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Two-center convergent close-coupling calculations for positron-lithium and positron-sodium collisions

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Synopsis The convergent close-coupling calculations of e^+-Li and e^+-Na collisions are reported. The target is treated as one active electron interacting with an inert ion core. The positronium formation channels are taken into account explicitly utilizing both negative- and positive-energy Laguerre-based states. A large number of channels and high partial waves are used to ensure the convergence of the cross sections.

The physics of positron collisions with atomic targets has attracted considerable interest during the past decade. In part this has been due to significant advances in experimental techniques and computational power available to researches. This permitted conducting new high-resolution experiments and computationally intensive calculations for a wide range of atomic and molecular targets. Also, the interest of the community has been motivated by a number of problems such as determining positron-atom bound states and anomalously high cross sections in positron scattering from macromolecules where agreement between the experiment and theory has not been reached.

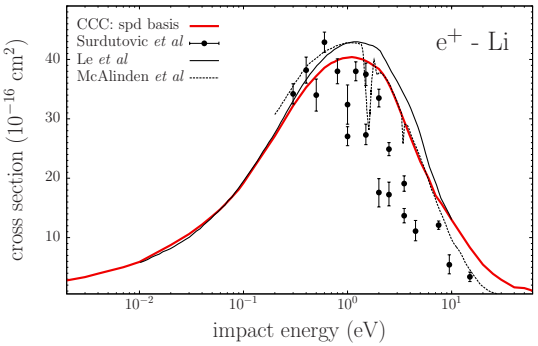

Figure 1. Total positronium formation cross section for e^+-Li calculated with the use of the CCC method [1] along with the experimental [2] and theoretical data [3, 4].

In this contribution we report our convergent close-coupling (CCC) results on positron scattering from atomic lithium and sodium. In positron collisions with alkalies both elastic and rearrangement channels are open at all incident energies. This generates a particular challenge for practical calculations since both centers, atom and positronium, can participate in a collision event on equal footing. To take this into account we use the two-center expansion for the wavefunction of interest

$$\Psi = \sum_{\alpha}^{N_\alpha} F_\alpha(\rho_\alpha)\psi_\alpha^{\mathbf{N}_\alpha}(\mathbf{r}_\alpha) + \sum_{\beta}^{\mathbf{N}_\beta} \mathbf{F}_\beta(\rho_\beta)\psi_\beta^{\mathbf{N}_\beta}(\mathbf{r}_\beta) \quad (1)$$

where $\psi_\alpha^{N_\alpha}$ and $\psi_\beta^{N_\beta}$ are atomic and positronium pseudostates, respectively, and F_α and F_β are their associated weight functions. Decomposition (1) results in a set of close-coupled equations for the T-matrix elements which we solve numerically.

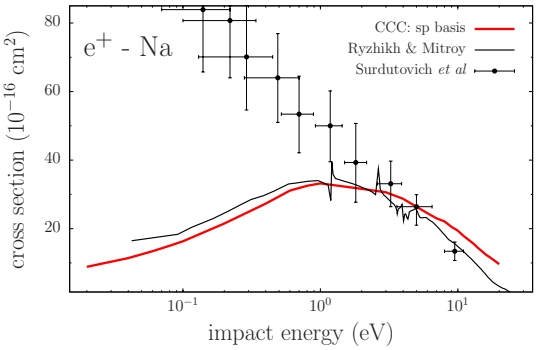

Figure 2. Same as Fig.1 but for e^+-Na scattering along with experimental and theoretical data from [2] and [5] respectively.

In Figures 1 and 2 we give our Ps formation results for Li and Na, respectively.

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