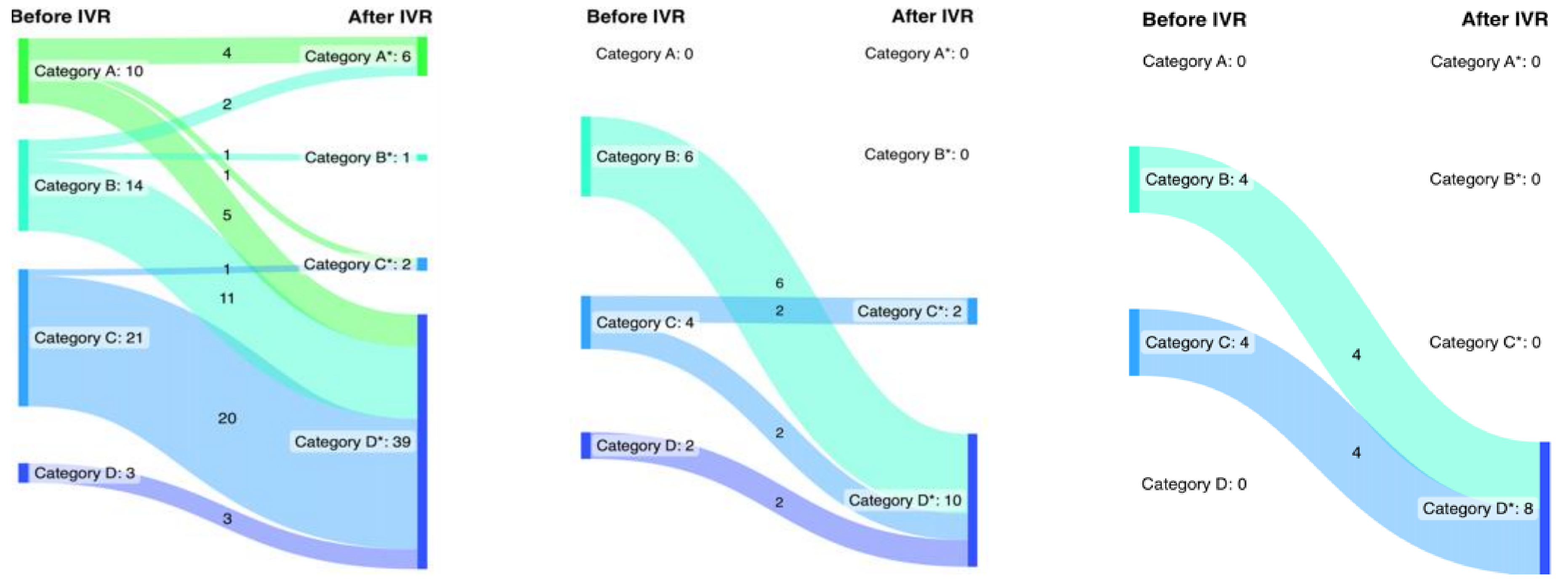
Research Question 1: Changes in Students' Conceptions of the Nature of Hydrogen Bonds Among Water Molecules in Snowflakes After Exploring the Concept in Collaborative IVR

Before IVR, students had varying conceptions of the nature of hydrogen bonds among water molecules in snowflakes, with most students exhibiting alternative conceptions of some form. For example, 10 students had difficulties drawing the structure of a water molecule and/or recognising that hydrogen bonds were non-covalent interactions between molecules (category A). Twenty-four students recognised that hydrogen bonds were electrostatic interactions between oxygen and hydrogen atoms in different molecules, but the students had alternative conceptions about the role of lone pairs in the formation of hydrogen bonds (category B). Other students (n = 34) explained that one water molecule in snowflakes would form multiple hydrogen bonds with other water molecules using individual lone pairs of electrons and hydrogen atoms. However, most of these students (n=29) explained hydrogen bonds as interactions in a flat plane (category C).

Table 5.3

Changes in Students' Conceptual Understanding of the Nature of Hydrogen Bonds Among Water Molecules in Snowflakes

(a) Individual activity (before and after IVR; n=48)	(b) Individual (before IVR) to collaborative (after IVR) activity (n=12)	(c) Collaborative activity (before and after IVR; n=8)



Note. Categories were based on the students' diagrams and accompanying verbal explanations as illustrated in the coding scheme in Table 5.1; Left (without asterisk) are categories before IVR; Right (with asterisk *) are categories after IVR; n = number of students

Category A: Uncertain of the structure of water molecules and/or the nature of intermolecular interactions

Category B: Uncertain of the role of lone pairs of electrons in forming hydrogen bonds

Category C: Molecules in snowflakes form hydrogen bonds in 2D space

Category D: Molecules in snowflakes form hydrogen bonds in 3D space

After IVR, there was a marked improvement in the students' conceptual understanding of the nature of hydrogen bonds among water molecules in snowflakes. Improvements in students' conceptual understanding were related to the intermolecular nature of hydrogen bonds, the role of lone pairs in the formation of hydrogen bonds, and molecular interactions in 3D space. In their post-interview diagrams and explanations, more students (61 after IVR vs 34 before IVR) explained that a hydrogen bond was formed between a lone pair of electrons in one water molecule and a hydrogen atom in a neighbouring water molecule (categories C* and D*). In addition, after IVR, more students (57 students in category D*) provided scientifically acceptable explanations of the nature of hydrogen bonds among water molecules. The 57 students described a hydrogen bond as an electrostatic force of attraction between molecules and recognised that each water molecule formed four hydrogen bonds with other molecules in 3D space. This number was exceptionally higher than the number of students who recognised the 3D nature of molecular interactions before IVR (5 students in category D).

As shown in Table 5.3, the changes in students' conceptual understanding of the nature of hydrogen bonds were partly influenced by the nature of students' preconceptions and the students' tendencies to collaborate with peers on the interview tasks. About half of the students who had difficulties with recognising the non-covalent nature of intermolecular interactions retained their preconceptions after IVR. On the other hand, students from other categories of preconceptions generally improved their understanding of the nature of hydrogen bonds after IVR. Also, students who collaborated with peers on the interview tasks tended to change their conceptual understanding more consistently than those who worked individually on the interview tasks. Below we elaborate on these findings:

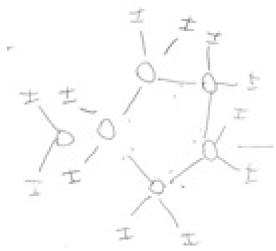
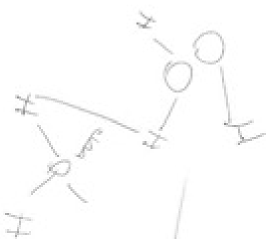
Changes in students' understanding of the nature of hydrogen bonds among water molecules in snowflakes based on the nature of students' preconceptions. Although some of the students initially in category A had an idea of the bent shape and the presence of lone pairs of electrons in water molecules, the students had difficulty in recognising the atoms between which hydrogen bonds form and the non-covalent nature of hydrogen bonds. In attempting to illustrate intermolecular interactions, the students connected oxygen atoms of different water molecules with solid lines, reasoning that the oxygen atoms would form bonds by sharing their nonbonding electrons.

After IVR, among the students initially in category A, six of them recognised a hydrogen bond as an attractive force between a lone pair of electrons on the oxygen atom in one molecule and a hydrogen atom of another water molecule, rather than as a covalent bond between molecules. Five of these six students discussed and/or illustrated that each water molecule in a snowflake formed hydrogen bonds with four other water molecules in 3D space. However, about half (n= 4) of the students initially in category A retained most of their preconceptions.

For example, in his diagram before IVR, Ross connected oxygen atoms of different molecules with solid lines (Table 5.4) and reasoned that water molecules would use the lone pairs of electrons on the oxygen atoms to bond covalently. Through IVR, Ross noticed that each water molecule in snowflakes formed four hydrogen bonds with neighbouring molecules in 3D space. However, after IVR, Ross connected hydrogen atoms of different molecules with a solid line and placed oxygen atoms of different molecules close to each other (Table 5.4). Ross's drawing showed that the student was still not able to discern how exactly the hydrogen bonds were formed between molecules.

Table 5.4

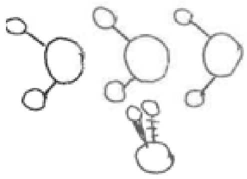
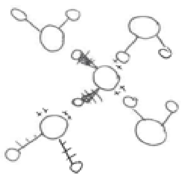
Retaining Preconceptions After IVR: Diagrams and Explanations Produced by Ross

	Diagram	Student's comment /explanation
Before IVR		"… the oxygen is just craving for more bonds because it has the two valence electrons"
After IVR		"There were four water molecules connected to the central water molecule… the molecules form layers and layers."

The 24 students who initially recognised that hydrogen bonds were electrostatic in nature but had alternative conceptions about the role of lone pairs in the formation of hydrogen bonds (category B) moved to different categories after IVR, such as category A or category D. After IVR, most of the students initially in category B (21 out of 24) recognised that a hydrogen bond is formed between a lone pair of electrons in one molecule and a hydrogen atom of a neighbouring water molecule. These students also recognised that each water molecule in snowflakes formed four hydrogen bonds in 3D space. For example, before IVR, Collin recognised polarity in a water molecule but imagined a water molecule as having only two partially charged regions. Collin reasoned that both lone pairs of electrons created a single negatively charged region and both hydrogen atoms of a water molecule collectively formed a partially positive region. Therefore, a water molecule would form multiple hydrogen bonds without directionality. To represent the nature of hydrogen bonds among water molecules, Collin drew other water molecules stacked around the central one (Table 5.5). After IVR, Collin improved his diagram and explanation to emphasise that, to form hydrogen bonds, individual hydrogen atoms were attracted to individual lone pairs of electrons (Table 5.5). While diagrammatically representing the molecular interactions after IVR, Collin also emphasised verbally that the molecules interacted in 3D space.

Table 5.5

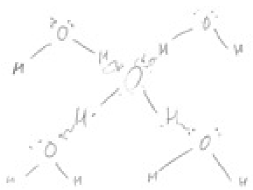
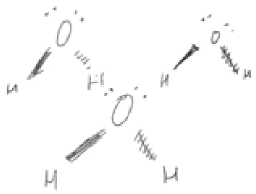
Recognition of the Role of Lone Pairs of Electrons in the Formation of Hydrogen Bonds After IVR: Diagrams and Explanations Produced by Collin

	Diagram	Student's comment/explanation
Before IVR		"There's both of the positive charge there [on the two H atoms] and both of the negative charge [on the O] that it would be stronger to have them together."
After IVR		"Each hydrogen is attracted to a lone pair … you have to draw them going in and out of the page as well ... these are hydrogens on the end there and they are coming out towards us."

Most of the students (26 out of 29) who initially recognised hydrogen bonds among water molecules as electrostatic interactions between lone pairs of electrons and hydrogen atoms but drew the diagrams as if molecules were interacting in 2D (category C) realized the 3D nature of molecular interactions after IVR. Attempting to illustrate the 3D molecular interactions on paper after IVR, most of the students explained that it was too difficult to draw in 3D. They instead explained verbally and with gestures that the molecules interacted in 3D. For example, even though Brian had a good understanding of the nature of hydrogen bonds in snowflakes before IVR, his diagram and explanation did not represent the molecules interacting in 3D. However, from IVR, Brian noticed that the molecules were interacting in 3D. Therefore, after IVR, Brian attempted to represent these interactions with dashed and wedged lines. He also verbally emphasised the 3D nature of molecular interactions (Table 5.6).

Table 5.6

Recognition of the 3D Nature of Molecular Interactions After IVR: Diagrams and Explanations Produced By Brian

	Diagram	Student's comment/explanation
Before IVR		"A lone pair attracts a hydrogen atom because it is positive … Each molecule has four opportunities for hydrogen bonding"
After IVR		"I forgot how to draw the ones into the page and out of the page … I mean the bonding was the same, it's just the 3D aspect of it compared to just lines … it is 3D, it's not a flat sheet"

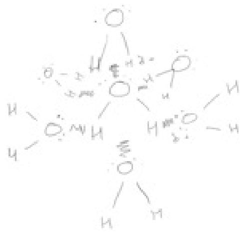
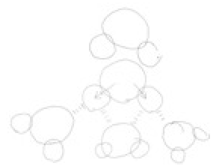
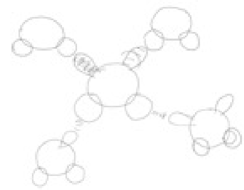
Comparison of the changes in students' individual and collaborative explanations of the nature of hydrogen bonds among water molecules in snowflakes**.** To assess students' learning through IVR, the students drew and explained their understanding in pre- and post-interviews. As shown in Table 5.3, most students (n = 48) preferred to draw individual diagrams and provide individual explanations in the pre- and post-interviews. Some students (n=12) worked individually before IVR but collaborated on the drawing tasks after IVR. Only eight students collaborated on the drawing tasks to create shared diagrams before and after IVR. Generally, students who struggled with the structure of a water molecule or had difficulties recognising the non-covalent nature of hydrogen bonds (category A) did not collaborate with peers. Similarly, only eight of the 29 students who already had a reasonable understanding of the nature of hydrogen bonds (category C) collaborated with peers in at least one interview session. Students who were initially in category B were more willing to collaborate with peers compared to those in other conceptual categories.

When students collaborated with peers on the diagram-drawing tasks, their understanding of the nature of hydrogen bonds improved more consistently after IVR compared to those who worked individually. For instance, three of the 14 students who were initially uncertain of the role of lone pairs (category B) and did not collaborate with the peers both before and after IVR either remained in the same category or moved to a category of lower conceptual understanding (Table 5.3a). On the other hand, all the 10 students who were initially in category B but collaborated on the diagram-drawing tasks in at least one of the interview sessions moved to category D of conceptual understanding after IVR (Tables 5.3b and 5.3c). These students recognised hydrogen bonds as interactions between lone pairs and hydrogen atoms and in 3D space. However, collaboration did not generate any new conceptual categories. In addition, the nature of the diagrams or verbal explanations created during the pre- and post-interviews did not differ much between the students who collaborated with peers and those who worked individually. For example, before IVR, the students Samson, Dom, and Sandra all exhibited alternative conceptions of the role of lone pairs of electrons in the formation of hydrogen bonds.

After IVR, the changes in conceptions of the nature of hydrogen bonds among water molecules that were held by Dom and Sandra (collaborative pair before and after IVR) also did not differ much from those held by Samson who worked individually on the diagram-drawing tasks before and after IVR (Table 5.7). After IVR, each of the students (Samson, Dom, and Sandra) recognised that a hydrogen bond was formed between a lone pair of electrons in one water molecule and a hydrogen atom of another water molecule. Each water molecule in snowflakes formed a maximum of four hydrogen bonds and that the interactions were in 3D space.

Table 5.7

Comparison of the Changes in Students' Conceptual Understanding Made by Individual and Collaborative Students

Samson (individual – before and after IVR)		Dom and Sandra (collaborative – before and after IVR)	
Diagrams and explanations before IVR			
	Samson: it [the water molecule] is polar, one [the H] side is slightly positive and the other [O] side is slightly negative … because opposites attract, slightly positive side will go to slightly negative side of the other water molecule		Sandra: (stacks a water molecule on top of a central molecule) there's the polarity difference, so that matches up. Can't remember if it's plus or minus, but yeah. [...] Dom: yeah, as you're saying [...] So, the negative dipole would be around the oxygen and the hydrogen would be positive. So, the hydrogens of the second molecule would be attracted towards the negatively negative area of the oxygen
Diagrams and explanations after IVR			
	Samson: it's hard to draw on 2D … there is only four molecules that can attach, and a bit more spread out, and yeah like individual [lone pairs to hydrogen atoms] … but it's not like 2D even if it's like aligned it's still [3D] (gestures molecules approaching from different angles)		Dom: You'd have one [lone pair] here, with the [incoming] hydrogen interacting with the lone pair. And another one, the fourth one coming from this kind of angle interacting with the other lone pair […] But of course, it's like tetrahedral shape. So, it's a bit hard on the paper. Sandra: I think two lone pairs, draw like that (draws two lobes on the first water molecule to show lone pairs). It is it's hard because it's not a flat shape like that, right? It's tetrahedral […] Dom: We can do … like shading and lines of what's coming out of the page and into the page (shades one of the lone pairs) …

Research Question 2: Changes in Students' Explanations of the Shape of Snowflakes After Exploring the Concept in Collaborative IVR.

Before IVR, the students had a wide range of ideas related to the formation of snowflakes. Some student participants (n=11) were not sure how they could explain the shape of snowflakes and did not attempt to provide explanations. Some of the students focused on explaining the overall flat appearance of snowflakes (n=17) and reasoned that molecules spread out in 2D, while some (n=12) focused on the macroscopic variations in the patterns of snowflakes. Other students (n=14) made efforts to explain the hexagonal symmetry in snowflakes but imagined that molecules were forming hexagonal shapes in 2D. Very few students recognised that the water molecules in snowflakes formed 3D lattices (n=4) or that tetrahedral units of molecules were the building blocks of the structures of snowflakes (n=3).

After IVR, the student participants were more confident to provide explanations for the shape of snowflakes; only three students did not attempt to provide explanations after IVR compared to 11 who did not provide explanations before IVR. After IVR, none of the students discussed molecules spreading out in a flat plane. Most students (n=50) explained that the submicroscopic structure of snowflakes was not 2D as many had initially imagined; therefore, many students shifted the focus from explaining the flat appearance of snowflakes to explaining other aspects of snowflakes such as the hexagonal symmetry and the variations in patterns (Table 5.8). In addition, after IVR, students tended to integrate multiple topics to explain the shape of snowflakes, instead of explaining individual features in the shape of snowflakes (such as the flat appearance of snowflakes only, the hexagonal symmetry only, or only the variations in the patterns in snowflakes). After IVR, students integrated topics such as hydrogen bonds, hexagonal shapes in 3D, and variations in patterns of snowflakes (n=16) to explain the shape of snowflakes. Other students integrated topics like hydrogen bonds, tetrahedral units, and hexagonal shapes in 3D (n=9); or hydrogen bonds, tetrahedral units, hexagonal shapes in 3D, and variations in snowflakes patterns (n=8) in their explanations.

Table 5.8

Changes in Students' Explanations of the Shape of Snowflakes After IVR

Category	Subcategory	Number of students	
		Before IVR	After IVR
Not sure		11	3
Incoherent or hard to categorise		7	7
Focus only on the appearance	flat structure	17	0
	variation in patterns	12	7
Explain molecular interactions in 3D	In terms of hydrogen bonds	1	2
	+ 3D lattices and the variations in patterns	3	3
Explain hexagonal symmetry	In terms of hydrogen bonds	13	13
	+ the variation in patterns	1	16
Recognise tetrahedral unit as the building block of snowflakes	In terms of hydrogen bonds or 3D lattice	1	0
	+ the hexagonal symmetry	0	9
	+ the variation in patterns	2	0
	+ the hexagonal symmetry and the variation in patterns	0	8

The 11 students who were initially not sure of the explanation of the shape of snowflakes moved to different levels of conceptual understanding after IVR. Some of the students did not attempt to explain the shape of snowflakes (n=3), gave incoherent explanations (n=1), or only explained the variations in snowflakes patterns (n=1). After IVR, more than half of the students in this category (6 out of 11) recognised that molecules interacted in 3D to form hexagonal patterns. For example, after IVR, Jill explained:

> "It [the central molecule] doesn't connect to six [other molecules]. [Before IVR], I wasn't sure how the lattice forms but … the hydrogen bonding between molecules allows the formation of a hexagonal lattice structure which forms the crystalline snowflakes, and the actual patterns and shapes are formed by the variations in temperature and humidity as the water gets drawn from the moisture, I guess"

Before IVR, some students (n=17) focused on the overall flat appearance of snowflakes. These students reasoned that molecules would spread out from a central molecule to form flat structures and often used gestures to illustrate molecules branching out in a flat plane, as if the thickness of a snowflake would be one layer of water molecules. However, after IVR, 12 of the 17 students in this category (e.g., Lucas) recognised that the molecules did not interact in 2D. Instead, the molecules interacted in 3D to form lattice structures and hexagonal patterns among molecules. These 12 students also explained variations in the patterns of snowflakes. The excerpts below show the changes in the explanation of the shape of snowflakes made by Lucas:

Before IVR

"I guess as it kind of cools down, they all (*pointing at his diagram*), the water [molecules] can compact a little bit and the bonds will be closer, and they will pack in a kind of shape like this (*points at the diagram*) so that they are spreading out as much as they can and sort of, evening out a little bit (*gestures molecules spreading out from the central molecule*)."

After IVR

"When the water molecules are kind of packed and you fit four on one, they end up forming that hexagonal kind of shape but then when that kind of builds on (*gestures water molecules building on the already existing chunk*), they can only fully pack when the temperature and humidity are right, so when there's low humidity and there's less water it tends to branch out a bit more because the lattices are not packing as much, I suppose, and back into the molecules, you form that hexagonal kind of shape …"

Those students who focused on the macroscopic variations in the patterns of snowflakes before IVR (n=12) used ideas such as differences in environmental conditions, differences in numbers of water molecules available or probabilities to explain the differences in snowflakes patterns. After IVR, some of the students in this category (n=4) not only explained the differences in snowflakes patterns but also recognised that, through hydrogen bonds, water molecules formed hexagonal shapes in 3D space. Moreover, about half of the students in this category (5 out of 12) recognised the tetrahedral unit as the basis for the snowflakes structure. For instance, before IVR, Kevin reasoned that water molecules may have different chances to interact; these different chances may explain why there are so many different patterns of snowflakes. After IVR, Kevin integrated several topics (hydrogen bonds, tetrahedral units, hexagonal shapes, and variation in patterns) to explain both the hexagonal symmetry in snowflakes and the variations in patterns of snowflakes. The excerpts below show the explanations provided by Kevin before IVR and after IVR.

Before IVR

"(*Looking at the images of snowflakes)* Yeah, when they [water molecules] interact with each other, like, come close enough and they get cold, like, it forms in every single angle, and it can form differently. For every time, it's a different chance of something else happening."

After IVR

"… So, the initial water molecules … bond to the hydrogen atoms and then the lone pairs and then it forms the tetrahedral, and then those tetrahedral shapes bond to another tetrahedral shape, and bond to another one … and it forms a hexagonal structure, and then it continues to expand. And then when different conditions hit the, to each point of that, it expands out slowly and forms different types of shapes. They're all very similar because they are experiencing the same conditions, as was said in the video."

Fourteen students explained the hexagonal symmetry in snowflakes before IVR but with different levels of success. Most of these students reasoned that molecules branched out in 2D from a central molecule to form flat hexagons, while some (e.g., Nelson) reasoned that six molecules could connect to one central molecule to result in the six branches that appear in each snowflake. After IVR, 13 of 14 the students in this category recognised that, by forming hydrogen bonds in 3D space, water molecules formed hexagonal shapes which explains the six-fold symmetry in snowflakes. Moreover, six of these 13 students also recognised that tetrahedral units were the basis of the snowflakes structure. The excerpts below show the explanations of the hexagonal symmetry given by Nelson before and after IVR:

Before IVR

"I think this middle one here *(points at the central water molecule in his drawing)*, will be the middle of the snowflake and that … like branches out. So, like different hydrogens will connect to the valence electrons forming a stem, like six stems off each one."

After IVR

"… hydrogen bonding occurring between …the valence electrons of the oxygen and the hydrogens … and then there's all that bonding, we end up forming like the hexagonal shape, which kind of helps explain that [the hexagonal shape of snowflakes] ...they [molecules] will bond together with other clusters at the correct orientation to form more hydrogen bonds and kind of just expand in a lattice structure … and that lattice structure will still go out. And then it kind of comes to our external factors that affect that final bit … because the actual flake is so small … the individual snowflakes [branches] experience like the same conditions which affect how the branch goes out ...”

The IVR program was designed to help students recognise the link between the macroscopic shapes of snowflakes and the interactions among water molecules. After IVR, most students made efforts to use their knowledge of hydrogen bond interactions among water molecules in 3D space to coherently explain the shape of snowflakes. However, some students (e.g., Harriet) provided very superficial explanations based on what they saw in IVR but did not clearly link their explanations to hydrogen bonds among molecules. Other students (n=7; e.g., Craig) simply described what they had seen/heard in the video at the end of the IVR activity regarding the factors that affect the way snowflakes grow. The excerpts below show explanations provided by Harriet and Craig after IVR:

> Harriet: “The basic structure is the hexagon to begin with. And then hexagons, hexagons together, like they have the pointy edges … and hexagons, hexagons together, planes are together … there's a plane, even the angles were different, like it wasn't like flat hexagons, it gives [the hexagonal] shape of snowflakes ...”

> Craig: “Snowflakes are made up of millions and millions of water molecules, and that’s how they get their shape. They grow in different environments which affects how they grow”

When designing the collaborative IVR program on snowflakes, we included multiple ‘hands-on’ tasks for students to complete, such as connecting many water molecules to form a 3D lattice structure. We anticipated that, as the students constructed larger molecular structures in IVR, they would improve their knowledge of the nature of hydrogen bonds and use it to develop a coherent understanding of the macroscopic scale snowflakes. Although most of the participating students achieved a much better understanding through the IVR activities (for example, 50 out of 68 students recognised the hexagonal arrangements among water molecules in 3D space as the reason for the hexagonal shape of snowflakes), the students explained the shape of snowflakes to different extents. Some of the students did not successfully integrate the idea of hydrogen bonds in their explanations after IVR. These students might have had difficulty demonstrating what they learnt or describing what they saw in the 3D virtual space. For other students, the connection between the molecular interactions and the shape of snowflakes might not have fully registered in their minds in the limited time available.

5.5. Discussion

In this study, we investigated how undergraduate chemistry students changed their conceptions of the nature of hydrogen bonds among water molecules after experiencing an IVR program on snowflakes. Firstly, the study found that the collaborative IVR experience helped most of the students to move towards a more scientifically accepted understanding of the nature of hydrogen bonds among water molecules in snowflakes. After IVR, more students (n=61) recognised hydrogen bonds as electrostatic, directional, and involving individual lone pairs of electrons compared to those (n = 34) who recognised this before IVR. The number of students who verbally discussed and/or represented molecular interactions in 3D also improved from five (5) before the IVR experience to 57 after the IVR experience.

Secondly, our findings showed that, through the collaborative IVR experience, most students built a coherent understanding of the shape of snowflakes. Before IVR, 11 students were not sure how to explain the shape of snowflake. Twenty-six students imagined that six water molecules connected to one molecule at the centre of a snowflake or that molecules spread out in a two-dimensional plane to form snowflakes. These students focused on the ideas that snowflakes had six branches and looked flat. Therefore, the students concluded that six molecules must be connecting to a central one to form hexagons, and/or that molecules branch out in a two-dimensional plane to form flat shapes. This finding is consistent with previous studies which reported that, when asked to explain complex macroscopic properties of substances, many students tend to rely on simple pattern recognition, superficial features, and heuristics rather than mechanistic reasoning (e.g., Cooper et al., 2013; McClary & Talanquer, 2011). After exploring the molecular structures in IVR, many of the students were able to integrate concepts of hydrogen bonds, 3D molecular interactions, and hexagonal patterns among water molecules in 3D space in their explanations of the shape of snowflakes.

The collaborative IVR experience may have supported students' understanding of the nature of hydrogen bonds among water molecules in several ways. For example, IVR showed the virtual water molecule models in three dimensions and provided visual cues to represent hydrogen bonds forming between lone pairs of electrons and hydrogen atoms. The students were also able to walk around the 3D structures to change perspectives and interact with the molecular structures by moving, flipping, rotating, and connecting them while discussing ideas with their partners in the same environment. These features may have helped the students to test their ideas in IVR, examine their preconceptions, and recognise how molecules interacted with each other and the arrangements of molecules in the structures formed. Consequently, most students were able to make positive changes to their diagrams and verbal explanations. Our findings are consistent with the argument that IVR not only supports development of practical skill-oriented knowledge as reported by Jensen and Konradsen (2018) but also the learning of abstract science concepts (Wu, Yu, et al., 2020). The present study lends support to previous studies which reported that IVR can improve students' understanding of abstract science concepts (Dede et al., 1997; Kozhevnikov et al., 2013; Tsivitanidou et al., 2021).

The study found that, amongst the 10 students who initially had difficulties with drawing the structure of a water molecule or distinguishing intermolecular from intramolecular interactions, four of them retained most of their preconceptions whereas the other six improved their understanding. Studies have reported that students' alternative conceptions may persist even after explicit instruction, and that changing these conceptions may be a gradual rather than a sudden process (Treagust & Duit, 2008). For meaningful learning to occur, learners need to make a connection between the new information and the existing prior knowledge (Taber, 2017). In the present study, some students may have failed to reconcile the new information provided in IVR with their own ideas or to interpret the relevant features in the molecular structures provided in IVR. This outcome is probably because the students had difficulties visualising basic concepts such as bonding and structure or polarity of water molecules.

Even though most students provided explanations that linked the nature of hydrogen bonds among molecules in 3D space to the shape of snowflakes after IVR, some students (n=3) were still unable to successfully explain the shape of snowflakes after the IVR experience. Some students identified relevant features such as the large number of molecules in snowflakes, hexagonal patterns of molecules, and the 3D nature of the molecular lattice but did not provide elaborate explanations in relation to hydrogen bonds or polarity of molecules. This result was unexpected. However, using the concept of hydrogen bonds to explain the shape of snowflakes is a complex task which requires integration of many chemistry concepts. Students' difficulties in coherently explaining structure-property relationships have been widely reported in previous studies (e.g., Cooper et al., 2013). Our findings suggest that a single exposure was not enough to help some of the students to make a clear link between the macroscopic and submicroscopic levels of snowflakes.

5.6. Implications

The intuitive nature of interactions and 3D visualisation capabilities of IVR hold promise in helping students visualise molecular interactions and improve their conceptual understanding of chemistry. In this study, we investigated undergraduate chemistry students' conceptions of the nature of hydrogen bonds in snowflakes before and after a collaborative IVR session. Before the IVR session, many students did not demonstrate a good grasp of the nature of hydrogen bonds among water molecules. However, by engaging in a series of hands-on activities with the models of water molecules in a collaborative IVR environment, many students tested their preconceptions and built a more scientific understanding of the nature of hydrogen bonds and the shape of snowflakes. For example, after IVR, about half of the students who initially had difficulties recognising the nature of hydrogen bonds as intermolecular interactions recognized that hydrogen bonds are not covalent in nature. Instead, hydrogen bonds were electrostatic forces of attraction between lone pairs of electrons and hydrogen atoms in neighbouring molecules. This research investigation with IVR has demonstrated the potential of this medium to challenge and address students' alternative conceptions in chemistry, such as those related to the concept of hydrogen bonds. Therefore, we recommend that IVR be further investigated with different chemistry content and in different contexts to further understand its potential.

Our findings also showed that learners may not benefit equally from IVR interventions. For instance, about half of the students who initially struggled with drawing the structure of a water molecule or recognising the nature of intermolecular interactions retained their preconceptions. In future studies, educators may wish to experiment with different strategies to support low prior knowledge learners in gaining the benefit of this novel technology when learning different science concepts. For example, purposefully designed activities to orient students to the target concepts in preparation for more independent learning in IVR have been reported to support science knowledge gains (e.g., Wu, Hu, et al., 2020). The benefit of other strategies such as scaffolding or explicit guidance to focus students' attention on the target features in the learning environment while they learn in IVR should also be explored further. In addition, as educators design to systematically investigate the educational benefits of IVR in future studies, they may wish to explore whether repeated use of IVR may further improve conceptual understanding.

In the present study, not many students collaborated on the pre- and post-interview tasks. However, students who collaborated on the diagram-drawing tasks tended to change their conceptions to scientifically accurate conceptions in a more consistent manner compared to students who worked individually on the tasks. Collaborating with peers may have allowed students to reflect on their learning from IVR or reinforce their understanding through discussion. This observation from our study is consistent with the findings of Klingenberg et al. (2020) who investigated students' learning of biology concepts with IVR. The authors reported that students who were asked to teach peers after individual play in IVR had higher learning outcome benefits compared to students who did not engage in the peer-teaching task after IVR (Klingenberg et al., 2020). In fact, peer-teaching has been identified as one of the strategies that can enhance students' learning (Fiorella & Mayer, 2016). In the present study, collaboration on post-IVR tasks may be considered as a form of reflection or peer-teaching; therefore, its role in students' learning with IVR needs to be investigated further in future studies. For example, future studies may want to experiment with different designs (for example, collaborative versus individual IVR designs) to explore whether collaboration in IVR leads to better learning gains.

5.7. Limitations

This study had some limitations. Firstly, learners were paired to complete the IVR learning tasks and the assessment tasks in pre- and post-interviews together. This was done to foster collaborative learning and to provide an opportunity for the students to consider and reflect on their understanding while explaining their ideas to the peers. However, during interviews, most students showed reluctance to collaborate with their peers and, instead, completed the diagrams and explanations individually. A small number of students switched from individual work in the pre-interview to collaborative work in the post-interview. Due to the variety in students' collaborative tendencies, the interviewer adjusted the assessment prompts from seeking collaborative responses to accommodating individual students' preferences. These variations made the interpretation of students' learning or the changes in their conceptions more complex than anticipated. Moreover, since the learners were paired, the verbal responses from each learner working individually during the pre- and post-interviews may have been influenced either directly or indirectly by the partners who were seated next to them. Secondly, although all the interactions were videotaped, this study did not investigate how learners interacted with the IVR environment to derive the learning benefits. In our future work, we intend to explore how each pair of learners constructed their understanding during the collaborative IVR experience. Thirdly, this study presents results from a single exposure of students to IVR. Educators warn that learning benefits may be partly influenced by the novelty of the learning technology (Clark, 1983). Based on the findings from this study, investigating conceptual benefits from IVR over multiple sessions is likely to demonstrate the power of IVR in supporting students' learning of science concepts. Lastly, in this study, we aimed to investigate how IVR changed the students' conceptual understanding rather than evaluate the effectiveness of IVR compared to other learning modes. In future studies, researchers may wish to include comparison groups to evaluate the learning benefits of IVR against alternative media.

5.8. Conclusions

The huge investment in technology development by major tech companies has made IVR technology more accessible for use in science classes. However, the evaluation of the educational benefits of IVR has been limited to motivation, engagement, and recall knowledge, therefore, providing limited justification for the huge investment in IVR. By analysing student-generated diagrams and verbal explanations before and after IVR, this study provides evidence that IVR can support students' conceptual understanding of abstract chemistry concepts such as the nature of hydrogen bonds among water molecules and the shape of snowflakes. The impact of IVR on students' conceptual understanding needs to be investigated further in different chemistry learning contexts and with different concepts. Educators may also want to experiment with the implementation of different scaffolding strategies to maximise the learning benefits of IVR. Such strategies may include pre-activities to orient students to the target concepts before exploring them in IVR or highlighting the important features in molecular structures in IVR designs to focus students' attention while exploring the science concepts in IVR.

Chapter 6. The Perceived Complexity of Learning Tasks Influences Students' Collaborative Interactions in Immersive Virtual Reality

After exploring the trends and gaps in the utilisation of IVR for science learning (Chapter 3), and the conceptual benefits of collaborative IVR (Chapters 4 and 5), Chapter 6 documented students' interactions as they completed chemistry learning tasks in different collaborative IVR environments. This chapter is in response to the fourth research question (*How do students interact to learn hydrogen bonding and enzyme-substrate reactions in collaborative IVR contexts?*[5]*;* please see Section 1.5*)*.

The content in this chapter has been published in the *Journal of Science Education and Technology*, a Q1 journal published by Springer. The content presented here is the version of the submitted article accepted by the journal. The table and figure numbers have been formatted for the chapter. The full citation of the published article is:

Matovu, H., Won, M., Hernandez-Alvarado, R. B., Ungu, D. A. K., Treagust, D. F., Tsai, C.-C., Mocerino, M., & Tasker, R. (2024). The perceived complexity of learning tasks influences students' collaborative interactions in immersive Virtual Reality. *Journal of Science Education and Technology*. Online first. https://doi.org/10.1007/s10956-024-10103-1.

[5] The fourth research question was addressed through two specific sub-questions (please see Section 2.3) and they are included in Section 6.3.

6.1. Abstract

This study investigated how different learning tasks influence students' collaborative interactions in immersive Virtual Reality (IVR). A set of chemistry learning activities was designed with IVR, and 35 pairs of undergraduate students went through the activities. Videos of students' interactions were analysed to identify patterns in students' physical, conceptual, and social interactions. When students were manipulating conceptually familiar virtual objects (several water molecules), they perceived the tasks as a simple extension of prior knowledge and did not attempt to explore the 3D visualisation much. They did not move around to take different perspectives, and conceptual discussions were brief. Their prior power relations (leader-follower) carried over in IVR environments. In contrast, when conceptually unfamiliar chemical structures (protein enzyme) were displayed, students perceived the tasks as complex, demanding a new mode of learning. They spontaneously moved around to explore and appreciate the 3D visualisation of IVR. Walking to different positions to observe the virtual objects from multiple angles, students engaged in more collaborative, exploratory conceptual discussions. As the perceived complexity of learning tasks or virtual objects triggers different collaborative interactions amongst students, careful considerations need to be placed on the design of IVR tasks to encourage productive collaborative learning.

Keywords: Immersive Virtual Reality; Human-Computer Interaction; Collaborative Learning; Chemistry Education

6.2. Introduction

Immersive Virtual Reality (IVR) technology for educational purposes has gained widespread popularity in recent years (Radianti et al., 2020). Using head-mount displays, IVR engrosses students in realistic-looking 3D computer-generated environments where they can interact intuitively. This enhances their feelings of "being there" in the virtual environment and actions having real consequences (Slater & Sanchez-Vives, 2016). The unique 3D visualisation and motion-tracking features of IVR present opportunities to address key educational challenges (Slater & Sanchez-Vives, 2016). Consequently, science educators have started to explore the educational possibilities of IVR to support students' visualisation of abstract concepts, enhance learners' engagement, or train practical skills (Matovu, Ungu, et al., 2023).

Of the different science learning areas, chemistry could significantly benefit from IVR. For instance, IVR can simulate 3D molecular structures, such as protein structures, which cannot be visualised or explored easily through other means (e.g., Qin et al., 2021). By transforming abstract chemistry concepts (e.g., molecules and their interactions) into tangible forms, IVR could support students' construction of useful mental models of the concepts (Mikropoulos & Natsis, 2011). Students can examine spatial relations (e.g., depth and angles) in 3D molecular structures from different viewpoints (Dede, 2009). Students can also manipulate the molecular structures in an embodied way to actively construct knowledge (Chen, 2010).

However, science education researchers have mainly provided one-time learning opportunities with IVR, without exploring how different learning tasks would influence students' experiences and learning (Matovu, Ungu, et al., 2023). The few researchers who provided multiple IVR opportunities to students (e.g., Huang et al., 2021; Pande et al., 2021) relied on pre-/post-knowledge tests without documenting how students' interactions in IVR evolved over the learning sessions. In addition, IVR-based learning activities have been designed and tested mostly for single users, without utilizing collaborative knowledge construction processes (Matovu, Ungu, et al., 2023; Won et al., 2023). Few researchers have explored students' collaboration to complete interactive science learning tasks in a shared IVR space (Southgate et al., 2019; Won et al., 2019). These studies relied on evaluations based on observations (Southgate et al., 2019) and interviews (Won et al., 2019), rather than comprehensively documenting students' interactions in IVR.

To gain a more balanced perspective of the educational potential of IVR, researchers need to explore how students' interactions change across different IVR-based learning contexts. By documenting changes in students' interactions with the nature of the learning tasks or virtual objects, educators can identify and design IVR-based learning tasks that can optimise students' collaborative interactions. In the present research, we designed a set of IVR-based learning tasks to help undergraduate students collaboratively learn chemistry topics on molecular interactions and evaluated the changes in students' collaborative interactions.

The present study was designed to support students' 3D visualisation of chemical structures and interactions. The skill to visualise these concepts is fundamental to the learning of chemistry yet challenging for many students (Wu & Shah, 2004). This study employed iVR to effectively represent molecular structures in tangible forms, enabling students to interact with these representations intuitively and support their understanding of intermolecular interactions.

The research study was also theoretically informed by the social constructivist theory of learning (Vygotsky, 1978), which emphasises social interactions as a driver of learning. Within iVR contexts, students were paired and encouraged to engage in coordinated efforts to create joint meanings and complete chemistry learning tasks. Such collaborative interactions involve a dynamic engagement with different ideas through verbal interactions, actions with artefacts, and non-verbal interactions, such as gestures and facial expressions (Hakkarainen et al., 2013; Roschelle & Teasley, 1995). Collaborating on learning tasks provides students with an opportunity to generate varied perspectives for consideration, engage in self-reflection, and organise and revise their understandings through reciprocal explanations (Webb, 2009, 2013).

6.3. Collaborative Interactions in Digital Learning Environments

Various forms of digital technologies offer opportunities for collaborative learning interactions in unique ways. Video conferencing platforms (e.g., *Zoom, or Skype*) allow students to communicate verbally and non-verbally in real time, but students are in different physical spaces and cannot manipulate shared objects. Multi-user virtual worlds on 2D screens (e.g., *Second Life, or River City*) provide a common ground for spatially distributed students to meet and work collaboratively on learning tasks (Dalgarno & Lee, 2010). However, in these environments, students are represented by avatars, communication is often through text, and students manipulate objects using a keyboard and mouse. In contrast, collaborative IVR platforms (e.g., *AltSpaceVR,* or *Engage VR*) allow students to physically walk into a shared virtual space to interact with peers in a first-person perspective, making them feel physically co-located with their peers (Šašinka et al., 2019). Students can communicate verbally with peers, use gestures for non-verbal communication, and use their “hands” to manipulate shared virtual objects and co-construct understanding (Maloney & Freeman, 2020). Students’ movements in the virtual space match their movements in the real world (Barreda-Ángeles et al., 2023; Won et al., 2019). As a result, collaborative interactions in IVR feel more “real” compared to other digital technologies (Barreda-Ángeles et al., 2023; Oh et al., 2018).

Although IVR could mimic face-to-face collaborative interactions, the implementation of social interactions in IVR for learning has been slow (Won et al., 2023). Efforts to incorporate social interactions mainly employed IVR designs where learners interacted with pedagogical agents for step-by-step guidance, rather than supporting collaborative knowledge construction with peers (e.g., Makransky, Wismer, et al., 2019). Some researchers incorporated peer-to-peer interactions by having one student in IVR and the other observing the virtual environment on a 2D screen (e.g., Price et al., 2020; Uz-Bilgin et al., 2020; Webb et al., 2022). The student using a 2D screen missed out on the opportunity to experience virtual objects from a first-person perspective.

Some educators have used opensource collaborative IVR platforms (e.g., *AltSpaceVR* or *Engage VR*) to engage students in social interactions (e.g., Barreda-Ángeles et al., 2023; Han et al., 2023; Ripka et al., 2020). However, these researchers used IVR as a place for distributed students to meet and brainstorm ideas, rather than as an environment to interact with virtual objects. Consequently, these studies have not explored how students utilise the unique IVR features (e.g., 3D visualisation and embodied movements) to collaboratively learn abstract science concepts.

Studies on technology-mediated collaborative learning also showed that assigning group tasks does not guarantee effective collaboration (Kreijns et al., 2003). For example, students who lack communication skills may struggle to negotiate ideas with others, leading to conflicts and unproductive conversations (e.g., Barron, 2003). In addition, some students may be less motivated to participate in collaborative activities, relying on the more active learners (X. Zhang et al., 2019). This can result in frustration for the active learners, who may also become less engaged (e.g., Lipponen et al., 2003).

Researchers note the importance of pedagogical considerations (e.g., task design) and social factors (e.g., group composition) in producing collaborative interactions when designing digital learning environments (Kirschner et al., 2008). For example, students' perceptions of task complexity influence how much effort they invest to complete the task. Tasks that are too easy, leave no room for student initiatives, or too closed offer little room for discussion and tend to limit collaboration (Kirschner et al., 2008). Too complex a task would also lead students to withdraw from tackling (Malmberg et al., 2022), but when the task requires students to draw from each member's perspectives, it tends to promote collaborative engagement (Care et al., 2015). A sense of cohesion amongst group members and relational history also contribute to collaborative interactions (Graesser et al., 2018; Kreijns et al., 2022). Yet, existing studies have not explored how the nature of learning tasks influenced collaborative interactions in IVR. More studies are needed to explore how such task-related factors influence students' collaborative interactions in IVR.

The present study explores how student pairs interact to complete chemistry tasks with different kinds of virtual objects in three IVR-based learning contexts. To illustrate the differences in students' interactions, this research focused on two of these IVR contexts, one with conceptually familiar virtual objects and one with conceptually unfamiliar virtual objects. The tasks targeted the topics of hydrogen bonds in water molecules and enzyme-substrate reactions, respectively. This research aimed to answer the following research questions:

1. How do students collaborate to learn intermolecular interactions with water molecules in immersive Virtual Reality?
2. How do students collaborate to learn the same concept with an enzyme and a substrate molecule in immersive Virtual Reality?

6.4. Methods

Participants and Data Collection Procedures

Seventy first- and second-year undergraduate chemistry students at a large public university in Australia volunteered to participate in this study. As part of their chemistry units for semester 1 (March–May 2021), the students in pairs completed three IVR sessions (snowflake IVR, taste receptor IVR, and protein IVR). Any two consecutive IVR sessions were spaced 2-3 weeks apart. Students selected convenient time slots outside their normal class schedules. Because of this flexibility, some students were paired with peers they had worked with prior (*friends*), while other pairs did not know each other (*strangers*). Participants worked with the same peers over the three IVR sessions.

Each IVR session involved a pre-interview (15-25 mins), an IVR learning activity (25-50 mins) and a post-interview (20-30 mins). In pre-interviews, students were introduced to the target topics and their prior understanding was evaluated. In pre-interview for the first IVR learning activity (snowflake IVR), students were asked to explain and illustrate how water molecules would interact in snowflakes. Similarly, before the last IVR learning activity (protein IVR), students were asked to describe and illustrate their understanding of enzyme-substrate reactions. After pre-interviews, participants were trained on using IVR controllers to manipulate virtual objects and were encouraged to discuss ideas with peers, move around the virtual space to explore objects from different perspectives, and immediately report any discomfort during IVR. Each student then donned an HTC VIVE Pro Eye headset with a wireless adaptor and two controllers for IVR-based learning. In IVR, students could walk around a 4m x 4m room to complete learning tasks. They could also see each other's avatars (floating headsets and hands) in a shared virtual space and communicate verbally. In post-interviews, students reflected on their learning experience and answered conceptual questions to evaluate their learning. All pre-/post-interviews and IVR activities were audio and video recorded. Videos of each student's view in IVR were also recorded using a screen-recording application.

The Collaborative IVR-Based Learning Tasks

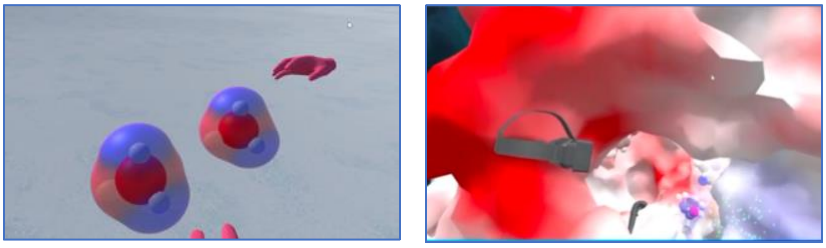
The three collaborative IVR activities were developed by the research team. First, storyboards were developed highlighting the target learning objectives, tasks, and instructions to students. The IVR programs were then developed in Unity® and were run with STEAM VR as the supporting platform. In each IVR activity, student pairs completed multiple interactive tasks. In snowflakes IVR, students explored the nature of hydrogen bonds between water molecules in snowflakes. The tasks included forming and exploring the strength of a hydrogen bond between two molecules (e.g., Figure 6.1**a**) and constructing a lattice structure of water molecules to explain the shape of snowflakes. In the second (taste receptor) IVR activity, students explored the concept of stereochemistry using the chemical phenylalanine. Learning tasks included constructing two enantiomeric forms of phenylalanine and fitting them in a model of a sweet taste receptor to identify the form that would activate the taste receptor. In the third (protein) IVR activity, students explored the reaction between an enzyme (acetylcholinesterase), and its substrate (acetylcholine) in relation to chemistry concepts. Learning tasks included exploring the structure and the best orientation of the substrate molecule to enter and react with the enzyme (e.g., Fig. 6.1**b**). In all the IVR learning environments, the key conceptual ideas were (1) molecular shapes and orientations; and (2) attractions between electron-rich (red) and electron-poor (blue) areas. To complete the key learning tasks in each IVR environment, students needed to apply these conceptual ideas to position the 3D molecules in optimal orientations so that they would interact.

Data Analysis

For each student pair, we first synchronised the videos of students' interactions in the physical space, audio records, and their views of the virtual world during each iVR activity. Synchronising these records facilitated the tracking of students' interactions in both the virtual and physical spaces simultaneously. The synchronised videos were then used to create multimodal transcripts (Cowan, 2014; Walkington et al., 2023) encompassing multiple forms of data. The data included students' talk, positions, visual foci, physical movements, gestures, interactions with virtual objects, and screenshots. This approach was chosen because social interactions are inherently complex and involve multiple communication modes (Jewitt, 2013). Multimodal transcripts, thus, make contextual information and moment-by-moment developments in students' collaborative interactions visible to aid the analysis (Walkington et al., 2023). For example, examining students' relative positions in the virtual and physical spaces allowed us to analyse students' perspectives of and proximity to virtual objects and peers during collaborative IVR activities. Students' speech, gestures, and interactions with virtual objects provided insights into students' ways of reasoning with molecular structures and how they responded to or built off each other's reasoning.

Figure 6.1

Some of the Learning Tasks Completed by Students in Snowflakes and Protein IVR Contexts



(a) (b)

Note. (a) Two water molecules in Snowflakes IVR. (b) Enzyme entrance in Protein IVR

The research team met to watch synchronised videos and identify some notable aspects in the interactions. We analysed the videos in terms of students' physical interactions (nature and sequence of movements, positions in IVR space, and actions with virtual objects), conceptual exploration (what chemistry concepts were discussed), and social dynamics (how peers generated, expressed, and elaborated ideas, negotiated control of virtual objects, and established consensus).

Based on the analyses of students' pre-interview diagrams and preliminary analyses of IVR session videos, we purposefully selected 10 out of the 35 student pairs for in-depth analysis. These pairs demonstrated a reasonable (but not comprehensive) understanding of the target topics in pre-interviews and engaged in deliberate conceptual explorations in IVR. The first author analysed interactions for all 10 pairs of students using a constant comparison method (Glaser, 1965) to identify any emerging patterns. Student-generated diagrams and responses during pre-/post-interviews were used to triangulate findings from the analysis of IVR session videos. Three researchers (HM, MW, and RBH-A) watched selected segments of IVR session videos together and discussed the patterns in students' interactions. The process was repeated over several months until an agreement was reached.

6.5. Findings

Our analysis showed that the different IVR-based learning contexts prompted different physical, conceptual, and social interactions among the students. When dealing with conceptually familiar virtual objects (water molecules) in snowflakes IVR, students engaged in short conceptual and physical explorations. Among strangers, the peer perceived as more knowledgeable dominated the generation of ideas and/or manipulation of objects but this dominance did not occur among friends. In an environment with conceptually unfamiliar virtual objects (enzyme and substrate structures) in protein IVR, students exerted more effort to collaborate and learn. Students explored the protein IVR environment extensively and integrated multiple chemistry concepts to complete the tasks. The dominance of one peer over another among strangers also disappeared.

We have arranged the results sections in two parts. **Part 1** illustrates students' interactions and social dynamics when exploring water molecules (conceptually familiar objects) in snowflake IVR. **Part 2** illustrates students' interactions and social dynamics when exploring enzyme and substrate molecules (conceptually unfamiliar objects) in protein IVR. In each part, we first provide an overview of students' interactions while completing the focal tasks in each learning environment. The findings are then illustrated with a more detailed analysis of one pair of students (pseudonyms Noah and Jesse).

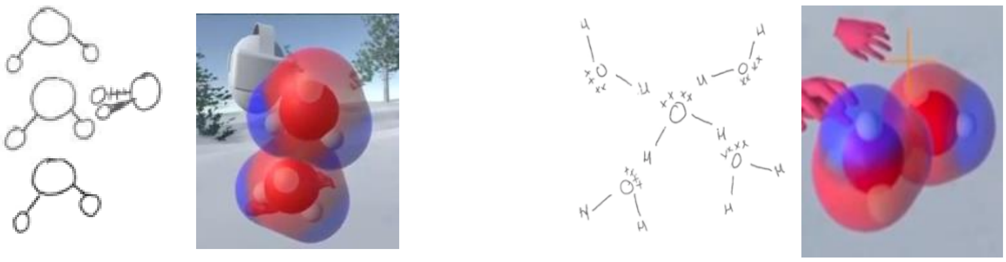
Part 1: Students' Interactions with Conceptually Familiar Virtual Objects

The focal task in the snowflakes IVR activity involved exploring the features of water molecules and the nature of hydrogen bonds between two water molecules. Although hydrogen bonds are a concept many students felt comfortable with, their diagrams and verbal explanations in the pre-interview showed varied levels of understanding. All ten pairs acknowledged that a hydrogen bond is an electrostatic intermolecular force, but many of them (seven pairs) were unsure of the role of lone pairs or the direction of a hydrogen bond. Only two pairs mentioned that hydrogen bonds would form because of molecular interactions in 3D space.

In IVR, students were amazed by the models of water molecules—the structure and electron density map were displayed in 3D. Students immediately grabbed one virtual water molecule each, rotating and pointing out the features (hydrogen atoms, oxygen atoms, lone pairs, red cloud for electron-rich, and blue cloud for electron-poor areas). When prompted to form a hydrogen bond, many students overlapped or stacked water molecules (e.g., Figure 6.2a). Even though they had a rough idea of the role of oxygen's lone pairs, they struggled to use that knowledge to form a hydrogen bond between two water molecules in the 3D IVR environment (Figure 6.2b). After several trial-and-error attempts, most students (8 pairs) managed to create a hydrogen bond by positioning water molecules at a reasonable distance and angle, but they did not change their perspectives to check the alignment of water molecules to take advantage of 3D visualisation. Since the water molecules looked simple and conceptually familiar, students felt that they had already explored the concepts through other media and that they could seamlessly apply their prior understanding to 3D objects. As such, in IVR, many tried to orient the molecules the same way they had represented them in their 2D diagrams, for example stacking molecules (Fig. 6.2a). Also, students did not feel compelled to walk around the virtual objects or explore different perspectives since they normally do not need to while drawing diagrams on paper or exploring the concepts on computer screens.

Figure 6.2.

Students' Initial Attempts at Forming a Hydrogen Bond Between Water Molecules



(a) (b)

Note. (a) Stacking molecules: Directly replicating 2D orientations in IVR. (b) Overlapping molecules: Difficulties applying prior knowledge in IVR.

Students' social dynamics showed distinct variations between strangers and friends. Among strangers, students who used keywords such as "electrostatic interactions" and "electronegativity" in pre-interviews were perceived as more knowledgeable by their peers and often assumed dominant roles. These leader-follower relations extended into IVR. As students explored hydrogen bonds between molecules, the peer perceived as more knowledgeable typically assumed a dominant role in manipulating molecules and generating ideas, while the less knowledgeable peer kept their ideas to themselves. Students with higher perceived prior knowledge felt confident to apply their knowledge in IVR and persuade their peers, while those perceived as less knowledgeable felt that their peers possessed enough prior knowledge to complete the IVR tasks. In contrast, such unequal relations were not evident among friends. Friends freely shared their thoughts and contributed equally in IVR. Perhaps the pre-existing rapport among friends facilitated communication and enabled them to work together effectively. For instance, a friend would know how to elicit ideas without claiming authority and would easily be able to detect divergent opinions.

The case of Noah and Jesse interacting with conceptually familiar virtual objects. Noah and Jesse were first-year chemical engineering majors who had not worked together before the IVR activities. Both had no prior experience with IVR but regularly played computer games. Before IVR, both illustrated each water molecule forming four hydrogen bonds but did not mention the 3D nature of these interactions (Fig. 6.2b). Jesse was more confident articulating his ideas and used more scientific language with keywords, such as "polarity" and "electronegativity". Recognising Jesse's proficiency, Noah was more reserved and perceived Jesse as more knowledgeable.

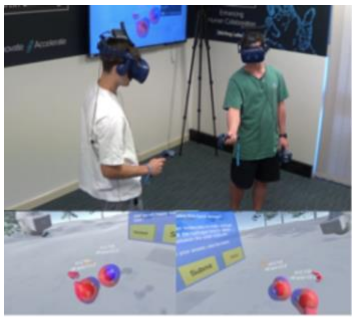
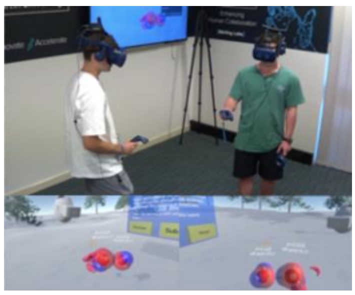
Water molecules in IVR are represented as white and red spheres (hydrogen and oxygen atoms) surrounded by blue and red clouds (electron density map over hydrogen and oxygen atoms). Upon seeing the water molecules in IVR, both students engaged in generating ideas but did not negotiate much. Jesse focused on the electron density map (the cloud): *"It does not look like normal atoms but a cloud of possibilities".* Noah remarked that he was not sure but identified the red sphere as the oxygen atom and the white spheres as the hydrogen atoms. Instead of acknowledging or building on Noah's idea, Jesse expanded his idea of the cloud: "*I think the cloud, the red [cloud] is oxygen, blue ones [clouds] are hydrogen, and the white ones (spheres) are bond sites.*" Without further discussion, Jesse then asked Noah to press the submit button and move to the next task. Jesse was confident that the concept was familiar—water molecules are only represented differently. Therefore, he did not feel compelled to explore the virtual objects or new ideas, which led him to miss out on the opportunity to recognise other concepts such as the lone pairs of electrons, or molecular geometry in the molecules. Moreover, the fact that Jesse focused on more advanced features (the cloud around the molecules) may have confirmed Noah's impression that Jesse understood the concepts better. Consequently, Noah did not negotiate much but simply followed the peer.

When prompted to form a hydrogen bond, the students took turns grabbing and orienting the two water molecules. Despite demonstrating a reasonable understanding of hydrogen bonds in their pre-interview diagrams, the students overlapped the molecules without aligning a hydrogen atom of one molecule with a lone pair of electrons on another molecule (Figure 6.2b). They might have found it hard to apply their prior knowledge in the 3D IVR environment. Each student then experimented with their ideas without narrating their actions. They did not negotiate much and simply moved to the next step even though no bond had formed.

Jesse’s dominance became more pronounced when the students were prompted to make the hydrogen bond stronger (Table 6.1). Jesse reflected on what they had achieved earlier and continued testing his ideas before the hydrogen bond (a green stick between molecules) suddenly formed (Turns 1-3). He then continued with the role of the “leader”, dominating the discussion about the features of the bond and prescribing further actions (Turns 4-9). Even after inviting the peer’s participation, Jesse kept manipulating virtual molecules (e.g., Turns 4-6). Conceptual discussion relied heavily on Jesse who introduced concepts, such as the formation of a hydrogen bond (Turn 6) or the effect of the angle between molecules on bond strength (Turn 8). Jesse’s dominance constrained the scope of conceptual exploration for Noah (Table 6.1).

Table 6.1

An Excerpt of Jesse and Noah's Interaction in Snowflakes IVR

Turn	Speaker	Transcript	Synchronised video shots
	VR:	How can you make this bond stronger? […]	
1	Jesse:	I’m not really sure if we did it right. Because (*pause*) … or maybe we could try different places (*moves one of the molecules around the other; after several trials, a bond suddenly forms).* Oh, I did it. Okay, I think that’s it.	
2	Noah:	Yeah	Turn 1: Jesse (green T-shirt) forms a hydrogen bond
3	Jesse:	So, the bond is yellow for the previous question (pause) in relation to the… Okay, so… (*adjusts the distance between the molecules; Noah observes*) […]	
4	Jesse:	Is it, is it that? Do you wanna try rotating it like this? (Gestures with the controller to show rotation then walks to move the molecules himself)	
5	Noah:	(surrenders control to Jesse) Yeah, you got it.	

6	Jesse:	*(manipulates the molecules)* Is it [hydrogen atom] reacting with this dot [the lone pair] here?	Turn 3-5: Noah observes as Jesse continues to manipulate objects
7	Noah:	Yeah, that one? Yeah.	
8	Jesse:	Okay. That one goes green. And it's yellow … (*briefly lowers his body to observe the bond and then stands up).* Okay, so it looks like the further you go, it turns green, and then it becomes stronger.	
9	Noah:	Yeah.	Turn 8: Jesse briefly lowers his body

Note. Video shots: Bottom left = Noah's view (white T-shirt); Bottom right = Jesse's view (green T-shirt)

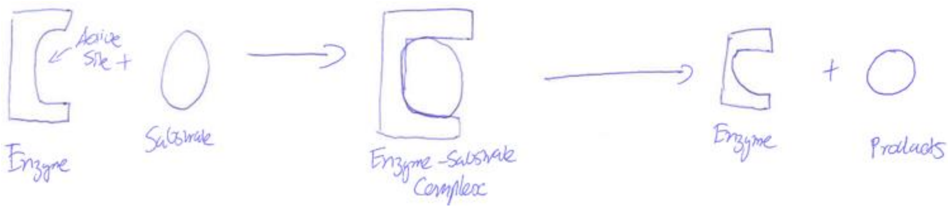
In terms of their physical movements, Noah and Jesse stood opposite each other and each stayed on a different side of the room as they explored ideas (refer to the synchronised video shots in Table 6.1). They did not walk around to observe the alignment between molecules from different directions, even though before IVR they had been given explicit instructions to walk around and change their perspectives. Instead, the students explored the virtual objects by rotating them. Even when Jesse lowered his body to observe the bond (Turn 8), it was only done for a brief moment, and he immediately went back to his initial posture.

Part 2: Students' Interactions with Conceptually Unfamiliar Objects

The focal task in the protein IVR activity required students to orient the substrate at the entrance of the enzyme for the catalytic reaction to occur. Before entering IVR, all students described enzymes as biological catalysts composed of amino acids. Most students (eight pairs) illustrated their ideas using simplistic diagrams explaining the lock-and-key mechanism (e.g., Figure 6.3). These diagrams emphasised that the shape of the substrate needed to match that of the enzyme for the reaction to occur. Students also explained that enzyme reactions are very fast due to enzymes providing alternative pathways to reduce the energy required for the reaction. However, students were unable to explain precisely what the enzymes looked like or how they provided these alternative reaction pathways.

Figure 6.3

An Example of Students' Illustrations of an Enzyme-Substrate Reaction Before IVR



In protein IVR, students were surprised by the intricate enzyme structure, making remarks like "*Whoa, this thing is massive*". The structure starkly contrasted with their expectations from simple 2D diagrams. When prompted to orient the substrate molecule at the entrance of the enzyme, students initially stood outside the massive enzyme structure and attempted to orient the substrate molecule based on the most salient features. Five pairs focused on the shape of the passageway, intuitively applying the lock-and-key concept to push the substrate through and test the best fit. Three pairs recognised the red (electron-rich) regions at the entrance and oriented the substrate with its blue (electron-poor) end facing those red regions. The remaining two pairs observed that inside the enzyme was mostly red (electron-rich). They initially oriented the substrate molecule with its blue (electron-poor) end entering the passageway first. Despite these initial differences, by looking at the complex enzyme structure, all student pairs recognised the importance of exploring the structure from different perspectives. During the interaction, students changed positions frequently to explore additional ideas. In addition, when encountering the resistance of the substrate at the entrance, students intuitively adjusted the angle of the molecule or tried different orientations.

In terms of their collaboration, students worked closely to complete the task. The students perceived the task as one requiring the consideration of multiple concepts before settling on a solution. Among strangers, the unequal relations exhibited when exploring water molecules disappeared. These students took turns manipulating the substrate, freely shared and elaborated on ideas, and negotiated to reach a consensus. Pairs who were friends also maintained their collaborative dynamics.

The case of Noah and Jesse interacting with conceptually unfamiliar virtual objects. Before IVR, both students had heard about enzyme-substrate reactions. They described enzymes as entities that speed up reactions in biological systems by providing alternative pathways in which a lower amount of energy is required for those reactions to proceed. However, the students could not elaborate on this process further. In addition, both students exhibited uncertainty regarding the actual structure of enzymes. Jesse described an enzyme as "*a bunch of amino acids together*" while Noah described it as "*a long chain of amino acids*".

Inside IVR, both students were surprised when they first saw the complex structure of the enzyme. They also appeared unsure of the best way to approach the task. Therefore, they equally contributed to the generation and exploration of ideas, taking turns manipulating molecules, and elaborating on ideas. For example, when determining the best orientation of the substrate at the entrance of the enzyme, Jesse and Noah were at the enzyme entrance, observing the concrete shape of the enzyme passageway. Noah tried to fit the bulky (blue) end of the substrate in the narrow passageway to meet the red areas inside the enzyme, but his attempt was unsuccessful because he did not consider the shape of the passageway (Table 6.2, Turn 1). Jesse, focusing on the shape of the passageway, took over control and tested the fit of the substrate with its skinny (red) end entering the enzyme first (Turn 2). Despite Jesse's attempt being successful, Noah still focused on the (red) appearance of the walls inside the enzyme. Noah flipped the substrate and re-oriented it with the bulky (blue) end entering the passageway first (Turns 3-4). When Jesse emphasised the role of orientation (Turn 5), Noah explained his reasoning integrating his idea of the red regions inside the enzyme and Jesse's idea of the shape of the passageway (Turn 6). This extract shows how students narrated their actions and built on each other's ideas. When ideas diverged, students made efforts to reconcile by elaborating on what they were doing.

The synchronised video shots in Table 6.2 also show that Noah and Jesse frequently changed their positions during the interaction. Looking at the unfamiliar, complex structures of the enzyme and substrate, the students perceived that the task demanded more physical and conceptual exploration and that there could be multiple possibilities. As a result, the students did not settle for simple solutions but, instead, pushed the substrate multiple times to test its fit and explored the virtual environment extensively. These actions allowed the students to identify and integrate different chemistry concepts. For instance, while taking turns testing the fit of the substrate (Turns 1-6), Jesse realised that staying at the entrance limited his perspective. Therefore, he walked into the enzyme to explore more ideas. There, Jesse confirmed Noah's reasoning after observing red regions inside the enzyme (Turns 7-10). Jesse then went back to the entrance and oriented the molecule as originally suggested by Noah.

Table 6.2

An Excerpt of Noah and Jesse's Interaction in Protein IVR

Turn	Speaker	Transcript	Synchronised video shots
1	Noah:	I think like that (orients the bulky end towards the tight-fit part of the passageway) … it kind of fits up there... it said it was like a tight fit. So, maybe like that. Oh, no.	
2	Jesse:	Let's try it this way. (Flips the substrate, pushes it with the skinny end going in first) So that's the only one that actually fits through (pulls the substrate out)	Turn 2: Jesse (black T-shirt) pushes the substrate with the skinny end entering first
		[...]	
3	Jesse:	Can you move this?	
4	Noah:	(Flips the substrate; moves the bulky end to enter the enzyme first)	
5	Jesse:	It needs to be at a particular angle. Ok?	
6	Noah:	(Drops the molecule) It has to be on a certain angle in order to attract like for the blue to attract the red kind of thing to be like kind of pulled in (Looks at Jesse).	Turn 4: Noah takes control; flips and orients the substrate with the bulky end going in first
7	Jesse:	um, and inside there's (ducks and walks into the reaction site) … a lot of red	
8	Noah:	A lot of red, yeah. So, I think the blue has to go in first and I think the angle just has to …	
9	Jesse:	(Walks back to the entrance)	Turn 7: Jesse ducks and walks to experience the journey of the substrate
10	Jesse:	(orients substrate with the bulky, blue end entering first) ... it looks like it will slot in (lowers his body to peep inside the enzyme). […]	

Note. Video shots: Bottom left = Noah's view (grey T-shit); Bottom right = Jesse's view (black T-shirt)

6.6. Discussion

In this study, we investigated how different learning tasks in different IVR contexts influenced students' collaborative interactions to learn abstract chemistry concepts. Our findings showed that students actively interacted with 3D objects in IVR to change their conceptual understanding. However, students' perceptions of the conceptual complexity of virtual objects prompted different physical, conceptual, and collaborative engagements while completing learning tasks in each IVR context.

Influence of the Nature of Learning Tasks on Students' Collaborative Interactions in IVR

In the IVR environment involving virtual objects that were conceptually familiar (water molecules), students perceived learning tasks as simple and engaged in short conceptual discussions and limited physical navigation. In contrast, when students encountered conceptually unfamiliar chemical structures (complex protein enzyme) in IVR, they recognised that there was no alternative way to explore such an object. Therefore, they engaged in exploratory embodied movements to fully appreciate the complex 3D structure. These findings were interesting considering that the molecular structures and their electron densities were represented similarly, and the target conceptual ideas were similar across the IVR learning activities. To form hydrogen bonds between water molecules, students needed to consider the composition and 3D shapes of water molecules, the attraction between oppositely charged (red and blue) areas, the role of lone pairs, and the distance and orientation between molecules. Similar considerations were needed to figure out the optimal orientation of the substrate molecule at the entrance of the enzyme. Based on our initial assessment, however, we expected that students would explore the virtual environment more actively for the water molecules task because, without moving around and bending their knees in and out, they could not effectively evaluate the impact of orientation and the distance between water molecules and complete the task. On the other hand, less movement was anticipated for the substrate molecule orientation task; to complete the task, students could rely only on the features at the entrance of the enzyme – electron density and shape of the entrance – without necessarily walking around. Yet, because the enzyme molecule appeared conceptually unfamiliar, students felt that the learning tasks in protein IVR demanded different problem-solving skills compared to water molecules. The students were compelled to explore the enzyme environment and collaborate extensively.

Findings from the current study remind us that utilising and evaluating the educational affordances of IVR needs to coincide with the careful design of the learning activities. Indeed, there have been several calls to carefully utilise the unique affordances of IVR to support learning (e.g., Dalgarno & Lee, 2010; Mikropoulos & Natsis, 2011). However, common IVR applications for science learning presented concepts (e.g., shapes of molecules as in Brown et al., 2021; Edwards et al., 2019; Fujiwara et al., 2020) that are easily accessible through existing media. These applications did not effectively utilise the unique value of IVR for 3D visualisation, but research studies tended to evaluate the educational benefits of IVR based on such IVR applications. Our findings in terms of the limited nature of students' interactions while exploring such simple and conceptually familiar objects in IVR could potentially explain why IVR was not superior to alternative media in terms of students' learning (e.g., Brown et al., 2021). To encourage students' exploratory interactions with concepts in IVR, interactive objects need to highlight the benefit of 3D visualisation in IVR which cannot otherwise be achieved.

Regarding students' social dynamics, previous studies have emphasised the influence of group composition on students' collaborative learning behaviours (e.g., Janssen et al., 2009; Ungu et al., 2023; Webb, 1991; Webb et al., 1998). For instance, students tend to be less critical of contributions made by unfamiliar peers (Janssen et al., 2009) and adopt expert-novice relations when they perceive a big gap in their abilities (Webb, 1991). Students also relied more on the information provided by their collaborators when they perceived these peers as more competent (Andrews & Rapp, 2014). Our findings in the present study were consistent with these observations but only when students explored conceptually familiar objects in IVR (e.g., two water molecules in snowflake IVR). When students encountered complex, unfamiliar structures in IVR (e.g., the entrance of enzyme in protein IVR), students perceived learning tasks as complex and prior unbalanced relations were modified.

Our findings suggest that, in IVR, the design of virtual objects and learning tasks influences students' tendencies to collaborate with peers. Therefore, to encourage students' collaborative interactions in IVR, learning tasks need to be designed so that the solutions are not so simple for individual students to accomplish without input from peers. This conclusion resonates with prior research on the impact of task design on students' collaborative interactions (e.g., Chizhik, 2001;

Cohen, 1994; Esmonde, 2009; Kirschner et al., 2004). Generally, tasks that no single individual feels sufficiently equipped to complete successfully alone elicit more student interactions than tasks that appear manageable to individuals (Care et al., 2015; Cohen et al., 1999; Scager et al., 2016). Even unfamiliar peers are forced to share resources, utilise each other's ideas, and facilitate each other's efforts (Cohen et al., 1999).

Affordances of Collaborative IVR for Learning Chemistry Concepts

The designed IVR environments showed concrete structures of molecules, such as the protein enzyme, and challenged students' imagination of the structures. In addition, the interactivity and embodied interactions with virtual objects supported by IVR gave students a sense of control over their learning and enhanced their comprehension of the target concepts (Johnson-Glenberg, 2018). By testing possibilities and observing consequences, students modified their conceptions of molecular interactions—for example, hydrogen bond formation in relation to orientation and distance of molecules; and influence of molecular structure and electron density in enzyme-substrate reactions. Moreover, the collaborative design allowed students to negotiate ideas and complement each other's spatial and conceptual perspectives. Our study lends support to research that suggests that interactive and collaborative IVR helps students visualise abstract science concepts and actively construct knowledge (Chen, 2010; Johnson-Glenberg, 2018; Matovu, Won, Treagust, Ungu, et al., 2023; Salzman et al., 1999).

6.7. Theoretical Contribution and Limitations of This Study

The present study showcases the unique capacity of IVR to engage students in exploring, problem-solving, and comprehending the complex 3D nature of chemical interactions, such as hydrogen bonds and enzyme-substrate reactions. Students were able to interact with otherwise abstract chemistry ideas in concrete forms to test their ideas and learn. In addition, most studies rely on pre-and post-tests to demonstrate the value of IVR, report individual students' experiences with IVR (e.g., Lui et al., 2020), or describe students' collaboration when one is using IVR and the other a 2D platform (e.g., Price et al., 2020; Uz-Bilgin et al., 2020). In contrast, the present study documents students' collaborative interactions and meaning-making processes when both students are present in the same IVR learning environment. In essence, the study highlights a paradigm shift in the conceptualisation and application of IVR in education, positioning it as a transformative medium to support collaborative learning experiences. Importantly, the study demonstrates the need for carefully crafted learning tasks in collaborative IVR contexts. The study, therefore, provides insights into how IVR-based learning tasks can be leveraged to promote collaborative learning interactions. At the same time, the study also demonstrates the importance of using synchronised videos and multimodal transcripts in analysing such students' interactions. Future studies may wish to adopt a similar approach to analyse students' interactions.

Nevertheless, the study suffered from some limitations. Firstly, this research study was conducted in a very specific educational context (undergraduate chemistry) which may limit the generalisability of the findings. Educators may want to further explore students' collaborative interactions in IVR in other educational contexts and with different learning content.

Secondly, students in the present study completed three IVR activities, starting with the snowflake IVR and ending with protein IVR. The students might have become more comfortable exploring virtual spaces and interacting with peers as they reached the last IVR activity (protein IVR). This familiarity with peers and the IVR environments can be a confounding variable in understanding the role of the complexity of virtual objects in students' interactions. Future studies may wish to change the order of the learning activities to isolate the effects of familiarity and complexity of virtual objects. This interplay of the nature of IVR context, perceived task complexity, and familiarity with IVR in our study highlights the complexity of analysing students' collaborative interactions in IVR.

In addition, the study reported here did not investigate how the nature of molecular representations used in IVR influenced students' interactions and learning. Chemical representations can vary in many ways, for example in terms of what molecular entities, properties, or attributes are represented, and what qualitative or quantitative information can be inferred (Talanquer, 2022). The molecular representations used in our IVR applications highlighted the particulate and electronic aspects of molecules, with emphasis on molecular size and shape, and electron densities. Changing the nature of representations to highlight different aspects might influence how students interact with, reason about, and make meaning from the representations (Talanquer, 2022). The present study, thus, paves the way for future researchers who may wish to investigate how different molecular representations could influence students' interactions and learning.

Furthermore, the present study did not thoroughly delve into the conceptual benefits and limitations of IVR. These aspects have been addressed in separate manuscripts. For instance, a prior study from our research team found that IVR helped most of the students to recognise the intermolecular nature of hydrogen bonds, the role of lone pairs of electrons in forming hydrogen bonds, and the 3D nature of hydrogen bonds (Authors, 2023b). However, a future study showing the direct relationship between students' collaborative interactions in IVR, and their pre-/post-test scores could offer further insights into the specific interactions that fostered distinct kinds of learning.

6.8. Conclusions

In this study, we designed multiple chemistry learning activities in IVR and investigated how students' perceptions of the complexity of learning tasks in different IVR contexts influenced their collaborative interactions. Utilising 3D visualisation, interactivity, embodied movements, and collaboration features of IVR helped students construct new understandings of molecular interactions. However, students' engagement in physical, conceptual, and collaborative exploration differed depending on the perceived complexity of virtual objects. This study shows that, although IVR programs for learning are designed with similar design features (such as interactivity, embodied movements, or collaboration), not all tasks can optimise collaborative interactions from learners. Only the tasks that highlighted the unique value of 3D visualisation in IVR – embodied exploration of complex 3D structures – prompted extensive interactions from students. To realise the educational benefits of IVR for science learning, educators need to pay careful attention to the design of interactive tasks in IVR.

Chapter 7. Discussion and Conclusion

The rapid development and adoption of IVR technology across various educational domains make it imperative to systematically explore when and how IVR can benefit learning. The aim of this thesis was to critically evaluate students' learning of molecular structures and interactions in collaborative IVR environments. These concepts are often challenging to learn because they require students to construct and manipulate mental images of molecules interacting in 3D. Since evaluating the educational benefit of a new learning medium such as IVR is a complex issue, four research questions were established, each addressed in one of four studies. Study 1 explored the current landscape of IVR utilisation in science education settings. Studies 2 and 3 systematically evaluated the level of students' conceptual understanding of molecular interactions before and after IVR, while Study 4 investigated the nature of students' interactions in different collaborative IVR learning contexts. The research questions addressed were:

- Study 1 – How do researchers design, implement, and evaluate IVR for science learning?
- Study 2 – What is the level of students' conceptual understanding of hydrogen bonds in snowflakes before a collaborative IVR experience?
- Study 3 – How does students' conceptual understanding of hydrogen bonds and the shape of snowflakes change after a collaborative IVR experience?
- Study 4 – How do students interact to learn hydrogen bonds and enzyme-substrate reactions in different collaborative IVR contexts?

The first section of this chapter summarises and discusses the findings from the four studies that answered each of the above research questions (Section 7.1). Then, an integrated discussion of all the studies (Section 7.2), and the implications of the findings for IVR designers, science educators and researchers (Section 7.3) are presented. The last sections present the limitations of the research in this thesis (Section 7.4) and conclude the research (Section 7.5).

7.1. Addressing the Four Research Questions

The Design, Implementation, and Evaluation of IVR for Science Learning

Research question 1, addressed in Study 1 (Chapter 3), emerged from an initial examination of the literature on the use of IVR in science education settings. Science educators utilised various types of IVR hardware, but it was unclear which design features were considered most compelling to achieve which learning goals. The existing literature review studies also evaluated IVR applications as if they were equivalent without any differentiation about their affordances or limitations (e.g., Di Natale et al., 2020; Radianti et al., 2020; Wu, Yu, et al., 2020). In addition, the evaluation of IVR-based learning in relation to conceptual understanding was not comprehensive, leaving doubts about the conceptual benefits of IVR. Moreover, most IVR applications were designed for individual students and the benefit of collaboration in IVR was largely unexplored.

To systematically identify trends and gaps in IVR design, implementation, and evaluation in science learning settings, a systematic literature review was conducted, covering 64 empirical studies published in the period 2016 to 2020. To evaluate the design of IVR applications, this research expanded upon the sensory, actional, narrative and social design considerations suggested by Dede and colleagues (2009; 2017). Ten concrete IVR design features were identified and evaluated – visual, audio, haptics, embodied actions, interactivity, virtual body, challenge, storyline, context, and social.

The systematic review revealed that science educators were making efforts to explore the educational benefits of IVR. Educators mainly adopted IVR to support students in visualising abstract concepts and to enhance learning experiences, but often integrated IVR features inconsistently; different designs were used to achieve similar learning objectives. IVR designs mostly integrated technological features (visual, audio, and interactivity), irrespective of the learning goal (Figure 3.2). Narrative and social design features were often underutilised; most IVR programs lacked relevant contexts and challenges and were designed for individual learners rather than peer collaboration. Won et al. (2023) also found visual, audio, and interactivity as the most readily adopted features in educational IVR designs, as well as variations in pedagogical approaches for achieving similar learning outcomes. These findings highlighted the need for educators and IVR designers to carefully consider IVR design features in relation to the target educational goals. In particular, the role of task design and collaborative learning in IVR needed to be explored more.

The review also identified that most IVR studies (43 out of 64) evaluated declarative knowledge irrespective of the target learning objectives (Table 3.4). In addition, the main assessment tool was multiple-choice or short-answer questions in pre-/post-tests, and the outcomes were mixed. Educators often use these tools because they are convenient for large-scale testing, but the tests are limited in terms of the level of conceptual understanding they assess (Martinez, 1999; Treagust, 1988). Conceptual understanding demands students to apply chemistry knowledge to novel situations, demonstrate critical thinking and reasoning, and translate freely across scales and representations (Holme et al., 2015; Nurrenbern & Robinson, 1998). Therefore, the systematic review revealed the need for IVR studies to employ strategies that would investigate at a deeper level students' knowledge structures.

Another trend observed in the literature was that students generally rated IVR highly on motivation and engagement (Table 3.5). However, this feedback was often based on one-time opportunities with IVR and self-report assessments, such as interviews, making it challenging to draw conclusions about the value of IVR. With one-time opportunities, students tend to rate novel technologies positively or exert more effort in learning (Clark, 1983; Clark, 2012). At the same time, some students who are unused to the tool may feel uncomfortable and may need more time to familiarise themselves with it (Hamilton et al., 2021; Han et al., 2022). In addition, although self-report evaluations illuminate participants' experiences of IVR-based learning, participants may rate learning experiences positively to appease researchers (Grimm, 2010). Consequently, an alternative way to evaluate students' learning experiences in IVR was necessary, such as documenting participants' interactions in varied IVR contexts, rather than solely relying on self-report measures and one-time experiences.

In summary, the comprehensive and systematic review of the literature involved in addressing research question 1 generated insights into how IVR was being employed and evaluated in science learning settings. It also provided the rationale for a more systematic investigation of what and how students learn in collaborative IVR learning environments.

Students' Conceptual Understanding of Hydrogen Bonds in Snowflakes Before Collaborative IVR Experiences

The mixed learning outcomes in IVR studies identified in the systematic review of the existing IVR studies (Section 3.5) made it hard to draw conclusions about the conceptual benefits of IVR. Therefore, research questions 2 and 3 were established to evaluate the conceptual benefits of IVR. Research question 2, addressed in Study 2 (Chapter 4), aimed at uncovering students' understanding of the hydrogen bonds in snowflakes before engaging in collaborative IVR activities. Diagram-drawing tasks accompanied by staged prompts were used to elicit students' ideas of hydrogen bonds in snowflakes and were triangulated with students' verbal explanations and gestures.

Study 2 revealed that, although most students were well acquainted with the structure of water molecules, they had alternative conceptions about the nature of molecular interactions (hydrogen bonds) in snowflakes (see Table 4.1). Some students were unsure of polarity in water molecules, the intermolecular nature of hydrogen bonds, the role of lone pairs of electrons in forming hydrogen bonds, or the 3D nature of hydrogen bonds. Only five out of 60 students explained or illustrated molecules interacting in 3D. These alternative conceptions confirmed that students indeed had difficulties in visualising the 3D molecular structures and interactions (hydrogen bonds) in snowflakes, consistent with previous studies (e.g., Wu et al., 2001; Wu & Shah, 2004).

The students' alternative conceptions of hydrogen bonds revealed in this study, such as uncertainty about the role of lone pairs of electrons, had gone unnoticed in previous literature on the topic (e.g., Cooper et al., 2015; Schmidt et al., 2009). This inclusion is likely because the unique prompts used in this study encouraged students to imagine and visualise molecular interactions without being constrained by their knowledge of complex chemical vocabulary. In contrast, other studies used terms like "intermolecular forces" or "hydrogen bonds" in their prompts. Such key terms can be misinterpreted by students, for example, a hydrogen bond as a chemical bond involving a hydrogen atom (e.g., Cooper et al., 2015). Moreover, the drawing task in this study also required students to illustrate the formation of hydrogen bonds in the context of many molecules, unlike in previous studies where students were required to represent only up to three molecules interacting (Williams et al., 2015). This unique challenge compelled students to consider the role of lone pairs of electrons and interactions in 3D.

Study 2 also demonstrated that, with the right prompts, students' conceptual understanding can effectively be assessed through student-generated diagrams. This approach aligns with previous research (e.g., Ainsworth et al., 2011; McLure et al., 2021b) which highlighted the value of diagram-drawing tasks in challenging students to visualise abstract science concepts, retrieve and link prior knowledge, and express their understanding in a novel way. Furthermore, this study nullified concerns that some researchers (e.g., Becker et al., 2016; Ehrlén, 2009) have about using 2D diagrams for investigating students' understanding. Ehrlén (2009) suggested that students might inconsistently rely on sociocultural resources when representing their understanding, while Becker et al. (2016) argued that interpreting students' understanding might be most effective when combined with other forms of communication, such as verbal explanations. In this study, the student-generated diagrams effectively captured students' understanding, as confirmed by their verbal explanations. Besides, 3D aspects are equally hard to represent through alternative modes, such as verbal or written explanations.

Overall, addressing research question 2 in Study 2 revealed the level of students' conceptual understanding of hydrogen bonds before IVR-based learning. A closer inspection of the change in students' conceptual understanding of hydrogen bonds after IVR was then conducted in the subsequent study.

Change in Students' Understanding of Hydrogen Bonds and the Shape of Snowflakes Through Collaborative IVR

Research question 3, addressed in Study 3 (Chapter 5), aimed to evaluate how a collaborative IVR experience impacted students' conceptual understanding of hydrogen bonds in snowflakes and the shape of snowflakes. In pairs, students completed multiple interactive tasks involving water molecules in Snowflakes IVR. Student-generated diagrams, gestures, and verbal explanations regarding hydrogen bonds and shapes of snowflakes before and after collaborative IVR were analysed to assess students' understanding.

Prior to the collaborative IVR experience, most students had difficulties comprehending hydrogen bonds and visualising 3D molecular interactions in snowflakes, as confirmed by the variety of their alternative conceptions identified in Study 2 (Section 4.5). In addition, most students were uncertain of the explanation of the shape of snowflakes while others reasoned that one water molecule connected to six others in a flat plane to form a flat shape with six branches (Table 5.8). This tendency to rely on surface features and heuristics rather than mechanistic reasoning to explain macroscopic phenomena is a common occurrence in science learning (Cooper et al., 2013; Talanquer, 2018).

Through the collaborative Snowflakes IVR experience, most students significantly improved their understanding of hydrogen bonds. After IVR, most students explained the intermolecular nature of hydrogen bonds, the role of a lone pair of electrons on the oxygen in hydrogen bonds, and hydrogen bonds as interactions in 3D space (Table 5.3). Furthermore, most students presented more scientific explanations of the intricate shapes of snowflakes after the collaborative

IVR experience (Section 5.8). For instance, none of the students mentioned molecules interacting in a flat plane to form snowflakes; instead, they incorporated ideas such as hydrogen bonding, tetrahedral units, 3D lattices, hexagonal patterns, or environmental conditions to explain the shape of snowflakes (Table 5.8). These results substantiated prior claims that collaborative and interactive IVR aids students in visualising abstract molecular interactions and enhances their conceptual understanding (e.g., Kozhevnikov et al., 2013; Salzman et al., 1999; Wu, Yu, et al., 2020). Importantly, by supporting students in developing a coherent explanation of snowflakes shapes, IVR helped students overcome the challenge of accumulating fragmented concepts, another prevalent concern in science education (Gilbert, 2006).

From Study 3, it was also observed that a very small number (four out of 10) of students who initially had difficulties with basic concepts such as the shape of a water molecule, or the intermolecular nature of interactions before IVR retained their prior conceptions. A small number of students were also not able to provide coherent explanations of snowflakes after IVR. Perhaps some of these students found it difficult to reconcile the new knowledge with their existing knowledge structures (Taber, 2017). Prior research also suggested that improving students' understanding can be a gradual process (Dickson et al., 2016; Treagust & Duit, 2008); some students can retain alternative conceptions even after explicit teaching (Dickson et al., 2016; Rushton et al., 2008). However, low prior knowledge students may benefit from carefully designed tasks to orient them to the target concepts before the collaborative IVR tasks (Wu, Hu, et al., 2020; Zambrano et al., 2019).

In sum, most students improved their understanding of hydrogen bonds in snowflakes and the shape of snowflakes through collaborative IVR-based learning. The findings suggested that by carefully utilising the features of IVR, such as 3D visualisation, interactivity, and collaboration as we did in this research, students' conceptual understanding of abstract concepts can be improved. However, a systematic exploration of how students construct knowledge in IVR was imperative to avoid misinterpreting the findings based on pre-/post-tests or speculating how IVR was used.

Students' Interactions to Learn Molecular Concepts in Different IVR Contexts

The systematic literature review (Study 1 in Chapter 3) revealed a lack of comprehensive documentation of students' learning processes in IVR. Therefore, research question 4, addressed in study 4 (Chapter 6) was established aiming to provide insights into the interaction process that underpins learning in IVR. Study 4 documented students' multimodal interactions in two distinct collaborative IVR contexts, one featuring conceptually familiar objects (water molecules in snowflakes IVR) and the other with conceptually unfamiliar objects (enzyme and substrate molecules in protein IVR).

Study 4 found that, within IVR, students actively manipulated virtual objects (familiar or unfamiliar) to observe them and inspect the outcomes of different orientations as they brainstormed ideas with peers. For instance, students experimented with various angles and distances between water molecules to understand the formation of hydrogen bonds (Table 6.1). Similarly, they pushed the substrate molecule through the enzyme passageway multiple times to explore the optimal orientation in terms of molecular shape and polarity of the enzyme and substrate (Table 6.2). Based on the constructivist perspective, emphasising active engagement with the environment as a fundamental aspect of knowledge construction (Chen, 2010; Jonassen, 1994), these active interactions contributed to the students' enhanced conceptual understanding of chemistry topics. For example, students' understanding of the nature of hydrogen bonds and their impact on the shape of snowflakes improved through the snowflakes IVR experience (Section 5.4 in Chapter 5). Other researchers also contend that such meaningful interactions with virtual objects in IVR can lead to improved conceptual understanding through embodied cognition (Johnson-Glenberg, 2019).

The study also revealed that the nature of students' physical, conceptual, and social interactions in IVR varied depending on the learning context. When students interacted with conceptually familiar objects (water molecules in snowflakes IVR), they perceived the concepts as a simple extension of their prior knowledge and engaged in limited physical, social, and conceptual explorations within the virtual environment. In contrast, when students encountered conceptually unfamiliar objects in the protein IVR environment, they recognised the necessity for extensive embodied exploration to comprehend these complex objects. The limited engagement of students when exploring water molecules in IVR observed could potentially explain why IVR did not always result in superior learning outcomes as observed in Table 3.4 (Chapter 3). Common IVR applications for learning chemistry often display simple molecules with which students are conceptually familiar and can easily be explored using alternative media like ball-and-stick models (e.g., Brown et al., 2021; Edwards et al., 2019; Fujiwara et al., 2020). In contrast, Study 4 employed IVR to support the exploration of complex objects (enzyme and substrate structures) that could not easily be explored through alternative media. Therefore, this study highlighted the unique benefit of IVR for embodied exploration of complex 3D concepts. Previous scholars have also consistently urged educators to carefully utilise the unique affordances of new technologies when designing learning tasks (Dalgarno & Lee, 2010; Mikropoulos & Natsis, 2011).

Distinct patterns were also observed in terms of the social dynamics the students exhibited in the different IVR contexts (Section 6.5). Students extended their real-world social dynamics when dealing with the conceptually familiar objects in snowflakes IVR. Among strangers the relations were unbalanced and, in each pair, the student with higher perceived prior knowledge dominated the interaction. This finding was consistent with previous studies on the influence of perceived "status" within the group on students' interactions; "more" knowledgeable peers often dominate collaborative interactions resulting in leader-follower dynamics (Cohen, 1994; Webb, 1982). However, in the IVR context with conceptually unfamiliar objects (complex enzyme and substrate molecules in protein IVR), previous power relations among strangers were modified (Section 6.5). Students perceived the learning tasks as novel and complex. Consequently, irrespective of their prior relations, students collaborated extensively, building on each other's ideas, and contributing equally to the manipulation of objects and idea generation. The finding aligns with the notion that complex tasks whose demands exceed individual students' capabilities tend to compel students to collaborate and leverage each other's skills (Care et al., 2015; Cohen, 1994).

7.2. Investigating the Potential of IVR for Enhancing Science Learning

This thesis aimed to critically evaluate students' learning of abstract science concepts – molecular structures and interactions – using collaborative IVR. The research in Study 1 (Chapter 3) set the stage for this research by examining trends and gaps in current IVR studies for science learning. Analysis of existent literature showed that science educators recognise the value of IVR in learning for achieving various learning objectives, such as supporting students' visualisation of abstract concepts, enhancing students' learning experiences, or training practical skills. However, various designs of IVR applications for science learning exist, potentially because IVR has only become more accessible recently and educators are still exploring its educational possibilities with various priorities (Won et al., 2023).

As one of the efforts to guide educators in designing IVR applications to achieve these goals, this thesis expanded Dede's (2009; 2017) framework of sensory, actional, narrative, and social IVR design considerations and identified a set of 10 design features that educators may consider in designing IVR applications (Table 3.2 in Chapter 3). Importantly, the research in this thesis demonstrated how these IVR design features of IVR may be used and how IVR-based learning may be evaluated in practice. With a focus on improving students' visualisation and conceptual understanding of abstract chemistry topics (molecular structures and interactions), three interactive and collaborative IVR applications were designed and empirically evaluated (Studies 2-4 in Chapters 4-6). The findings from Studies 2 and 3 (Chapters 4 and 5) combined showed that collaborative IVR applications helped students transition from non-scientific conceptions to a more coherent and scientific understanding of molecular interactions (hydrogen bonds in snowflakes).

The positive conceptual outcomes of IVR can be attributed to the deliberate integration of not just the technological features but also theory-driven pedagogical aspects (task design and social interactions) in the designs of the IVR applications used in this research. Many previous scholars also argued that moving away from the technocentric approach of designing learning media would allow educators to design productive and meaningful learning experiences (Fowler, 2015; Kirschner et al., 2004). Mayes and Fowler (1999), for example, argue that technology designs can promote conceptual learning if educators deliberately consider learning in three phases: conceptualisation, construction, and dialogue. For learners to attain an advanced conceptual understanding, concepts should be presented in a manner that allows the exploration of different possibilities enabling conceptualisation. Learners should also be given opportunities to activate and apply these concepts through such actions as problem-solving to facilitate knowledge construction. In addition, learning technologies should encourage learners to integrate their conceptual learning into a social context through collaborative interactions and dialogue (Fowler, 2015; Mayes & Fowler, 1999).

In many other studies, pedagogical considerations are often not given enough attention. For example, reviews of literature on the educational applications of desktop VR technologies showed that pedagogical considerations were not always evident in the ways that these technologies were designed, implemented, and evaluated (Fowler, 2015; Mikropoulos & Natsis, 2011). With more advanced technology, such as IVR, similar trends can also be observed. For instance, educators often consider only sensory and actional features – such as representational fidelity (environment, user, objects, audio and haptics) and user interaction (e.g., embodied actions, navigation, object manipulation) – as the key features of IVR (e.g., Lui et al., 2023; Makransky & Petersen, 2021). The analysis of the design features integrated in current IVR applications in Study 1 also showed that science educators mainly integrated 3D visuals and interactivity features, with a limited focus on content/task design considerations or collaborative learning (Figure 3.2 in Chapter 3). Moreover, about half of the studies reviewed in this thesis did not explicitly mention the pedagogical frameworks guiding the designs, implementation, or evaluation of IVR in science learning (Section 3.5).

When designing the IVR applications following pedagogical and technological considerations, we expected that students would recognise the benefit of IVR as we intended, for example, by interrogating their ideas through active manipulation of objects and sharing ideas with peers. The analyses of students' learning outcomes (Studies 2 and 3) and interactions in IVR showed that most students realised the unique learning experiences provided by IVR. In addition, Study 4 found that, within IVR environments, many students explored 3D spatial patterns and features in molecules, interacted with the molecular structures in an embodied way to test and revise their ideas, and engaged in social interactions to co-construct knowledge (Section 6.5 in Chapter 6). These findings demonstrated that carefully utilising the possibilities of IVR (e.g., 3D visualisation, interactivity), and pedagogical considerations (e.g., problem-solving tasks and collaboration) can indeed provide students with opportunities to construct conceptual understanding.

However, there were also complexities and variations in terms of students' interactions, knowledge-co-construction, and learning. As discussed in Study 4 (Section 6.5), students in this research engaged in limited physical, conceptual, and social explorations when they perceived learning objects as conceptually familiar and the learning tasks as simple. Yet, when they encountered objects that could not easily be explored through alternative means (protein enzyme and substrate), the students recognised the benefit of IVR and engaged in extensive exploration and collaboration (Section 6.5). In addition, Study 3 showed that a small number of students did not gain significant learning benefits after experiencing IVR. These complexities demonstrated that achieving superior learning outcomes does not come from simply asking students to wear IVR headsets. For students to engage in intentional and extensive interactions as may be desired by educators, the perceived benefit of IVR must be clear to the students (Study 4). In addition, the methods used to evaluate students' learning in IVR need to be carefully considered. Investigating students' learning processes in IVR may reveal insights that may not be obvious by simply looking at pre-/post-test scores, such as the influence of task design on students' learning as discussed in Study 4.

Taken together, although this thesis demonstrates benefits of using IVR for learning abstract science concepts, it also demonstrates that effectively designing and evaluating IVR is not a trivial matter. For instance, in this research, analysing students' learning interactions in IVR was not straightforward. Due to the paucity in the literature on students' dynamic and collaborative interactions in IVR, several analytical frameworks were explored but many could not successfully capture the complexity of students' interactions in collaborative IVR settings. However, the use of multimodal transcripts (Walkington et al., 2023) created from the synchronised videos of students' interactions during IVR (Section 6.4) proved an invaluable approach. As elaborated in Sections 6.4 and 6.5, these transcripts allowed students' interactions to be tracked on a moment-by-moment basis. In future, educators and researchers may want to combine this approach with more objective methods, such as eye-tracking (Clay et al., 2019; Shadiev & Li, 2023), to better monitor students' attention and learning behaviours while in IVR.

This research work also demonstrates that it takes significant skills to explore at a deeper level what students learn from IVR. Common approaches to evaluating students' learning in IVR using multiple-choice or short-answer questions often failed to demonstrate the benefit of IVR for learning science concepts (Study 1). In contrast, the findings in studies 2 and 3 validated prior claims that asking students to express what they have learnt from IVR through student-generated representations, such as diagrams, is a valuable approach in investigating students' learning benefits (e.g., Ainsworth et al., 2011; Ainsworth & Scheiter, 2021; McLure et al., 2021b). In this research, prompting students to illustrate their understanding through diagrams, verbal explanations, and gestures before and after IVR allowed us to thematically establish the different ways in which students imagined molecular structures and interactions (Sections 4.5 and 5.5). However, these findings need to be treated with some caution. Gilbert and Watts (1983) argue that the ideas displayed by students when they are interrogated may change depending on the nature of the activities in which they are engaged or the social context of the investigation. Therefore, the students' alternative conceptions documented in this thesis may not be static and could change depending on the prompts given (Kuiper, 1994). Despite their potentially tentative nature, these students' ideas were important as they revealed some of the ways students imagined molecular interactions in the context of many molecules. Understanding such students' explanatory frameworks of how the world works guides educators' efforts when designing strategies to support students' learning more effectively (Libarkin & Kurdziel, 2001).

It is also crucial to acknowledge the existing barriers to diversity and inclusion in the integration of IVR in education. For example, many science teachers still struggle to imagine how they could design or integrate IVR in their classrooms (Bower et al., 2020). Therefore, sufficient training needs to be provided to teachers before they can implement this innovative technology in their classes. Limited resources, especially in low-socioeconomic-status institutions also limit many students' access to IVR's transformative impact (Richter et al., 2023; Rojas-Sánchez et al., 2023). For example, the high financial and technical costs associated with sophisticated (interactive and collaborative) IVR applications and high-end equipment, such as those used in this research, pose a significant hindrance (Won et al., 2023). Although more affordable alternatives, such as mobile-phone-based IVR headsets or stand-alone headsets (e.g., Meta Quest 3) exist, they have limited processing power and may not support complex IVR interactions (Angelov et al., 2020) like those employed in this research. Such disparities in accessibility to IVR may exacerbate the educational divide between privileged and underprivileged students. As the IVR industry continues to evolve, collaborative efforts amongst stakeholders in the educational technology sector (e.g., designers, researchers, and educators) may help to bridge such gaps in access to IVR.

7.3. Implications of This Research

This thesis started off by elaborating on the challenges students often have in learning chemistry concepts. The findings in study 2 (Section 4.5) confirmed that students had difficulties visualising 3D molecular interactions before exploring the concepts in collaborative IVR. For example, many students reasoned about molecules without clear consideration of orientations and angles in 3D. In addition, if students had any mental image of enzyme-substrate reactions, it was in the form of a simple lock-and-key model (Figure 6.3). However, after using collaborative IVR, students appreciated the 3D nature of molecular interactions and provided coherent explanations of molecular phenomena (Section 5.4). Taken together, these findings highlight the need for teachers to emphasise the 3D nature of molecular interactions when teaching chemistry. The findings also underscore the benefit of using 3D visualisation technologies, such as collaborative IVR, for supporting students' visualisation of abstract chemistry concepts.

This research found that some science educators already recognise the value of 3D visualisation in IVR for supporting students' learning, but there are inconsistencies in IVR design approaches for achieving similar learning objectives (Section 3.5). To optimise the learning benefits of IVR, it is essential to align key features of IVR with the rationale for adopting IVR. For instance, this thesis demonstrated that when the focus is on 3D visualisation of abstract concepts, designing interactive virtual objects that clearly demonstrate the benefit of IVR ensures that students make efforts to explore concepts (Section 6.5) and obtain the benefit of IVR (Section 5.4). The expanded IVR design framework comprising the set of 10 concrete features in Study 1 (Section 3.3), or similar versions (e.g., Won et al., 2023), are useful starting points for identifying what features to include in IVR designs to achieve the target learning objectives. Given that educators do not always control IVR application design, collaborative research projects between educators and designers need to be prioritised.

As demonstrated in this thesis (e.g., Section 5.4), carefully designing and evaluating collaborative IVR can enhance students' understanding of abstract chemistry topics. Therefore, exploration of the educational potential of IVR for learning other science topics is a worthwhile endeavour. However, this research also found that some students with low prior knowledge did not benefit much from IVR (Table 5.3). Several strategies may be explored to support students' learning with IVR. For instance, educators may wish to consider integrating IVR as a part of a teaching-learning schedule that involves orientation, exploration of IVR, and reflection. Orientation activities may help low prior knowledge learners build just enough knowledge to make sense of the molecular features in IVR, while reflection activities could help learners solidify their understanding. For example, reflection by talking to peers helps students reorganise what they have learnt into coherent structures and results in better learning outcomes (Fiorella & Mayer, 2016). There is evidence from the present research that collaborative reflection activities after IVR could enhance students' learning benefits (Section 5.4). When students collaborated to produce shared diagrams in pre- and post-interviews, they improved their understanding more consistently to the highest possible level (category D). In contrast, students who created individual diagrams before and after IVR demonstrated variable conceptual changes (Table 5.3). In addition, designers and educators may wish to experiment with various ways of scaffolding students as they progress through the IVR learning tasks, such as using adaptive prompts, to enhance their learning.

The findings from this research also have implications for the approaches used to evaluate IVR-based learning. The research in Paper 1 revealed a misalignment where many educators assess declarative knowledge regardless of the rationale for adopting IVR, and a reliance on multiple-choice or short-answer questions for evaluating knowledge gains from IVR (Section 3.5). These trends may have contributed to inconsistent findings in IVR studies. Therefore, to achieve the desired learning outcomes, IVR designers and educators need to carefully align the assessments closely with the target learning objectives. In the research in this thesis, student-generated representations provided valuable insights not captured by traditional tests and interviews (Section 4.5). Educators and researchers may want to consider using student-generated representations for assessing students' knowledge of other science concepts learned in IVR.

In investigating students' learning, this thesis demonstrated the benefit of asking students to imagine and illustrate molecular interactions in contexts that involve many molecules. When students are tasked to draw diagrams involving only one or two molecules, they can provide reasonable representations of molecular interactions, even when they have alternative conceptions. However, when challenged to connect many molecules, their true understanding becomes apparent, as was the case in this research (Sections 4.5 and 5.4). In addition, this research showed the benefit of using staged prompts to accompany diagram-drawing tasks. The prompts used in this thesis (Appendix A) were thoughtfully designed to encourage students to imagine molecular structures and interactions. The prompts also helped students to integrate knowledge, without burdening them with complex chemistry terminologies. Researchers and educators may find it valuable to employ similar prompts and diagram-drawing tasks when investigating students' understanding of other concepts. Other scholars have also argued that prompts to scaffold diagram-drawing activities help to increase the correlation between the diagrams and other student-generated representations such as written explanations (Noyes & Cooper, 2019).

Furthermore, this thesis introduced a method for exploring in-depth students' collaborative knowledge-construction process in a shared IVR environment (Section 6.4). The findings based on students' physical, social, and conceptual explorations shed light on how the design of learning tasks influences students' learning. This thesis, therefore, highlights the need for researchers to move beyond pre- and post-tests and investigate the processes of knowledge construction in IVR. More objective approaches, such as eye tracking or motion tracking, could also be applied to monitor students' attention and learning processes in IVR. Such knowledge can be used to help guide the effective design of IVR environments.

By investigating students' knowledge construction processes in IVR, the research in this thesis also generated implications for task design in IVR-based learning (narrative design feature). The findings from this research suggest that collaborative tasks should highlight the benefit of IVR for exploring science concepts and be complex enough so that students realise the need to collaborate with peers (Section 6.5). Complex tasks, like those involving conceptually unfamiliar virtual objects, have been shown to promote peer engagement (Care et al., 2015; Cohen, 1994). However, educators may also want to design tasks with conceptually familiar objects. In such as case, educators, and designers of IVR environments should design tasks that go beyond simple exploration. For instance, the tasks may be designed to involve problem-solving to stimulate students' engagement. In addition, the assignment of roles can also foster interaction and more balanced contributions to collaborative learning tasks (Cohen, 1994). Therefore, educators may also experiment with assigning specific actions for individual students to complete in alternation to encourage individual students' participation in collaborative IVR-based learning tasks.

7.4. Limitations of This Research

The research in this thesis suffered some limitations which could be addressed in future studies. First, the research was conducted in a very specific educational context (undergraduate chemistry) which allowed a thorough investigation of what and how students learn in IVR. While this research generated important insights, the specificity of its context may limit the generalisability of the findings. Therefore, further research in varied educational contexts, such as high school chemistry, with different learning content may provide more knowledge about the educational potential of IVR for learning science concepts.

Secondly, learners were paired to complete all the IVR-based learning sessions and assessment (interview) tasks with their peers. This decision was taken to provide an opportunity for students to construct knowledge together and reflect on their learning by explaining it to each other. However, as discussed in Section 5.4, most students preferred to draw individual diagrams and generate individual explanations, forcing the researcher to adapt the prompts depending on students' preferences. Previous studies indeed highlighted that grouping students does not guarantee spontaneous collaboration (Cohen, 1994; Gijlers & de Jong, 2005; Ungu et al., 2023). The variety of students' collaborative tendencies also made the interpretation of students' learning much more complex than anticipated. Besides, since learners were interviewed in pairs, verbal responses from individual students during the pre-and post-interviews may have influenced those of their peers, either directly or indirectly. Therefore, in future studies, researchers may wish to systematically evaluate students' learning in collaborative or individual interview settings.

In addition, this thesis only investigated the influence of task design on students' collaborative interactions while learning in IVR. Exploring the impact of group composition, such as pairing students with varying levels of prior knowledge, on students' interactions in IVR could yield valuable insights not covered in this thesis. The research needs to be expanded to encompass a broader range of students' characteristics (beyond prior knowledge, such as collaborative tendencies, or gaming experience) and their influence on learning and interactions within collaborative IVR. Furthermore, establishing a direct connection between the learning outcomes obtained by students on pre-/post-tests and their interactions in IVR can provide insights into what kind of learning interactions promoted students' learning in IVR and understanding the underlying concepts. As discussed in Section 6.5, in the snowflake IVR activity, students with "higher" prior knowledge dominated the interaction, while those with lower prior knowledge lacked the confidence to contribute significantly. The unbalanced nature of the interaction may have limited opportunities for the low prior knowledge students to explore their ideas and enhance their conceptual understanding (Cohen, 1994; Webb, 1982). This could explain why some low prior knowledge students did not benefit much from IVR (section 5.4), although this could not be confirmed by the research in this thesis.

When exploring the role of the IVR context in students' interactions in IVR in Study 4, students completed two IVR activities with the same peers before exploring complex virtual objects (enzyme and substrate molecules) in protein IVR. Therefore, there were potential limitations resulting from the way the IVR activities were sequenced. For instance, as students completed more learning activities in IVR, they may have become familiar with learning with their peers in IVR and exploring IVR environments. This familiarity with the IVR environment and with peers may have been a confounding factor in the results presented. Therefore, a comparative study where the order of learning activities is interchanged (simple to complex vs. complex to simple) can help to clearly identify the effects of the nature of virtual objects and familiarity on students' interactions.

Moreover, there were potential limitations stemming from the nature of molecular representations used in IVR in this research. As discussed in Section 6.7, chemical representations may vary in many aspects, including the nature of atomic or molecular components highlighted, molecular attributes emphasised, or the kind of information communicated implicitly or explicitly by the representations (Talanquer, 2022). The chemical representations used in the IVR applications in this research were designed to highlight particulate molecular structures and their electron densities in 3D. These representations also allowed students to touch them, drag them, and explore possibilities. Consequently, the interactions observed among students (Section 6.5) or the learning that they achieved (Section 5.5) may apply only to such forms of chemical representations in IVR. Variations in the representations or the properties of molecules highlighted may influence students' interactions and reasoning with the structures (Talanquer, 2022). Future studies may wish to explore how different forms of molecular representations in IVR influence students' learning and interactions in IVR.

7.5. Conclusion

The integration of IVR technology into teaching and learning holds the promise of enhancing understanding of complex science topics. This thesis aimed to evaluate how students learn challenging chemistry concepts, molecular structures and interactions, using collaborative IVR. This research program commenced with Study 1, a critical and systematic examination of the existing literature regarding the design, implementation, and evaluation of IVR-based learning in the broader context of science education. The review of the literature revealed inconsistencies and, sometimes, misalignments between IVR design choices, the rationales behind its adoption, and the methods employed to assess its effectiveness. This investigation underscored the significance of carefully aligning IVR design with educational goals. It also highlighted the need for a more systematic assessment of the potential of IVR for improving conceptual understanding in terms of learning outcomes and processes.

To systematically investigate what students learn in collaborative IVR, Studies 2 and 3 investigated students' understanding of hydrogen bonds in snowflakes and shapes of snowflakes before and after engaging in collaborative IVR-based learning. Study 2 revealed many alternative conceptions of hydrogen bonds, some of which had not been documented previously. For instance, most students were unsure of the role of lone pairs in forming hydrogen bonds or the 3D nature of these molecular interactions. The subsequent study (Study 3), revealed that a collaborative IVR experience facilitated students' understanding of hydrogen bonds, helping students to change from alternative conceptions to more scientifically accepted conceptual models. The study highlighted that when IVR is carefully designed to leverage its features, such as 3D visualisation, interactivity, embodied movements, and collaboration, students can significantly improve their conceptual understanding of challenging chemistry topics.

The fourth study (Chapter 6) delved into how students interacted in different collaborative IVR contexts to learn hydrogen bonds in snowflakes, and enzyme-substrate reactions. The investigation found that IVR provided opportunities for students to actively experiment with virtual objects to test and revise their conceptions, demonstrating the unique role of IVR in supporting constructivist learning. The study also emphasised the importance of leveraging the capabilities of IVR when designing learning tasks; students embraced the unique value of IVR for embodied exploration of complex ideas when they were presented with conceptually unfamiliar objects. This investigation also highlighted the importance of addressing power imbalances in collaborative IVR tasks by designing tasks complex enough to promote collaborative engagement or assigning students roles (specific tasks to individuals) to encourage equitable participation.

Overall, this thesis is built on a comprehensive review of the literature on the design of IVR learning environments, chemistry learning and assessment, as well as pedagogical theories. By critically and systematically evaluating IVR-based learning, the thesis has contributed to a more critical understanding of conceptual benefits of IVR in science learning and the unique opportunities IVR offers for active learning of scientific concepts. The thesis also demonstrated the importance of thoughtfully crafting IVR experiences to capitalise on its unique capabilities to foster learning interactions and enhance learning. The research also underscores the need for careful consideration of content choice, orientation and reflection activities, and assessment methods when implementing IVR-based learning in the relevant educational contexts. Therefore, this thesis paves the way for more effective and innovative use of IVR for science teaching and learning.

References

Abraham, M., Varghese, V., & Tang, H. (2010). Using molecular representations to aid student understanding of stereochemical concepts. *Journal of Chemical Education*, *87*(12), 1425-1429. https://doi.org/10.1021/ed100497f.

Adams, N. E. (2015). Bloom's taxonomy of cognitive learning objectives. *Journal of the Medical Library Association*, *103*(3), 152-153. https://doi.org/10.3163/1536-5050.103.3.010.

Ahn, S. J., Bostick, J., Ogle, E., Nowak, K. L., McGillicuddy, K. T., & Bailenson, J. N. (2016). Experiencing nature: Embodying animals in immersive virtual environments increases inclusion of nature in self and involvement with nature. *Journal of Computer-Mediated Communication*, *21*(6), 399-419. https://doi.org/10.1111/jcc4.12173.

Ainsworth, S. (1999). The functions of multiple representations. *Computers & Education*, *33*(2), 131-152. https://doi.org/10.1016/S0360-1315(99)00029-9.

Ainsworth, S. (2006). DeFT: A conceptual framework for considering learning with multiple representations. *Learning and Instruction*, *16*(3), 183-198. https://doi.org/10.1016/j.learninstruc.2006.03.001.

Ainsworth, S. (2018). Multiple representations and multimedia learning. In F. Fischer, C. E. Hmelo-Silver, S. R. Goldman, & P. Reimann (Eds.), *International handbook of the learning sciences* (pp. 96-105). Routledge. https://doi.org/10.4324/9781315617572-10.

Ainsworth, S., Prain, V., & Tytler, R. (2011). Drawing to learn in science. *Science*, *333*(6046), 1096-1097. https://doi.org/10.1126/science.1204153.

Ainsworth, S. E., & Scheiter, K. (2021). Learning by drawing visual representations: Potential, purposes, and practical implications. *Current Directions in Psychological Science*, *30*(1), 61-67. https://doi.org/10.1177/0963721420979582.

Al-Balushi, S. M., & Al-Hajri, S. H. (2014). Associating animations with concrete models to enhance students' comprehension of different visual representations in organic chemistry. *Chemistry Education Research and Practice*, *15*(1), 47-58. https://doi.org/10.1039/C3RP00074E.

Allred, Z. D. R., & Bretz, S. L. (2019). University chemistry students' interpretations of multiple representations of the helium atom [10.1039/C8RP00296G]. *Chemistry Education Research and Practice*, *20*(2), 358-368. https://doi.org/10.1039/C8RP00296G.

Anderson, L. W., & Krathwohl, D. R. (2001). *A taxonomy for learning, teaching, and assessing: A revision of Bloom's taxonomy of educational objectives*. Longman.

Anderson, T., & Shattuck, J. (2012). Design-based research: A decade of progress in education research? *Educational Researcher*, *41*(1), 16-25. https://doi.org/10.3102/0013189X11428813.

Andrade, D. V. F., Freire, S., & Baptista, M. (2021). Constructing scientific explanations for chemical phenomena through drawings among 8th-grade students. *EURASIA Journal of Mathematics, Science and Technology Education*, *17*(1), em1937. https://doi.org/10.29333/ejmste/9614.

Andreasen, N. K., Baceviciute, S., Pande, P., & Makransky, G. (2019, March 23-27). *Virtual reality instruction followed by enactment can increase procedural knowledge in a science lesson* [Paper presentation]. 2019 26th IEEE Conference on Virtual Reality and 3D User Interfaces, Osaka, Japan. https://doi.org/10.1109/VR.2019.8797755.

Andrews, J. J., & Rapp, D. N. (2014). Partner characteristics and social contagion: Does group composition matter? *Applied Cognitive Psychology*, *28*(4), 505-517. https://doi.org/10.1002/acp.3024.

Angelov, V., Petkov, E., Shipkovenski, G., & Kalushkov, T. (2020, 26-28 June). *Modern Virtual Reality headsets* [Paper presentation]. 2020 International Congress on Human-Computer Interaction, Optimization and Robotic Applications (HORA), Turkey. https://doi.org/10.1109/HORA49412.2020.9152604.

Artun, H., Durukan, A., & Temur, A. (2020). Effects of virtual reality enriched science laboratory activities on pre-service science teachers' science process skills. *Education and Information Technologies*, *25*, 5477–5498. https://doi.org/10.1007/s10639-020-10220-5.

Bagher, M. M., Sajjadi, P., Carr, J., La Femina, P., & Klippel, A. (2020, June). *Fostering penetrative thinking in geosciences through immersive experiences: A case study in visualizing earthquake locations in 3D* [Paper presentation]. 6th International Conference of the Immersive Learning Research Network (iLRN), San Luis Obispo, CA, USA. https://doi.org/10.23919/iLRN47897.2020.9155123.

Barnea, N. (2000). Teaching and learning about chemistry and modelling with a computer managed modelling system. In J. K. Gilbert & C. J. Boulter (Eds.), *Developing models in science education* (pp. 307-323). Springer. https://doi.org/10.1007/978-94-010-0876-1_16.

Barreda-Ángeles, M., Horneber, S., & Hartmann, T. (2023). Easily applicable social virtual reality and social presence in online higher education during the covid-19 pandemic: A qualitative study. *Computers & Education: X Reality*, *2*, 100024. https://doi.org/10.1016/j.cexr.2023.100024.

Barron, B. (2003). When smart groups fail. *Journal of the Learning Sciences*, *12*(3), 307-359. https://doi.org/10.1207/S15327809JLS1203_1.

Bateman, J., Wildfeuer, J., & Hiippala, T. (2017). *Multimodality: Foundations, research and analysis–A problem-oriented introduction*. Walter de Gruyter.

Becker, N., Noyes, K., & Cooper, M. (2016). Characterizing students' mechanistic reasoning about London dispersion forces. *Journal of Chemical Education*, *93*(10), 1713-1724. https://doi.org/10.1021/acs.jchemed.6b00298.

Bennie, S. J., Ranaghan, K. E., Deeks, H., Goldsmith, H. E., O'Connor, M. B., Mulholland, A. J., & Glowacki, D. R. (2019). Teaching enzyme catalysis using interactive molecular dynamics in virtual reality. *Journal of Chemical Education*, *96*(11), 2488-2496. https://doi.org/10.1021/acs.jchemed.9b00181.

Bhattacharjee, D., Paul, A., Kim, J. H., & Karthigaikumar, P. (2018). An immersive learning model using evolutionary learning [Article]. *Computers and Electrical Engineering*, *65*, 236-249. https://doi.org/10.1016/j.compeleceng.2017.08.023.

Bibic, L., Druskis, J., Walpole, S., Angulo, J., & Stokes, L. (2019). Bug off pain: An educational virtual reality game on spider venoms and chronic pain for public engagement. *Journal of Chemical Education*, *96*(7), 1486-1490. https://doi.org/10.1021/acs.jchemed.8b00905.

Blackman, A., Bottle, S. E., Schmid, S., Mocerino, M., & Wille, U. (2019). *Chemistry* (4 ed.). Wiley.

Boda, P. A., & Brown, B. (2020a). Designing for relationality in virtual reality: Context-specific learning as a primer for content relevancy. *Journal of Science Education and Technology*, *29*(5), 691-702. https://doi.org/10.1007/s10956-020-09849-1.

Boda, P. A., & Brown, B. (2020b). Priming urban learners' attitudes toward the relevancy of science: A mixed-methods study testing the importance of context. *Journal of Research in Science Teaching*, *57*(4), 567-596. https://doi.org/10.1002/tea.21604.

Boukhechem, M.-S., & Dumon, A. (2016). To what degree does handling concrete molecular models promote the ability to translate and coordinate between 2D and 3D molecular structure representations? A case study with Algerian students [10.1039/C5RP00180C]. *Chemistry Education Research and Practice*, *17*(4), 862-877. https://doi.org/10.1039/C5RP00180C.

Boukhechem, M.-S., Dumon, A., & Zouikri, M. (2011). The acquisition of stereochemical knowledge by Algerian students intending to teach physical sciences. *Chemistry Education Research and Practice*, *12*(3), 331-343. https://doi.org/10.1039/C1RP90040D.

Bower, M., DeWitt, D., & Lai, J. W. M. (2020). Reasons associated with preservice teachers' intention to use immersive virtual reality in education. *British Journal of Educational Technology*, *51*(6), 2215-2233. https://doi.org/10.1111/bjet.13009.

Bowman, D. A., & McMahan, R. P. (2007). Virtual reality: How much immersion is enough? *Computer*, *40*(7), 36-43. https://doi.org/10.1109/MC.2007.257.

Brady, J., & Senese, F. (2004). *Chemistry: Matter and its changes*. Wiley.

Brinkmann, S. (2013). *Qualitative interviewing*. Oxford University Press.

Brown, C. E., Alrmuny, D., Williams, M. K., Whaley, B., & Hyslop, R. M. (2021). Visualizing molecular structures and shapes: A comparison of virtual reality, computer simulation, and traditional modeling. *Chemistry Teacher International*, *3*(1), 69-80. https://doi.org/10.1515/cti-2019-0009.

Brown, T. L., LeMay, H. E., Bursten, E. B., Murphy, C., & Woodward, P. (2013). *Chemistry: The central science* (Vol. 3). Pearson.

Broyer, R. M., Miller, K., Ramachandran, S., Fu, S., Howell, K., & Cutchin, S. (2020). Using virtual reality to demonstrate glove hygiene in introductory chemistry laboratories. *Journal of Chemical Education*, *98*(1), 224–229. https://doi.org/10.1021/acs.jchemed.0c00137.

Care, E., Griffin, P., Scoular, C., Awwal, N., & Zoanetti, N. (2015). Collaborative problem solving tasks. In P. Griffin & E. Care (Eds.), *Assessment and teaching of 21st century skills: Methods and approach* (pp. 85-104). Springer. https://doi.org/10.1007/978-94-017-9395-7_4.

Carter, C. S., Larussa, M. A., & Bodner, G. M. (1987). A study of two measures of spatial ability as predictors of success in different levels of general chemistry. *Journal of Research in Science Teaching*, *24*(7), 645-657. https://doi.org/10.1002/tea.3660240705.

Cassidy, K. C., Šefčík, J., Raghav, Y., Chang, A., & Durrant, J. D. (2020). ProteinVR: Web-based molecular visualization in Virtual Reality. *PLoS computational biology*, *16*(3), e1007747. https://doi.org/10.1371/journal.pcbi.1007747.

Chang, H.-Y., Lin, T.-J., Lee, M.-H., Lee, S. W.-Y., Lin, T.-C., Tan, A.-L., & Tsai, C.-C. (2020). A systematic review of trends and findings in research employing drawing assessment in science education. *Studies in Science Education*, *56*(1), 77-110. https://doi.org/10.1080/03057267.2020.1735822.

Chavez, B., & Bayona, S. (2018). Virtual reality in the learning process. In A. Rocha, H. Adeli, L. Reis, & S. Costanzo (Eds.), *Trends and advances in information systems and technologies. WorldCIST'18 2018. Advances in intelligent systems and computing* (Vol. 746, pp. 1345-1356). Springer. https://doi.org/10.1007/978-3-319-77712-2_129.

Checa, D., & Bustillo, A. (2020). A review of immersive virtual reality serious games to enhance learning and training. *Multimedia Tools and Applications*, *79*(9), 5501-5527. https://doi.org/10.1007/s11042-019-08348-9.

Chen, C. J. (2010). Theoretical bases for using Virtual Reality in education. *Themes in Science and Technology Education*, *2*(1-2), 71-90. http://earthlab.uoi.gr/ojs/theste/index.php/theste/article/view/23

Chen, J., Wang, M., Kirschner, P. A., & Tsai, C.-C. (2018). The role of collaboration, computer use, learning environments, and supporting strategies in CSCL: A meta-analysis. *Review of Educational Research* *88*(6), 799-843. https://doi.org/10.3102/0034654318791584.

Cheng, K. H., & Tsai, C. C. (2020). Students' motivational beliefs and strategies, perceived immersion and attitudes towards science learning with immersive virtual reality: A partial least squares analysis. *British Journal of Educational Technology*, *51*(6), 2140-2159. https://doi.org/10.1111/bjet.12956.

Cheng, M., & Gilbert, J. K. (2009). Towards a Better Utilization of Diagrams in Research into the Use of Representative Levels in Chemical Education. In J. K. Gilbert & D. Treagust (Eds.), *Multiple representations in chemical education* (pp. 55-73). Springer. https://doi.org/10.1007/978-1-4020-8872-8_4.

Chittleborough, G., & Treagust, D. (2008). Correct interpretation of chemical diagrams requires transforming from one level of representation to another. *Research in Science Education*, *38*(4), 463-482. https://doi.org/10.1007/s11165-007-9059-4.

Chizhik, A. W. (2001). Equity and status in group collaboration: Learning through explanations depends on task characteristics. *Social Psychology of Education*, *5*(2), 179-200. https://doi.org/10.1023/A:1014405118351.

Choi, K., Yoon, Y. J., Song, O. Y., & Choi, S. M. (2018). Interactive and immersive learning using 360° virtual reality contents on mobile platforms. *Mobile Information Systems*, *2018*, 1-12, Article 2306031. https://doi.org/10.1155/2018/2306031.

Clark, R. E. (1983). Reconsidering research on learning from media. *Review of Educational Research*, *53*(4), 445-459. https://doi.org/10.3102/00346543053004445.

Clark, R. E. (1994). Media will never influence learning. *Educational Technology Research and Development*, *42*(2), 21-29. https://doi.org/10.1007/BF02299088.

Clark, R. E. (2012). Media are "mere vehicles". In R. E. Clark (Ed.), *Learning from media: Arguments, analysis, and evidence* (Vol. 2, pp. 1-12). Information Age Publishing.

Clay, V., König, P., & König, S. (2019). Eye tracking in Virtual Reality. *Journal of Eye Movement Research*, *12*(1). https://doi.org/10.16910/jemr.12.1.3.

Coban, M., Bolat, Y. I., & Goksu, I. (2022). The potential of immersive virtual reality to enhance learning: A meta-analysis. *Educational Research Review*, *36*, 100452. https://doi.org/10.1016/j.edurev.2022.100452.

Cohen, E. G. (1994). Restructuring the classroom: Conditions for productive small groups. *Review of Educational Research*, *64*(1), 1-35. https://doi.org/10.3102/00346543064001001.

Cohen, E. G., Lotan, R. A., Scarloss, B. A., & Arellano, A. R. (1999). Complex instruction: Equity in cooperative learning classrooms. *Theory into practice*, *38*(2), 80-86. https://doi.org/10.1080/00405849909543836.

Cohen, L., Manion, L., & Morrison, K. (2018). *Research methods in education*. Routledge.

Cooper, M. M., Corley, L. M., & Underwood, S. M. (2013). An investigation of college chemistry students' understanding of structure–property relationships. *Journal of Research in Science Teaching*, *50*(6), 699-721. https://doi.org/10.1002/tea.21093.

Cooper, M. M., Stieff, M., & DeSutter, D. (2017). Sketching the invisible to predict the visible: From drawing to modeling in chemistry. *Topics in Cognitive Science*, *9*(4), 902-920. https://doi.org/10.1111/tops.12285.

Cooper, M. M., Williams, L. C., & Underwood, S. M. (2015). Student understanding of intermolecular forces: A multimodal study. *Journal of Chemical Education*, *92*(8), 1288-1298. https://doi.org/10.1021/acs.jchemed.5b00169.

Cowan, K. (2014). Multimodal transcription of video: examining interaction in early years classrooms. *Classroom Discourse*, *5*(1), 6-21. https://doi.org/10.1080/19463014.2013.859846.

Creswell, J. W. (2013). *Qualitative inquiry and research design: Choosing among five approaches*. SAGE Publications.

Csikszentmihalyi, M. (1990). *Flow: The psychology of optimal experience*. Harper & Row.

Csikszentmihalyi, M. (2014). *Applications of flow in human development and education*. Springer.

Cummings, J. J., & Bailenson, J. N. (2016). How immersive is enough? A meta-analysis of the effect of immersive technology on user presence. *Media Psychology*, *19*(2), 272-309. https://doi.org/10.1080/15213269.2015.1015740.

Dalgarno, B., & Lee, M. J. (2010). What are the learning affordances of 3-D virtual environments? *British Journal of Educational Technology*, *41*(1), 10-32. https://doi.org/10.1111/j.1467-8535.2009.01038.x.

Davidowitz, B., Chittleborough, G., & Murray, E. (2010). Student-generated submicro diagrams: a useful tool for teaching and learning chemical equations and stoichiometry [10.1039/C005464J]. *Chemistry Education Research and Practice*, *11*(3), 154-164. https://doi.org/10.1039/C005464J.

Dede, C., Salzman, M., Loftin, R. B., & Ash, K. (1997). Using virtual reality technology to convey abstract scientific concepts. In M. J. Jacobson, R. B. Kozma, & L. Erlbaum (Eds.), *Learning the sciences of the 21st century: Research, design, and implementing advanced technology learning environments* (pp. 1-44). Lawrence Erlbaum.

Dede, C. J. (2009). Immersive interfaces for engagement and learning. *Science*, *323*(5910), 66-69. https://doi.org/10.1126/science.1167311.

Dede, C. J., Jacobson, J., & Richards, J. (2017). Introduction: Virtual, augmented, and mixed realities in education. In D. Liu, C. Dede, R. Huang, & J. Richards (Eds.), *Virtual, augmented, and mixed realities in education* (pp. 1-16). Springer. https://doi.org/10.1007/978-981-10-5490-7_1.

Denscombe, M. (2017). *The good research guide: For small-scale social research projects*. McGraw-Hill Education.

Denzin, N. K., & Lincoln, Y. S. (2005). *The SAGE handbook of qualitative research*. SAGE.

Derman, A., & Ebenezer, J. (2020). The effect of multiple representations of physical and chemical changes on the development of primary pre-service teachers cognitive structures. *Research in Science Education*, *50*(4), 1575-1601. https://doi.org/10.1007/s11165-018-9744-5.

Derman, A., Koçak, N., & Eilks, I. (2019). Insights into components of prospective science teachers' mental models and their preferred visual representations of atoms. *Education Sciences*, *9*(2), Article 154. https://www.mdpi.com/2227-7102/9/2/154

Derry, S. J., Pea, R. D., Barron, B., Engle, R. A., Erickson, F., Goldman, R., Hall, R., Koschmann, T., Lemke, J. L., Sherin, M. G., & Sherin, B. L. (2010). Conducting video research in the learning sciences: Guidance on selection, analysis, technology, and ethics. *Journal of the Learning Sciences*, *19*(1), 3-53. https://doi.org/10.1080/10508400903452884.

Di Natale, A. F., Repetto, C., Riva, G., & Villani, D. (2020). Immersive Virtual Reality in K-12 and higher education: A 10-year systematic review of empirical research. *British Journal of Educational Technology*, *51*(6), 2006-2033. https://doi.org/10.1111/bjet.13030.

Dickson, H., Thompson, C. D., & O'Toole, P. (2016). A picture is worth a thousand words: Investigating first year chemistry students' ability to visually express their understanding of chemistry concepts. *International Journal of Innovation in Science and Mathematics Education*, *24*(1), 12-23. https://openjournals.library.usyd.edu.au/index.php/CAL/article/view/9043

Duis, J. M. (2011). Organic chemistry educators' perspectives on fundamental concepts and misconceptions: An exploratory study. *Journal of Chemical Education*, *88*(3), 346-350. https://doi.org/10.1021/ed1007266.

Duit, R., & Treagust, D. F. (2003). Conceptual change: A powerful framework for improving science teaching and learning. *International Journal of Science Education*, *25*(6), 671-688. https://doi.org/10.1080/09500690305016.

Dunnagan, C. L., Dannenberg, D. A., Cuales, M. P., Earnest, A. D., Gurnsey, R. M., & Gallardo-Williams, M. T. (2020). Production and evaluation of a realistic immersive virtual reality organic chemistry laboratory experience: Infrared spectroscopy. *Journal of Chemical Education*, *97*(1), 258-262. https://doi.org/10.1021/acs.jchemed.9b00705.

Durmaz, M. (2018). Determination of prospective chemistry teachers' cognitive Structures and misconceptions about stereochemistry. *Journal of Education and Training Studies*, *6*(9), 13-20. https://doi.org/doi.org/10.11114/jets.v6i9.3353.

Echeverri-Jimenez, E., & Oliver-Hoyo, M. (2023). Visual-spatial skills, strategies, and challenges to extract, represent, and predict stereochemical outcomes of cycloadditions using a hexagonal prism reference frame. *Journal of Chemical Education*, *100*(7), 2483-2494. https://doi.org/10.1021/acs.jchemed.2c00398.

Edwards, B. I., Bielawski, K. S., Prada, R., & Cheok, A. D. (2019). Haptic virtual reality and immersive learning for enhanced organic chemistry instruction. *Virtual Reality*, *23*, 363-373. https://doi.org/10.1007/s10055-018-0345-4.

Ehrlén, K. (2009). Drawings as representations of children's conceptions. *International Journal of Science Education*, *31*(1), 41-57. https://doi.org/10.1080/09500690701630455.

Elford, D., Lancaster, S. J., & Jones, G. A. (2021). Stereoisomers, not stereo enigmas: A stereochemistry escape activity incorporating augmented and immersive virtual reality. *Journal of Chemical Education*, *98*(5), 1691-1704. https://doi.org/10.1021/acs.jchemed.0c01283.

Esmonde, I. (2009). Mathematics learning in groups: Analyzing equity in two cooperative activity structures. *Journal of the Learning Sciences*, *18*(2), 247-284. https://doi.org/10.1080/10508400902797958.

Farland-Smith, D. (2012). Development and field test of the modified Draw-a-Scientist Test and the Draw-a-Scientist Rubric. *School Science and Mathematics*, *112*(2), 109-116. https://doi.org/10.1111/j.1949-8594.2011.00124.x.

Feng, Z., González, V. A., Amor, R., Spearpoint, M., Thomas, J., Sacks, R., Lovreglio, R., & Cabrera-Guerrero, G. (2020). An immersive virtual reality serious game to enhance earthquake behavioral responses and post-earthquake evacuation preparedness in buildings. *Advanced Engineering Informatics*, *45*, 101118. https://doi.org/10.1016/j.aei.2020.101118.

Ferrell, J. B., Campbell, J. P., McCarthy, D. R., McKay, K. T., Hensinger, M., Srinivasan, R., Zhao, X., Wurthmann, A., Li, J., & Schneebeli, S. T. (2019). Chemical exploration with virtual reality in organic teaching laboratories. *Journal of Chemical Education*, *96*(9), 1961-1966. https://doi.org/10.1021/acs.jchemed.9b00036.

Filter, E., Eckes, A., Fiebelkorn, F., & Büssing, A. G. (2020). Virtual reality nature experiences involving wolves on YouTube: Presence, emotions, and attitudes in immersive and nonimmersive settings. *Sustainability*, *12*(9), 3823. https://doi.org/10.3390/su12093823.

Finson, K. D. (2002). Drawing a scientist: What we do and do not know after fifty years of drawings. *School Science and Mathematics*, *102*(7), 335-345. https://doi.org/10.1111/j.1949-8594.2002.tb18217.x.

Fiorella, L., & Mayer, R. E. (2016). Eight ways to promote generative learning. *Educational Psychology Review*, *28*(4), 717-741. https://doi.org/10.1007/s10648-015-9348-9.

Fokides, E., & Kefallinou, M. (2020). Examining the impact of spherical videos in teaching endangered species/environmental education to primary school students. *Journal of Information Technology Education: Research*, *19*, 427-450. https://doi.org/10.28945/4612.

Fombona-Pascual, A., Fombona, J., & Vázquez-Cano, E. (2022). VR in chemistry, a review of scientific research on advanced atomic/molecular visualization. *Chemistry Education Research and Practice*, *23*(2), 300-312. https://doi.org/10.1039/D1RP00317H.

Fowler, C. (2015). Virtual Reality and learning: Where is the pedagogy? *British Journal of Educational Technology*, *46*(2), 412-422. https://doi.org/10.1111/bjet.12135.

Freina, L., & Ott, M. (2015, April). *A literature review on immersive Virtual Reality in education: State of the art and perspectives* [Paper presentation]. The International Scientific Conference on eLearning and

Software for Education, Bucharest, Romania. https://progesis.itd.cnr.it/download/eLSE%202015%20Freina%20Ott%20Paper.pdf.

Fujiwara, D., Kellar, K., Humer, I., Pietroszek, K., & Eckhardt, C. (2020). VSEPR theory, an interactive and immersive virtual reality. In D. Economou, A. Klippel, H. Dodds, A. Peña-Rios, M. J. W, D. Beck, J. Pirker, A. Dengel, T. M. Peres, & J. Richter (Eds.), *Proceedings of 6th international conference of the Immersive Learning Research Network (iLRN)* (pp. 140-146). IEEE. https://doi.org/10.23919/iLRN47897.2020.9155185.

Furió, C., & Calatayud, M. L. (1996). Difficulties with the geometry and polarity of molecules: Beyond misconceptions. *Journal of Chemical Education*, *73*(1), 36. https://doi.org/10.1021/ed073p36.

Gandhi, H. A., Jakymiw, S., Barrett, R., Mahaseth, H., & White, A. D. (2020). Real-time interactive simulation and visualization of organic molecules. *Journal of Chemical Education*, *97*(11), 4189–4195. https://doi.org/10.1021/acs.jchemed.9b01161.

Garzón, J. (2021). An overview of twenty-five years of augmented reality in education. *Multimodal Technologies and Interaction*, *5*(7), Article 37. https://doi.org/10.3390/mti5070037.

Gijlers, H., & de Jong, T. (2005). The relation between prior knowledge and students' collaborative discovery learning processes. *Journal of Research in Science Teaching*, *42*(3), 264-282. https://doi.org/10.1002/tea.20056.

Gilbert, J. K. (2006). On the nature of “context” in chemical education. *International Journal of Science Education*, *28*(9), 957-976. https://doi.org/10.1080/09500690600702470.

Gilbert, J. K., & Treagust, D. F. (2009). *Multiple representations in chemical education* (Vol. 4). Springer.

Gilbert, J. K., & Watts, D. M. (1983). Concepts, misconceptions and alternative conceptions: Changing perspectives in science education. *Studies in Science Education*, *10*, 61-98. https://doi.org/10.1080/03057268308559905.

Glaser, B. G. (1965). The constant comparative method of qualitative analysis. *Social Problems*, *12*(4), 436-445. https://doi.org/10.2307/798843.

Gobert, J. D., & Clement, J. J. (1999). Effects of student-generated diagrams versus student-generated summaries on conceptual understanding of causal and dynamic knowledge in plate tectonics. *Journal of Research in Science Teaching*, *36*(1), 39-53. https://doi.org/10.1002/(SICI)1098-2736(199901)36:1.

Gochman, S. R., Morano Lord, M., Goyal, N., Chow, K., Cooper, B. K., Gray, L. K., Guo, S. X., Hill, K. A., Liao, S. K., Peng, S., Seong, H. J., Wang, A., Yoon, E. K., Zhang, S., Lobel, E., Tregubov, T., & Dominy, N. J. (2019). Tarsier Goggles: A virtual reality tool for experiencing the optics of a dark-adapted primate visual system. *Evolution: Education and Outreach*, *12*(1), Article 9. https://doi.org/10.1186/s12052-019-0101-6.

Graesser, A. C., Fiore, S. M., Greiff, S., Andrews-Todd, J., Foltz, P. W., & Hesse, F. W. (2018). Advancing the science of collaborative problem solving. *Psychological Science in the Public Interest*, *19*(2), 59-92. https://doi.org/10.1177/1529100618808244.

Grimm, P. (2010). Social desirability bias. In N. J. Sheth & K. N. Malhotra (Eds.), *Wiley international encyclopedia of marketing*. Wiley. https://onlinelibrary.wiley.com/doi/abs/10.1002/9781444316568.wiem02057

Hakkarainen, K., Paavola, S., Kangas, K., & Seitamaa-Hakkarainen, P. (2013). Toward collaborative knowledge creation. In C. E. Hmelo-Silver, C. A. Chinn, C. K. K. Chan, & A. O’Donnell (Eds.), *International handbook of collaborative learning* (pp. 57-73). Routledge. https://doi.org/10.4324/9780203837290.

Hamilton, D., McKechnie, J., Edgerton, E., & Wilson, C. (2021). Immersive virtual reality as a pedagogical tool in education: A systematic literature review of quantitative learning outcomes and experimental design. *Journal of Computers in Education*, *8*(1), 1-32. https://doi.org/10.1007/s40692-020-00169-2.

Han, E., Miller, M. R., DeVeaux, C., Jun, H., Nowak, K. L., Hancock, J. T., Ram, N., & Bailenson, J. N. (2023). People, places, and time: a large-scale, longitudinal study of transformed avatars and environmental context in group interaction in the metaverse. *Journal of Computer-Mediated Communication*, *28*(2), zmac031. https://doi.org/10.1093/jcmc/zmac031.

Han, E., Nowak, K. L., & Bailenson, J. N. (2022). Prerequisites for learning in networked immersive Virtual Reality. *Technology, Mind, and Behavior*, *3*(4), 1-14. https://doi.org/10.1037/tmb0000094.

Han, P.-H., Chen, Y.-S., Liu, I.-S., Jang, Y.-P., Tsai, L., Chang, A., & Hung, Y.-P. (2019). A compelling virtual tour of the Dunhuang Cave with an immersive head-mounted display. *IEEE Computer Graphics and Applications*, *40*(1), 40-55. https://doi.org/10.1109/MCG.2019.2936753.

Han, Y., Shi, Y., Wang, J., Liu, Y., & Wang, Y. (2020). First-person perspective physics learning platform based on virtual reality. In P. Zaphiris & A. Ioannou (Eds.), *Learning and collaboration technologies. Human and technology ecosystems. HCII 2020. Lecture notes in computer science* (Vol. 12206, pp. 435-447). Springer. https://doi.org/10.1007/978-3-030-50506-6_30.

Harle, M., & Towns, M. (2011). A review of spatial ability literature, Its connection to chemistry, and implications for instruction. *Journal of Chemical Education*, *88*(3), 351-360. https://doi.org/10.1021/ed900003n.

Henderleiter, J., Smart, R., Anderson, J., & Elian, O. (2001). How do organic chemistry students understand and apply hydrogen bonding? *Journal of Chemical Education*, *78*(8), 1126. https://doi.org/10.1021/ed078p1126.

Holme, T. A., Luxford, C. J., & Brandriet, A. (2015). Defining conceptual understanding in general chemistry. *Journal of Chemical Education*, *92*(9), 1477-1483. https://doi.org/10.1021/acs.jchemed.5b00218.

Hsu, W. C., Tseng, C. M., & Kang, S. C. (2018). Using exaggerated feedback in a virtual reality environment to enhance behavior intention of water-conservation. *Educational Technology and Society*, *21*(4), 187-203. https://www.jstor.org/stable/26511548

Huang, H.-M., Rauch, U., & Liaw, S.-S. (2010). Investigating learners' attitudes toward virtual reality learning environments: Based on a constructivist approach. *Computers & Education*, *55*(3), 1171-1182. https://doi.org/10.1016/j.compedu.2010.05.014.

Huang, K. T., Ball, C., Francis, J., Ratan, R., Boumis, J., & Fordham, J. (2019). Augmented versus virtual reality in education: An exploratory study examining science knowledge retention when using augmented reality/virtual reality mobile applications. *Cyberpsychology, Behavior, and Social Networking*, *22*(2), 105-110. https://doi.org/10.1089/cyber.2018.0150.

Huang, W. (2019). Examining the impact of head-mounted display virtual reality on the science self-efficacy of high schoolers. *Interactive Learning Environments*, *2019*, 1-13. https://doi.org/10.1080/10494820.2019.1641525.

Huang, W., Roscoe, R. D., Johnson-Glenberg, M. C., & Craig, S. D. (2021). Motivation, engagement, and performance across multiple virtual reality sessions and levels of immersion. *Journal of Computer Assisted Learning*, *37*(3), 745-758. https://doi.org/10.1111/jcal.12520.

Janssen, J., Erkens, G., Kirschner, P. A., & Kanselaar, G. (2009). Influence of group member familiarity on online collaborative learning. *Computers in Human Behavior*, *25*(1), 161-170. https://doi.org/10.1016/j.chb.2008.08.010.

Jensen, L., & Konradsen, F. (2018). A review of the use of virtual reality head-mounted displays in education and training. *Education and Information Technologies*, *23*(4), 1515-1529. https://doi.org/10.1007/s10639-017-9676-0.

Jewitt, C. (2013). Multimodal methods for researching digital technologies. In S. Price, C. Jewitt, & B. Brown (Eds.), *The SAGE handbook of digital technology research* (pp. 250-265). SAGE. https://doi.org/10.4135/9781446282229.n18

Johnson-Glenberg, M. C. (2018). Immersive VR and education: Embodied design principles that include gesture and hand controls. *Frontiers in Robotics and AI*, *5*, Article 81. https://doi.org/10.3389/frobt.2018.00081.

Johnson-Glenberg, M. C. (2019). The necessary nine: Design principles for embodied VR and active STEM education. In P. Díaz, A. Ioannou, K. K. Bhagat, & J. M. Spector (Eds.), *Learning in a digital world: Perspective on interactive technologies for formal and informal education* (pp. 83-112). Springer. https://doi.org/10.1007/978-981-13-8265-9_5.

Johnstone, A. H. (1991). Why is science difficult to learn? Things are seldom what they seem. *Journal of Computer Assisted Learning*, *7*(2), 75-83. https://doi.org/10.1111/j.1365-2729.1991.tb00230.x.

Jonassen, D. H. (1994). Thinking technology: Toward a constructivist design model. *Educational Technology*, *34*(4), 34-37. https://doi.org/https://www.learntechlib.org/p/171050/.

Jong, M. S. Y., Tsai, C. C., Xie, H., & Kwan-Kit Wong, F. (2020). Integrating interactive learner-immersed video-based virtual reality into learning and teaching of physical geography. *British Journal of Educational Technology*, *51*(6), 2064-2079. https://doi.org/10.1111/bjet.12947.

Kader, S. N., Ng, W. B., Tan, S. W. L., & Fung, F. M. (2020). Building an interactive immersive virtual reality crime scene for future chemists to learn forensic science chemistry. *Journal of Chemical Education*, *97*(9), 2651–2656. https://doi.org/10.1021/acs.jchemed.0c00817.

Kelly, R. M., Barrera, J. H., & Mohamed, S. C. (2010). An analysis of undergraduate general chemistry students' misconceptions of the submicroscopic level of precipitation reactions. *Journal of Chemical Education*, *87*(1), 113-118. https://doi.org/10.1021/ed800011a.

Kern, A. L., Wood, N. B., Roehrig, G. H., & Nyachwaya, J. (2010). A qualitative report of the ways high school chemistry students attempt to represent a chemical reaction at the atomic/molecular level. *Chemistry Education Research and Practice*, *11*(3), 165-172. https://doi.org/10.1039/C005465H.

Kirschner, P., Strijbos, J.-W., Kreijns, K., & Beers, P. J. (2004). Designing electronic collaborative learning environments. *Educational Technology Research and Development*, *52*(3), 47-66. https://doi.org/10.1007/BF02504675.

Kirschner, P. A., Beers, P. J., Boshuizen, H. P. A., & Gijselaers, W. H. (2008). Coercing shared knowledge in collaborative learning environments. *Computers in Human Behavior*, *24*(2), 403-420. https://doi.org/10.1016/j.chb.2007.01.028.

Klingenberg, S., Jørgensen, M. L., Dandanell, G., Skriver, K., Mottelson, A., & Makransky, G. (2020). Investigating the effect of teaching as a generative learning strategy when learning through desktop and immersive VR: A media and methods experiment. *British Journal of Educational Technology*, *51*(6), 2115-2138. https://doi.org/10.1111/bjet.13029.

Klippel, A., Zhao, J., Oprean, D., Wallgrün, J. O., Stubbs, C., La Femina, P., & Jackson, K. L. (2019). The value of being there: Toward a science of immersive virtual field trips. *Virtual Reality*, *24*, 753–770. https://doi.org/10.1007/s10055-019-00418-5.

Klippel, A., Zhao, J. Y., Jackson, K. L., La Femina, P., Stubbs, C., Wetzel, R., Blair, J., Wallgrun, J. O., & Oprean, D. (2019). Transforming earth science education through immersive experiences: Delivering on a long held promise. *Journal of Educational Computing Research*, *57*(7), 1745-1771. https://doi.org/10.1177%2F0735633119854025

Kozhevnikov, M., Gurlitt, J., & Kozhevnikov, M. (2013). Learning relative motion concepts in immersive and non-immersive virtual environments [journal article]. *Journal of Science Education and Technology*, *22*(6), 952-962. https://doi.org/10.1007/s10956-013-9441-0.

Kozma, R. (2003). The material features of multiple representations and their cognitive and social affordances for science understanding. *Learning and Instruction*, *13*(2), 205-226. https://doi.org/10.1016/S0959-4752(02)00021-X.

Kozma, R., Chin, E., Russell, J., & Marx, N. (2000). The roles of representations and tools in the chemistry laboratory and their implications for chemistry learning. *Journal of the Learning Sciences*, *9*(2), 105-143. https://doi.org/10.1207/s15327809jls0902_1.

Kozma, R. B., & Russell, J. (1997). Multimedia and understanding: Expert and novice responses to different representations of chemical phenomena. *Journal of Research in Science Teaching*, *34*(9), 949-968. https://doi.org/10.1002/(SICI)1098-2736(199711)34:9%3C949::AID-TEA7%3E3.0.CO;2-U

Krämer, N. C. (2017). The Immersive power of social interaction. In D. Liu, C. Dede, R. Huang, & J. Richards (Eds.), *Virtual, augmented, and mixed realities in education* (pp. 55-70). Springer. https://doi.org/10.1007/978-981-10-5490-7_4.

Krathwohl, D. R. (2002). A revision of bloom's taxonomy: An overview. *Theory Into Practice 41*(4), 212-218. https://doi.org/10.1207/s15430421tip4104_2.

Krauss, S. E. (2005). Research paradigms and meaning making: A primer. *The qualitative report*, *10*(4), 758-770. http://www.nova.edu/ssss/QR/QR10-4/krauss.pdf

Kreijns, K., Kirschner, P. A., & Jochems, W. (2003). Identifying the pitfalls for social interaction in computer-supported collaborative learning environments: A review of the research. *Computers in Human Behavior*, *19*(3), 335-353. https://doi.org/10.1016/S0747-5632(02)00057-2.

Kreijns, K., Xu, K., & Weidlich, J. (2022). Social presence: Conceptualization and measurement. *Educational Psychology Review*, *34*(1), 139-170. https://doi.org/10.1007/s10648-021-09623-8.

Kress, G. (2010). *Multimodality: A social semiotic approach to contemporary communication*. Routledge.

Krippendorff, K. (2018). *Content analysis: An introduction to its methodology*. SAGE.

Krupić, D., Žuro, B., & Corr, P. J. (2021). Anxiety and threat magnification in subjective and physiological responses of fear of heights induced by virtual reality. *Personality and Individual Differences*, *169*, Article 109720. https://doi.org/10.1016/j.paid.2019.109720.

Kuiper, J. (1994). Student ideas of science concepts: Alternative frameworks? *International Journal of Science Education*, *16*(3), 279-292. https://doi.org/10.1080/0950069940160303.

Kuo, Y.-R., Won, M., Zadnik, M., Siddiqui, S., & Treagust, D. F. (2017). Learning optics with multiple representations: Not as simple as expected. In D. F. Treagust, R. Duit, & H. E. Fischer (Eds.), *Multiple representations in physics education* (pp. 123-138). Springer. https://doi.org/10.1007/978-3-319-58914-5_6.

Kwon, C. (2019). Verification of the possibility and effectiveness of experiential learning using HMD-based immersive VR technologies. *Virtual Reality*, *23*(1), 101-118. https://doi.org/10.1007/s10055-018-0364-1.

Lamb, R., Antonenko, P., Etopio, E., & Seccia, A. (2018). Comparison of virtual reality and hands on activities in science education via functional near infrared spectroscopy. *Computers & Education*, *124*, 14-26. https://doi.org/10.1016/j.compedu.2018.05.014.

Lamb, R. L., Etopio, E., Hand, B., & Yoon, S. Y. (2019). Virtual reality simulation: Effects on academic performance within two domains of writing in science. *Journal of Science Education and Technology*, *28*(4), 371-381. https://doi.org/10.1007/s10956-019-09774-y.

Laricheva, E. N., & Ilikchyan, A. (2023). Exploring the effect of Virtual Reality on learning in general chemistry students with low visual-spatial skills. *Journal of Chemical Education*, *100*(2), 589-596. https://doi.org/10.1021/acs.jchemed.2c00732.

Lee, K. M. (2004). Presence, explicated. *Communication Theory 14*(1), 27-50. https://doi.org/10.1111/j.1468-2885.2004.tb00302.x.

Lee, Y., Kim, S. K., & Eom, M.-R. (2020). Usability of mental illness simulation involving scenarios with patients with schizophrenia via immersive virtual reality: A mixed methods study. *PLoS One*, *15*(9), e0238437. https://doi.org/10.1371/journal.pone.0238437.

Libarkin, J. C., & Kurdziel, J. P. (2001). Research methodologies in science education: Assessing students' alternative conceptions. *Journal of Geoscience Education*, *49*(4), 378-383. https://doi.org/10.1080/10899995.2001.12028050.

Lipponen, L., Rahikainen, M., Lallimo, J., & Hakkarainen, K. (2003). Patterns of participation and discourse in elementary students' computer-supported collaborative learning. *Learning and Instruction*, *13*(5), 487-509. https://doi.org/10.1016/S0959-4752(02)00042-7.

Liu, R., Wang, L., Lei, J., Wang, Q., & Ren, Y. (2020). Effects of an immersive virtual reality-based classroom on students' learning performance in science lessons. *British Journal of Educational Technology*, *51*(6), 2034-2049. https://doi.org/10.1111/bjet.13028.

Liu, Y., Won, M., & Treagust, D. F. (2014). Secondary biology teachers' use of different types of diagrams for different purposes. In B. Eilam & J. K. Gilbert (Eds.), *Science teachers' use of visual representations* (pp. 103-121). Springer International Publishing. https://doi.org/10.1007/978-3-319-06526-7_5.

Lohre, R., Bois, A. J., Athwal, G. S., & Goel, D. P. (2020). Improved complex skill acquisition by immersive virtual reality training: a randomized controlled trial. *Journal of Bone and Joint Surgery*, *102*(6), e26. https://doi.org/10.2106/JBJS.19.00982.

Lui, A. L. C., Not, C., & Wong, G. K. W. (2023). Theory-based learning design with immersive Virtual Reality in science education: A systematic review. *Journal of Science Education and Technology*, *32*(3), 390-432. https://doi.org/10.1007/s10956-023-10035-2.

Lui, M., McEwen, R., & Mullally, M. (2020). Immersive virtual reality for supporting complex scientific knowledge: Augmenting our understanding with physiological monitoring. *British Journal of Educational Technology*, *51*(6), 2180–2198. https://doi.org/10.1111/bjet.13022.

Madden, J., Pandita, S., Schuldt, J. P., Kim, B., Won, A. S., & Holmes, N. G. (2020). Ready student one: Exploring the predictors of student learning in virtual reality. *PLoS One*, *15*(3), Article e0229788. https://doi.org/10.1371/journal.pone.0229788.

Makransky, G., Borre-Gude, S., & Mayer, R. E. (2019). Motivational and cognitive benefits of training in immersive virtual reality based on multiple assessments. *Journal of Computer Assisted Learning*, *35*(6), 691-707. https://doi.org/10.1111/jcal.12375.

Makransky, G., & Lilleholt, L. (2018). A structural equation modeling investigation of the emotional value of immersive virtual reality in education. *Educational Technology Research and Development*, *66*(5), 1141-1164. https://doi.org/10.1007/s11423-018-9581-2.

Makransky, G., & Petersen, G. B. (2021). The cognitive affective model of immersive learning (CAMIL): a Theoretical research-based model of learning in immersive virtual reality. *Educational Psychology Review*, *33*(3), 937-958. https://doi.org/10.1007/s10648-020-09586-2.

Makransky, G., Petersen, G. B., & Klingenberg, S. (2020). Can an immersive virtual reality simulation increase students' interest and career aspirations in science? *British Journal of Educational Technology*, *51*(6), 2079-2097. https://doi.org/10.1111/bjet.12954.

Makransky, G., Terkildsen, T. S., & Mayer, R. E. (2019). Adding immersive virtual reality to a science lab simulation causes more presence but less learning. *Learning and Instruction*, *60*, 225-236. https://doi.org/10.1016/j.learninstruc.2017.12.007.

Makransky, G., Wismer, P., & Mayer, R. E. (2019). A gender matching effect in learning with pedagogical agents in an immersive virtual reality science simulation. *Journal of Computer Assisted Learning*, *35*(3), 349-358. https://doi.org/10.1111/jcal.12335.

Malmberg, J., Haataja, E., & Järvelä, S. (2022). Exploring the connection between task difficulty, task perceptions, physiological arousal and learning outcomes in collaborative learning situations. *Metacognition and Learning*, *17*(3), 793-811. https://doi.org/10.1007/s11409-022-09320-z.

Maloney, D., & Freeman, G. (2020). Falling asleep together: What makes activities in social virtual reality meaningful to users. In P. Mirza-Babaei, V. McArthur, V. V. Abeele, & M. Birk (Eds.), *Proceedings of the annual symposium on computer-human interaction in play* (pp. 510–521). Association for Computing Machinery. https://doi.org/10.1145/3410404.3414266.

Markic, S., & Eilks, I. (2015). Evaluating drawings to explore chemistry teachers' pedagogical attitudes. In M. Kahveci & M. Orgill (Eds.), *Affective dimensions in chemistry education* (pp. 259-278). Springer. https://doi.org/10.1007/978-3-662-45085-7_13.

Markowitz, D. M., Laha, R., Perone, B. P., Pea, R. D., & Bailenson, J. N. (2018). Immersive virtual reality field trips facilitate learning about climate change. *Frontiers in Psychology*, *9*, Article 2364. https://doi.org/10.3389/fpsyg.2018.02364.

Martín-Gutiérrez, J., Mora, C. E., Añorbe-Díaz, B., & González-Marrero, A. (2017). Virtual technologies trends in education. *EURASIA Journal of Mathematics, Science and Technology Education*, *13*(2), 469-486. https://doi.org/10.12973/eurasia.2017.00626a.

Martinez, M. E. (1999). Cognition and the question of test item format. *Educational Psychologist*, *34*(4), 207-218. https://doi.org/10.1207/s15326985ep3404_2.

Matovu, H., Ungu, D. A. K., Won, M., Tsai, C.-C., Treagust, D. F., Mocerino, M., & Tasker, R. (2023). Immersive Virtual Reality for science learning: Design, implementation, and evaluation. *Studies in Science Education*, *59*(2), 205-244. https://doi.org/10.1080/03057267.2022.2082680.

Matovu, H., Won, M., Treagust, D. F., Mocerino, M., Ungu, D. A. K., Tsai, C.-C., & Tasker, R. (2023). Analysis of students' diagrams of water molecules in snowflakes to reveal their conceptual understanding of hydrogen bonds. *Chemistry Education Research and Practice*, *24*(2), 437-452. https://doi.org/10.1039/d2rp00175f.

Matovu, H., Won, M., Treagust, D. F., Ungu, D. A. K., Mocerino, M., Tsai, C.-C., & Tasker, R. (2023). Change in students' explanation of the shape of snowflakes after collaborative immersive virtual reality. *Chemistry Education Research and Practice*, *24*(2), 509-525. https://doi.org/10.1039/D2RP00176D.

Mayer, R. E. (2005). Cognitive theory of multimedia learning. In R. E. Mayer (Ed.), *The Cambridge handbook of multimedia learning* (Vol. 41, pp. 31-48). Cambridge University Press.

Mayes, J. T., & Fowler, C. J. (1999). Learning technology and usability: A framework for understanding courseware. *Interacting with Computers*, *11*(5), 485-497. https://doi.org/10.1016/s0953-5438(98)00065-4.

McClary, L., & Talanquer, V. (2011). College chemistry students' mental models of acids and acid strength. *Journal of Research in Science Teaching*, *48*(4), 396-413. https://doi.org/10.1002/tea.20407.

McLure, F., Won, M., & Treagust, D. F. (2021a). Analysis of students' diagrams explaining scientific phenomena. *Research in Science Education*, *52*(4), 1225-1241. https://doi.org/10.1007/s11165-021-10004-y.

McLure, F., Won, M., & Treagust, D. F. (2021b). What students' diagrams reveal about their sense-making of plate tectonics in lower secondary science. *International Journal of Science Education*, *43*(16), 2684-2705. https://doi.org/10.1080/09500693.2021.1983922.

Merchant, Z., Goetz, E. T., Keeney-Kennicutt, W., Cifuentes, L., Kwok, O.-m., & Davis, T. J. (2013). Exploring 3-D virtual reality technology for spatial ability and chemistry achievement. *Journal of Computer Assisted Learning*, *29*(6), 579-590. https://doi.org/10.1111/jcal.12018.

Merriam, S. B., & Tisdell, E. J. (2015). *Qualitative research: A guide to design and implementation*. John Wiley & Sons.

Meyer, O. A., Omdahl, M. K., & Makransky, G. (2019). Investigating the effect of pre-training when learning through immersive virtual reality and video: A media and methods experiment. *Computers & Education*, *140*, Article 103603. https://doi.org/10.1016/j.compedu.2019.103603.

Mikropoulos, T. A., & Natsis, A. (2011). Educational virtual environments: A ten-year review of empirical research (1999–2009). *Computers & Education*, *56*(3), 769-780. https://doi.org/10.1016/j.compedu.2010.10.020.

Miller, D. I., Nolla, K. M., Eagly, A. H., & Uttal, D. H. (2018). The development of children's gender-science stereotypes: A Meta-analysis of 5 decades of U.S. Draw-A-Scientist studies. *Child Development*, *89*(6), 1943-1955. https://doi.org/10.1111/cdev.13039.

Mistry, N., Singh, R., & Ridley, J. (2020). A web-based stereochemistry tool to improve students' ability to draw Newman projections and chair conformations and assign R/S Labels. *Journal of Chemical Education*. https://doi.org/10.1021/acs.jchemed.9b00688

Nakhleh, M. B. (1992). Why some students don't learn chemistry: Chemical misconceptions. *Journal of Chemical Education*, *69*(3), 191. https://doi.org/10.1021/ed069p191.

Nicoll, G. (2003). A qualitative investigation of undergraduate chemistry students' macroscopic interpretations of the submicroscopic structures of molecules. *Journal of Chemical Education*, *80*(2), 205. https://doi.org/10.1021/ed080p205.

Nie, J., & Wu, B. (2020). Investigating the effect of immersive virtual reality and planning on the outcomes of simulation-based learning: A media and method experiment. *IEEE Xplore*, 329-332. https://doi.org/10.1109/ICALT49669.2020.00106.

Norris, S. (2002). The implication of visual research for discourse analysis: transcription beyond language. *Visual Communication*, *1*(1), 97-121. https://doi.org/10.1177/147035720200100108.

Nowak, G. J., Evans, N. J., Wojdynski, B. W., Ahn, S. J. G., Len-Rios, M. E., Carera, K., Hale, S., & McFalls, D. (2020). Using immersive virtual reality to improve the beliefs and intentions of influenza vaccine avoidant 18-to-49-year-olds: Considerations, effects, and lessons learned. *Vaccine*, *38*(5), 1225-1233. https://doi.org/10.1016/j.vaccine.2019.11.009.

Noyes, K., & Cooper, M. M. (2019). Investigating student understanding of London dispersion forces: A longitudinal study. *Journal of Chemical Education*, *96*(9), 1821-1832. https://doi.org/10.1021/acs.jchemed.9b00455.

Nurrenbern, S. C., & Robinson, W. R. (1998). Conceptual questions and challenge problems. *Journal of Chemical Education*, *75*(11), 1502. https://doi.org/10.1021/ed075p1502.

Nyachwaya, J. M., Mohamed, A.-R., Roehrig, G. H., Wood, N. B., Kern, A. L., & Schneider, J. L. (2011). The development of an open-ended drawing tool: an alternative diagnostic tool for assessing students' understanding of the particulate nature of matter. *Chemistry Education Research and Practice*, *12*(2), 121-132. https://doi.org/10.1039/C1RP90017J.

Oh, C. S., Bailenson, J. N., & Welch, G. F. (2018). A systematic review of social presence: Definition, antecedents, and implications. *Frontiers in Robotics and AI*, *5*, Article 114. https://doi.org/10.3389/frobt.2018.00114.

Olimpo, J. T., Kumi, B. C., Wroblewski, R., & Dixon, B. L. (2015). Examining the relationship between 2D diagrammatic conventions and students' success on representational translation tasks in organic chemistry. *Chemistry Education Research and Practice*, *16*(1), 143-153. https://doi.org/10.1039/C4RP00169A.

Oliver-Hoyo, M., & Sloan, C. (2014). The development of a Visual-Perceptual Chemistry Specific (VPCS) assessment tool. *Journal of Research in Science Teaching*, *51*(8), 963-981. https://doi.org/10.1002/tea.21154.

Othman, J., Treagust, D. F., & Chandrasegaran, A. L. (2008). An investigation into the relationship between students' conceptions of the particulate nature of matter and their understanding of chemical bonding. *International Journal of Science Education*, *30*(11), 1531-1550. https://doi.org/10.1080/09500690701459897.

Page, M. J., McKenzie, J. E., Bossuyt, P. M., Boutron, I., Hoffmann, T. C., Mulrow, C. D., Shamseer, L., Tetzlaff, J. M., Akl, E. A., Brennan, S. E., Chou, R., Glanville, J., Grimshaw, J. M., Hróbjartsson, A., Lalu, M. M., Li, T., Loder, E. W., Mayo-Wilson, E., McDonald, S., . . . Moher, D. (2021). The PRISMA 2020 statement: An updated guideline for reporting systematic reviews. *International Journal of Surgery*, *88*, 105906. https://doi.org/10.1016/j.ijsu.2021.105906.

Pande, P., Thit, A., Sørensen, A. E., Mojsoska, B., Moeller, M. E., & Jepsen, P. M. (2021). Long-term effectiveness of immersive VR simulations in undergraduate science learning: Lessons from a media-comparison study. *Research in Learning Technology*, *29*. https://doi.org/10.25304/rlt.v29.2482.

Papachristos, N. M., Vrellis, I., & Mikropoulos, T. A. (2017, July). *A comparison between Oculus Rift and a low-cost smartphone VR headset: Immersive user experience and learning* [Paper presentation]. 2017 IEEE 17th International Conference on Advanced Learning Technologies (ICALT), Timisoara, Romania. https://doi.org/10.1109/ICALT.2017.145.

Parong, J., & Mayer, R. E. (2018). Learning science in immersive virtual reality. *Journal of Educational Psychology*, *110*(6), 785-797. https://doi.org/10.1037/edu0000241.

Parong, J., & Mayer, R. E. (2020). Cognitive and affective processes for learning science in immersive virtual reality. *Journal of Computer Assisted Learning*, *37*(1), 226-241. https://doi.org/10.1111/jcal.12482.

Pellas, N., Dengel, A., & Christopoulos, A. (2020). A Scoping Review of Immersive Virtual Reality in STEM Education. *IEEE Transactions on Learning Technologies*, *13*(4), 748-761. https://doi.org/10.1109/TLT.2020.3019405.

Petersen, G. B., Klingenberg, S., Mayer, R. E., & Makransky, G. (2020). The virtual field trip: Investigating how to optimize immersive virtual learning in climate change education. *British Journal of Educational Technology*, *51*(6), 2099-2115. https://doi.org/10.1111/bjet.12991.

Pirker, J., Holly, M. S., Hipp, P., Konig, C., Jeitler, D., & Gutl, C. (2018). Improving physics education through different immersive and engaging laboratory setups. In M. E. Auer & T. Tsiatsos (Eds.), *Interactive mobile communication technologies and learning* (Vol. 725, pp. 443-454). Springer. https://doi.org/10.1007/978-3-319-75175-7_44.

Pirker, J., Lesjak, I., & Gütl, C. (2017). An educational physics laboratory in mobile versus room scale virtual reality - A comparative study. *International Journal of Online Engineering*, *13*(8), 106-120. https://doi.org/10.3991/ijoe.v13i08.7371.

Price, S., Yiannoutsou, N., & Vezzoli, Y. (2020). Making the body tangible: Elementary geometry learning through VR. *Digital Experiences in Mathematics Education*, *6*(2), 213-232. https://doi.org/10.1007/s40751-020-00071-7.

Pritchard, A. (2017). *Ways of learning: Learning theories for the classroom*. Routledge.

Qin, T., Cook, M., & Courtney, M. (2021). Exploring chemistry with wireless, PC-less portable Virtual Reality laboratories. *Journal of Chemical Education*, *98*(2), 521-529. https://doi.org/10.1021/acs.jchemed.0c00954.

Quillin, K., & Thomas, S. (2015). Drawing-to-learn: A framework for using drawings to promote model-based reasoning in biology. *CBE—Life Sciences Education*, *14*(1), es2. https://doi.org/10.1187/cbe.14-08-0128.

Radianti, J., Majchrzak, T. A., Fromm, J., & Wohlgenannt, I. (2020). A systematic review of immersive virtual reality applications for higher education: Design elements, lessons learned, and research agenda. *Computers & Education*, *147*, 103778. https://doi.org/10.1016/j.compedu.2019.103778.

Reeves, S. M., Crippen, K. J., & McCray, E. D. (2021). The varied experience of undergraduate students learning chemistry in virtual reality laboratories. *Computers & Education*, *175*, 104320. https://doi.org/10.1016/j.compedu.2021.104320.

Reinisch, B., Krell, M., Hergert, S., Gogolin, S., & Krüger, D. (2017). Methodical challenges concerning the Draw-A-Scientist Test: A critical view about the assessment and evaluation of learners' conceptions of scientists. *International Journal of Science Education*, *39*(14), 1952-1975. https://doi.org/10.1080/09500693.2017.1362712.

Richter, J., Sharabi, L., Luchmun, R., Geiger, T., Hale, A., & Hall, A. R. (2023). Virtual Reality as a tool for promoting diversity, equity, and inclusion within the higher education landscape. In J. Jovanovic, I.-A. Chounta, J. Uhomoibhi, & B. McLaren (Eds.), *Proceedings of the 15th International Conference on Computer Supported Education (CSEDU 2023)* (Vol. 2, pp. 574-580). https://doi.org/10.5220/0011995900003470.

Ripka, G., Grafe, S., & Latoschik, M. E. (2020). Preservice teachers' encounter with Social VR – Exploring virtual teaching and learning processes in initial teacher education. In E. Langran (Ed.), *Proceedings of SITE interactive 2020 online conference* (pp. 549-562). Association for the Advancement of Computing in Education (AACE). https://www.learntechlib.org/p/218201

Rodrigues, I., & Prada, R. (2018, November). *Virtual Reality game to teach organic chemistry* [Paper presentation]. VJ2018 — 10th Conference on Video Games Sciences and Arts, Porto, Portugal. https://vj2018.fba.up.pt/files/Papers/Pages%20from%20VJ2018-Proceedings-full-13.pdf.

Rojas-Sánchez, M. A., Palos-Sánchez, P. R., & Folgado-Fernández, J. A. (2023). Systematic literature review and bibliometric analysis on virtual reality and education. *Education and Information Technologies*, *28*(1), 155-192. https://doi.org/10.1007/s10639-022-11167-5.

Roschelle, J., & Teasley, S. D. (1995). The construction of shared knowledge in collaborative problem solving. In C. O'Malley (Ed.), *Computer supported collaborative learning* (pp. 69-97). Springer. https://doi.org/10.1007/978-3-642-85098-1_5.

Roth, W.-M. (2008). The nature of scientific conceptions: A discursive psychological perspective. *Educational Research Review*, *3*(1), 30-50. https://doi.org/10.1016/j.edurev.2007.10.002.

Rupp, M. A., Odette, K. L., Kozachuk, J., Michaelis, J. R., Smither, J. A., & McConnell, D. S. (2019). Investigating learning outcomes and subjective experiences in 360-degree videos. *Computers & Education*, *128*, 256-268. https://doi.org/10.1016/j.compedu.2018.09.015.

Rushton, G. T., Hardy, R. C., Gwaltney, K. P., & Lewis, S. E. (2008). Alternative conceptions of organic chemistry topics among fourth year chemistry students. *Chemistry Education Research and Practice*, *9*(2), 122-130. https://doi.org/10.1039/B806228P.

Rychkova, A., Korotkikh, A., Mironov, A., Smolin, A., Maksimenko, N., & Kurushkin, M. (2020). Orbital battleship: A multiplayer guessing game in immersive virtual reality. *Journal of Chemical Education*, *97*(11), 4184–4188. https://doi.org/10.1021/acs.jchemed.0c00866.

Salvadori, A., Fusè, M., Mancini, G., Rampino, S., & Barone, V. (2018). Diving into chemical bonding: An immersive analysis of the electron charge rearrangement through virtual reality. *Journal of Computational Chemistry* *39*(31), 2607-2617. https://doi.org/10.1002/jcc.25523.

Salzman, M. C., Dede, C., Loftin, R. B., & Chen, J. (1999). A model for understanding how virtual reality aids complex conceptual learning. *Presence: Teleoperators and Virtual Environments*, *8*(3), 293-316. https://doi.org/10.1162/105474699566242.

Sanchez-Vives, M. V., & Slater, M. (2005). From presence to consciousness through virtual reality. *Nature Reviews Neuroscience*, *6*(4), 332-339. https://doi.org/10.1038/nrn1651.

Šašinka, Č., Stachoň, Z., Sedlák, M., Chmelík, J., Herman, L., Kubíček, P., Šašinková, A., Doležal, M., Tejkl, H., & Urbánek, T. (2019). Collaborative immersive virtual environments for education in geography.

ISPRS International Journal of Geo-Information, *8*(3), 1-25, Article 3. https://doi.org/10.3390/ijgi8010003.

Savickiene, I. (2010). Conception of learning outcomes in the Bloom's taxonomy affective domain. *Quality of Higher Education*, *7*, 37-59. https://eric.ed.gov/?id=EJ900258

Scager, K., Boonstra, J., Peeters, T., Vulperhorst, J., & Wiegant, F. (2016). Collaborative learning in higher education: Evoking positive interdependence. *CBE—Life Sciences Education*, *15*(4), ar69. https://doi.org/10.1187/cbe.16-07-0219.

Schmidt, H.-J., Kaufmann, B., & Treagust, D. F. (2009). Students' understanding of boiling points and intermolecular forces. *Chemistry Education Research and Practice*, *10*(4), 265-272. https://doi.org/10.1039/B920829C.

Schmidt, M. (2008). The Sankey diagram in energy and material flow management. *Journal of Industrial Ecology*, *12*(2), 173-185. https://doi.org/10.1111/j.1530-9290.2008.00015.x.

Schunk, D. H. (2012). *Learning theories an educational perspective sixth edition*. Pearson.

Seritan, S., Wang, Y., Ford, J. E., Valentini, A., Gold, T., & Martínez, T. J. (2021). InteraChem: Virtual reality visualizer for reactive interactive molecular dynamics. *Journal of Chemical Education*, *98*(11), 3486–3492. https://doi.org/10.1021/acs.jchemed.1c00654.

Shadiev, R., & Li, D. (2023). A review study on eye-tracking technology usage in immersive Virtual Reality learning environments. *Computers & Education*, *196*, 104681. https://doi.org/10.1016/j.compedu.2022.104681.

Sharma, L., Jin, R., Prabhakaran, B., & Gans, M. (2018, April). LearnDNA: An interactive VR application for learning DNA structure. Proceedings of the 3rd International Workshop on Interactive and Spatial Computing, Richardson Texas.

Slater, M. (2017). Implicit learning through embodiment in immersive virtual reality. In D. Liu, C. Dede, R. Huang, & J. Richards (Eds.), *Virtual, augmented, and mixed realities in education* (pp. 19-33). Springer. https://doi.org/10.1007/978-981-10-5490-7_2.

Slater, M., Banakou, D., Beacco, A., Gallego, J., Macia-Varela, F., & Oliva, R. (2022). A separate reality: An update on place illusion and plausibility in Virtual Reality. *Frontiers in Virtual Reality*, *3*. https://doi.org/10.3389/frvir.2022.914392.

Slater, M., & Sanchez-Vives, M. V. (2016). Enhancing our lives with immersive virtual reality. *Frontiers in Robotics and AI*, *3*, Article 74. https://doi.org/10.3389/frobt.2016.00074

Slater, M., & Wilbur, S. (1997). A framework for immersive virtual environments (FIVE): Speculations on the role of presence in virtual environments. *Presence: Teleoperators & Virtual Environments*, *6*(6), 603-616. https://doi.org/10.1162/pres.1997.6.6.603.

Southgate, E., Smith, S. P., Cividino, C., Saxby, S., Kilham, J., Eather, G., Scevak, J., Summerville, D., Buchanan, R., & Bergin, C. (2019). Embedding immersive virtual reality in classrooms: Ethical, organisational and educational lessons in bridging research and practice. *International Journal of Child-Computer Interaction*, *19*, 19-29. https://doi.org/10.1016/j.ijcci.2018.10.002.

Stieff, M., Scopelitis, S., Lira, M. E., & Dane, D. (2016). Improving Representational Competence with Concrete Models. *Science Education*, *100*(2), 344-363. https://doi.org/10.1002/sce.21203.

Stull, A. T., Hegarty, M., Dixon, B., & Stieff, M. (2012). Representational translation with concrete models in organic chemistry. *Cognition and Instruction*, *30*(4), 404-434. https://doi.org/10.1080/07370008.2012.719956.

Suh, A., & Prophet, J. (2018). The state of immersive technology research: A literature analysis. *Computers in Human Behavior*, *86*, 77-90. https://doi.org/10.1016/j.chb.2018.04.019.

Sun, J., Li, H., Liu, Z. H., Cai, S., & Li, X. W. (2017). An empirical case on integration of immersive virtual environment into primary school science class. In W. Chen, J. C. Yang, A. F. M. Ayub, S. L. Wong, &

A. Mitrovic (Eds.), *Proceedings of the 25th international conference on computers in education* (pp. 566-575). Asia-Pacific Society for Computers in Education. https://aic-fe.bnu.edu.cn/docs/20181011172544773030.pdf

Taber, K. S. (1998). An alternative conceptual framework from chemistry education. *International Journal of Science Education*, *20*(5), 597-608. https://doi.org/10.1080/0950069980200507.

Taber, K. S. (2017). The nature of student conceptions in science. In S. K. Taber & B. Akpan (Eds.), *Science education. New directions in mathematics and science education* (pp. 119-131). Sense Publishers. https://doi.org/10.1007/978-94-6300-749-8_9.

Taber, K. S. (2019). Alternative conceptions and the learning of chemistry. *Israel Journal of Chemistry*, *59*(6-7), 450-469. https://doi.org/10.1002/ijch.201800046.

Talanquer, V. (2006). Commonsense chemistry: A model for understanding students' alternative conceptions. *Journal of Chemical Education*, *83*(5), 811. https://doi.org/10.1021/ed083p811.

Talanquer, V. (2018). Exploring mechanistic reasoning in chemistry. In J. Yeo, T. W. Teo, & K.-S. Tang (Eds.), *Science education research and practice in Asia-Pacific and beyond* (pp. 39-52). Springer. https://doi.org/10.1007/978-981-10-5149-4_3.

Talanquer, V. (2022). The complexity of reasoning about and with chemical representations. *JACS Au*, *2*(12), 2658-2669. https://doi.org/10.1021/jacsau.2c00498.

Tenzin, S., Won, M., & Treagust, D. (2022). Hair-raising fun: Making sense of student-generated diagrams. *The Science Teacher*, *90*(1), 48-54. https://doi.org/10.1080/00368555.2022.12293727.

Thayban, T., Habiddin, H., Utomo, Y., & Muarifin, M. (2021). Understanding of symmetry: Measuring the contribution of virtual and concrete models for students with different spatial abilities. *Acta Chimica Slovenica*, *68*(3), 1-8. https://doi.org/10.17344/acsi.2021.6836.

Thompson, M., Wang, A., Bilgin, C. U., Anteneh, M., Roy, D., Tan, P., Eberhart, R., & Klopfer, E. (2020). Influence of virtual reality on high school students' conceptions of cells. *Journal of Universal Computer Science*, *26*(8), 929-946. https://doi.org/https://hdl.handle.net/1721.1/130512.

Tippett, C. D. (2016). What recent research on diagrams suggests about learning with rather than learning from visual representations in science. *International Journal of Science Education*, *38*(5), 725-746. https://doi.org/10.1080/09500693.2016.1158435.

Treagust, D. F. (1988). Development and use of diagnostic tests to evaluate students’ misconceptions in science. *International Journal of Science Education*, *10*(2), 159-169. https://doi.org/10.1080/0950069880100204.

Treagust, D. F., & Duit, R. (2008). Conceptual change: A discussion of theoretical, methodological and practical challenges for science education. *Cultural Studies of Science Education*, *3*(2), 297-328. https://doi.org/10.1007/s11422-008-9090-4.

Treagust, D. F., & Won, M. (2023). Paradigms in science education research. In G. N. Lederman, L. D. Zeidler, & S. J. Lederman (Eds.), *Handbook of research on science education* (pp. 3-27). Routledge.

Treagust, D. F., Won, M., & McLure, F. (2017). Multiple representations and students’ conceptual change in science. In G. T. Amin & O. Levrini (Eds.), *Converging perspectives on conceptual change: Mapping an emerging paradigm in the learning sciences* (pp. 121-128). Routledge.

Tsivitanidou, O. E., Georgiou, Y., & Ioannou, A. (2021). A Learning experience in inquiry-based physics with immersive virtual reality: Student perceptions and an interaction effect between conceptual gains and attitudinal profiles. *Journal of Science Education and Technology*, *30*(6), 841-861. https://doi.org/10.1007/s10956-021-09924-1.

Tuckey, H. (1993). Studies involving three-dimensional visualisation skills in chemistry: A review. *Studies in Science Education*, *21*(1), 99-121. https://doi.org/10.1080/03057269308560015.

Tytler, R., Prain, V., Aranda, G., Ferguson, J., & Gorur, R. (2020). Drawing to reason and learn in science. *Journal of Research in Science Teaching*, *57*(2), 209-231. https://doi.org/10.1002/tea.21590.

Tytler, R., Prain, V., Hubber, P., & Waldrip, B. (2013). *Constructing representations to learn in science*. Sense Publishers.

Ungu, D. A. K., Won, M., Treagust, D. F., Mocerino, M., Matovu, H., Tsai, C.-C., & Tasker, R. (2023). Students' use of magnetic models to learn hydrogen bonding and the formation of snowflakes. *Journal of Chemical Education*, *100*(7), 2504-2519. https://doi.org/10.1021/acs.jchemed.2c00697.

Uz-Bilgin, C., Thompson, M., & Anteneh, M. (2020). Exploring how role and background influence through analysis of spatial dialogue in collaborative problem-solving games. *Journal of Science Education and Technology*, *29*, 813–826. https://doi.org/10.1007/s10956-020-09861-5.

Van Meter, P., & Garner, J. (2005). The promise and practice of learner-generated drawing: Literature review and synthesis. *Educational Psychology Review*, *17*(4), 285-325. https://doi.org/10.1007/s10648-005-8136-3.

Villena-Taranilla, R., Tirado-Olivares, S., Cózar-Gutiérrez, R., & González-Calero, J. A. (2022). Effects of virtual reality on learning outcomes in K-6 education: A meta-analysis. *Educational Research Review*, *35*, 100434. https://doi.org/10.1016/j.edurev.2022.100434.

Vygotsky, L. S. (1978). *Mind in society: The development of higher psychological processes*. Harvard University Press.

Walkington, C., Nathan, M. J., Huang, W., Hunnicutt, J., & Washington, J. (2023). Multimodal analysis of interaction data from embodied education technologies. *Educational Technology Research and Development*. https://doi.org/10.1007/s11423-023-10254-9.

Wang, F., & Hannafin, M. J. (2005). Design-based research and technology-enhanced learning environments. *Educational Technology Research and Development*, *53*(4), 5-23. https://doi.org/10.1007/BF02504682.

Webb, M., Tracey, M., Harwin, W., Tokatli, O., Hwang, F., Johnson, R., Barrett, N., & Jones, C. (2022). Haptic-enabled collaborative learning in virtual reality for schools. *Education and Information Technologies*, *27*(1), 937-960. https://doi.org/10.1007/s10639-021-10639-4.

Webb, N. M. (1982). Student interaction and learning in small groups. *Review of Educational Research*, *52*(3), 421-445. https://doi.org/10.3102/00346543052003421.

Webb, N. M. (1991). Task-related verbal interaction and mathematics learning in small groups. *Journal of Research in Mathematics Education*, *22*(5), 366-389. https://doi.org/10.5951/jresematheduc.22.5.0366.

Webb, N. M. (2009). The teacher's role in promoting collaborative dialogue in the classroom. *British Journal of Educational Psychology*, *79*(1), 1-28. https://doi.org/10.1348/000709908X380772.

Webb, N. M. (2013). Information processing approaches to collaborative learning. In C. E. Hmelo-Silver, C. A. Chinn, C. K. K. Chan, & A. O'Donnell (Eds.), *The international handbook of collaborative learning* (pp. 19-40). Routledge. https://doi.org/10.4324/9780203837290.

Webb, N. M., Nemer, K. M., Chizhik, A. W., & Sugrue, B. (1998). Equity issues in collaborative group assessment: Group composition and performance. *American Educational Research Journal*, *35*(4), 607-651. https://doi.org/10.3102/00028312035004607.

Webster, R. (2016). Declarative knowledge acquisition in immersive virtual learning environments. *Interactive Learning Environments*, *24*(6), 1319-1333. https://doi.org/10.1080/10494820.2014.994533.

Williams, L. C., Underwood, S. M., Klymkowsky, M. W., & Cooper, M. M. (2015). Are noncovalent interactions an Achilles heel in chemistry education? A comparison of instructional approaches. *Journal of Chemical Education*, *92*(12), 1979-1987. https://doi.org/10.1021/acs.jchemed.5b00619.

Winn, W. (1993). *A conceptual basis for educational applications of Virtual Reality: Technical publication R-93-9*. Human Interface Technology Laboratory of the Washington Technology Center, Seattle: University of Washington. http://www.hitl.washington.edu/projects/education/winn/winn-paper.html~

Won, M., Mocerino, M., Tang, K.-S., Treagust, D. F., & Tasker, R. (2019). Interactive immersive virtual reality to enhance students' visualisation of complex molecules. In M. Schultz, S. Schmid, & G. A. Lawrie (Eds.), *Research and practice in chemistry education* (pp. 51-64). Springer. https://doi.org/10.1007/978-981-13-6998-8_4.

Won, M., Ungu, D. A. K., Matovu, H., Treagust, D. F., Tsai, C.-C., Park, J., Mocerino, M., & Tasker, R. (2023). Diverse approaches to learning with immersive Virtual Reality identified from a systematic review. *Computers & Education*, *195*, 104701. https://doi.org/10.1016/j.compedu.2022.104701.

Won, M., Yoon, H., & Treagust, D. F. (2014). Students' learning strategies with multiple Representations: Explanations of the human breathing mechanism. *Science Education*, *98*(5), 840-866. https://doi.org/10.1002/sce.21128.

Wu, B., Hu, Y., & Wang, M. (2020). How do head-mounted displays and planning strategy influence problem-solving-based learning in introductory electrical circuit design? *Educational Technology & Society*, *23*(3), 40-52. https://www.jstor.org/stable/26926425

Wu, B., Yu, X., & Gu, X. (2020). Effectiveness of immersive virtual reality using head-mounted displays on learning performance: A meta-analysis. *British Journal of Educational Technology*, *51*(6), 1991-2005. https://doi.org/10.1111/bjet.13023.

Wu, H.-K., Krajcik, J. S., & Soloway, E. (2001). Promoting understanding of chemical representations: Students' use of a visualization tool in the classroom. *Journal of Research in Science Teaching*, *38*(7), 821-842. https://doi.org/10.1002/tea.1033.

Wu, H.-K., & Shah, P. (2004). Exploring visuospatial thinking in chemistry learning. *Science Education*, *88*(3), 465-492. https://doi.org/10.1002/sce.10126.

Wu, S. P. W., & Rau, M. A. (2019). How students learn content in science, technology, engineering, and mathematics (STEM) through drawing activities. *Educational Psychology Review*, *31*(1), 87-120. https://doi.org/10.1007/s10648-019-09467-3.

Xiao, Y., & Watson, M. (2019). Guidance on conducting a systematic literature review. *Journal of Planning Education and Research*, *39*(1), 93-112. https://doi.org/10.1177/0739456x17723971.

Yin, R. K. (2009). *Case study research: Design and methods* (4 ed., Vol. 5). SAGE publications.

Yu, Z., & Lin, X. (2020). Impact of environmental education with VR equipment on learning performance and environmental identity. In Z. Xu, R. Parizi, M. Hammoudeh, & O. Loyola-González (Eds.), *Cyber security intelligence and analytics. CSIA 2020. Advances in intelligent systems and computing* (Vol. 1147, pp. 3-9). Springer. https://doi.org/10.1007/978-3-030-43309-3_1.

Zambrano, R. J., Kirschner, F., Sweller, J., & Kirschner, P. A. (2019). Effects of prior knowledge on collaborative and individual learning. *Learning and Instruction*, *63*, 101214. https://doi.org/10.1016/j.learninstruc.2019.05.011.

Zhang, L., Bowman, D. A., & Jones, C. N. (2019, September). *Exploring effects of interactivity on learning with interactive storytelling in immersive virtual reality* [Paper presentation]. 2019 11th International Conference on Virtual Worlds and Games for Serious Applications (VS-Games), Vienna, Austria.

Zhang, X., Meng, Y., Ordóñez de Pablos, P., & Sun, Y. (2019). Learning analytics in collaborative learning supported by Slack: From the perspective of engagement. *Computers in Human Behavior*, *92*, 625-633. https://doi.org/10.1016/j.chb.2017.08.012.

Zhao, J., LaFemina, P., Carr, J., Sajjadi, P., Wallgrün, J. O., & Klippel, A. (2020, March). *Learning in the field: Comparison of desktop, immersive virtual reality, and actual field trips for place-based STEM education* [Paper presentation]. 2020 IEEE Conference on Virtual Reality and 3D User Interfaces (VR), Atlanta, GA, USA.

Zhao, J., Lin, L., Sun, J., & Liao, Y. (2020). Using the summarizing strategy to engage learners: Empirical evidence in an immersive virtual reality environment. *The Asia-Pacific Education Researcher*, *29*(5), 473-482. https://doi.org/10.1007/s40299-020-00499-w.

Zhao, R., Chu, Q., & Chen, D. (2022). Exploring chemical reactions in virtual reality. *Journal of Chemical Education*, *99*(4), 1635-1641. https://doi.org/10.1021/acs.jchemed.1c01040.

Zheng, L., Xie, T., & Liu, G. (2018). Affordances of virtual reality for collaborative learning. In T. Nishimori, Z. Li, J. C. Liu, L. Liu, H. Zhang, & C. Yin (Eds.), *International Joint Conference on Information, Media and Engineering (ICIME 2018)* (pp. 6-10). IEEE Computer Society. https://doi.org/10.1109/ICIME.2018.00011.

Zinchenko, Y. P., Khoroshikh, P. P., Sergievich, A. A., Smirnov, A. S., Tumyalis, A. V., Kovalev, A. I., Gutnikov, S. A., & Golokhvast, K. S. (2020). Virtual reality is more efficient in learning human heart anatomy especially for subjects with low baseline knowledge. *New Ideas in Psychology*, *59*, Article 100786. https://doi.org/10.1016/j.newideapsych.2020.100786.

Appendix A: Pre-Interview prompts

Snowflakes IVR Pre-interview

The prompts were adjusted depending on the willingness of the students to collaborate with peers.

1. We are going to explore how we can use the chemistry concepts we have learnt to explain the unique shape of snowflakes. Have you seen snow before? Where?
2. Here I have some images of snowflakes (*the interviewer displays pictures of some of the shapes of snowflakes*). What do you notice about the shapes of snowflakes? Discuss your ideas.
3. To explain the shape of snowflakes, let's start with the chemistry concepts we have learned so far and see how we can build on those. Imagine I am a year 11 (high school) student, what can you tell me about a water molecule?
4. Please draw the water molecule you have described at the centre of the piece of paper. [Feel free to work together to create a combined diagram if you wish].

   Why is the water molecule shaped like that? [Explain to your partner]
5. Now, let's imagine that this water molecule is at a very low temperature, say close to its freezing point, and we have another water molecule coming close to the first one to interact with it, how would you draw the interaction between those two water molecules?

   Why would the molecules interact like that? [Explain to your partner]
6. We have another molecule coming close to the first one. Is it still possible for it to interact with the first molecule? How would you draw the interaction between the third water molecule and the first one? [Please explain to your partner why the molecules would interact like this.]
   (The students were prompted to add more water molecules to the central water molecule until the students said that no more water molecules would interact with the central molecule, with reasons)
7. How do you think the interactions you have illustrated in the diagram would be translated into the shape of snowflakes?

Protein VR Pre-interview

1. In today's activity we are going to explore an important enzyme reaction in our bodies and why nerve agents are very harmful in our bodies. What do you know about enzymes? *(biological catalysts, highly specific, denatured at high temperatures, e.t.c.)*
2. In general terms, how do enzymes work? Please draw a diagram to illustrate what you mean.
3. You have mentioned that enzymes are catalysts—the breakdown of substrate molecules by enzymes is a very fast reaction. The same reaction, if carried out in a laboratory, takes hours. Why do you think this is the case? How can you explain this difference in reaction rates with and without an enzyme?
4. Have you heard about the enzyme acetylcholinesterase before? What does it do?
5. In our bodies, a molecule acetylcholine is released by nerve cells to get muscles to contract. Once this message has been received, acetylcholine needs to be rapidly removed—we do not want to have repeated and uncontrolled muscle contraction caused by continually receiving the message to contract. The enzyme acetylcholinesterase puts a stop to this message by breaking acetylcholine down into its components.
6. Because of its role in our bodies, acetylcholinesterase has been targeted by snake venoms, and chemical weapons such as sarin gas. These chemicals bind irreversibly to the enzyme, causing death in minutes. We are going to explore the structures of acetylcholine and acetylcholinesterase, its enzyme, taking note of their shapes and regions of high and low electron density and how these factors influence the catalytic reaction. Before we go to the VR, let's first go through a short activity. I have a model of acetylcholine *[Give them a model of ACh]*
   (a) Explore the model. What features of this molecule do you notice?
   (b) Which part of the acetylcholine molecule is electron-rich, and which part is electron-poor? Discuss with your peer.
   (c) As a protein, the enzyme acetylcholinesterase has many other amino acids, some react with ACh, and others offer a supporting role. Based on electron density, how do you think ACh will interact with the other amino acids in the catalytic chamber?
7. You have shared very good ideas. Let's go to the VR and explore these ideas more.

Appendix B: Post-Interview Prompts

Snowflakes IVR Post-Interview

1. What do you think you have learned from the IVR activity?
2. Now that you have explored the nature of interactions amongst water molecules, please look at your initial diagram.
    a) Are you still happy with the diagram? Please explain.
    b) How would you improve the diagram? Please explain the changes you have made.
3. Imagine that I am a year 11 student who knows about the structure and polarity of a water molecule. Starting with the structure and polarity of a water molecule, how would you explain to me why snowflakes are shaped the way they are? You may also use a diagram, if you can, to explain to me.

Protein IVR Post-Interview

1. How was the experience?
2. Which part of the learning activity was the most informative and which one was the most challenging. Why?
3. In terms of the learning, what do you think you learnt from the IVR activity? How did IVR help you learn this?
4. Still about the learning from IVR, (*If they drew diagrams of the enzyme reaction in the pre-interview*) please look at your diagram of the mechanism of an enzyme reaction again, are you still happy with it? Why or why not? How would you improve it? *[Ask them if they want to draw]*
5. (If they did not draw at the pre-interview): Imagine I am a friend from your chemistry class who has not done this activity. What would you tell me about the structure of the enzyme?
6. Before IVR, we talked about the differences between an enzyme-catalysed reaction and a similar reaction conducted in the lab without an enzyme. The reaction between the enzyme and acetylcholine is very fast. The breakdown of acetylcholine in the laboratory takes hours. Having completed the IVR activity, how can you explain the difference in rates of reaction in the two conditions?

7. The next task is going to be challenging. However, it is important for us to know what benefit you got from the IVR activity so that we can improve it. With me here, I have physical models of the amino acids in the catalytic chamber of acetylcholine and a model of acetylcholine. *[Show the students the models of the amino acids, tryptophan, serine, histidine, and glutamate; and a model of acetylcholine]*. Can you please describe the role of each of these amino acids in the catalytic reaction? I am not looking for a step-by-step mechanism of the reaction but a general idea of how these amino acids help in the reaction.
8. You have studied complex molecular systems (such as enzymes) in your chemistry (or biochemistry) classes before. How does studying these concepts in VR compare to the ways used in your chemistry classes?

Appendix C: Copyright Approval

Chemistry education research and practice

Article: Analysis of students' diagrams of water molecules in snowflakes to reveal their conceptual understanding of hydrogen bonds

GENERAL INFORMATION

Request ID	600145185	**Request Date**	19 Nov 2023
Request Status	Accepted	**Price**	0.00 AUD

> ALL DETAILS

COMMENTS

Add Comment / Attachment

22 Nov 2023 7:17:40 PM, by Publisher Representative

Permission is granted as long as the article is fully acknowledged and a link is given back to the article on our Platform. Please go to rsc.li/permissions for details. Please note that if the material specified above or any part of it appears with credit or acknowledgement to a third party then you must also secure permission from that third party before reproducing that material.

View Less

Chemistry education research and practice

Article: Change in students' explanation of the shape of snowflakes after collaborative immersive virtual reality

GENERAL INFORMATION

Request ID	600145186	**Request Date**	19 Nov 2023
Request Status	Accepted	**Price**	0.00 AUD

> ALL DETAILS

COMMENTS

Add Comment / Attachment

22 Nov 2023 7:17:03 PM, by Publisher Representative

Permission is granted as long as the article is fully acknowledged and a link is given back to the article on our Platform. Please go to rsc.li/permissions for details. Please note that if the material specified above or any part of it appears with credit or acknowledgement to a third party then you must also secure permission from that third party before reproducing that material.

View Less