

High-Precision Cross Sections for Low-Energy Electron–Atom Collisions.

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Domain : Low-Energy Electron–Atom Interactions

In recent years, much progress has been achieved in calculating reliable cross-section data for electron scattering from atoms and ions. In particular, the “convergent close-coupling” (CCC) [1] and “*R*-matrix with pseudo-states” (RMPS) [2] methods have been extremely successful in describing elastic scattering as well as electron-impact excitation and ionization of light quasi-one and quasi-two electron targets, such as atomic hydrogen, helium, the alkalis, and the alkali-earth elements. However, accurate calculations of electron collisions with more complex targets, notably the heavy noble gases Ne–Xe, heavy quasi-one electron targets such as Zn, Ba, or Hg, and transition metals such as Fe or Mo [3], continue to be a major challenge.

We have further developed a new version of the *R*-matrix (close-coupling) method, using a *B*-spline basis with non-orthogonal sets of term-dependent orbitals [4-6]. This method allows us to generate target descriptions of unprecedented accuracy in collision calculations. Example results for some of the systems mentioned above illustrate that the flexibility of the *B*-spline *R*-matrix (BSR) method to describe both the *N*-electron target and the (*N*+1)-electron collision problems is of crucial importance for obtaining highly accurate cross sections, particularly in the low-energy near-threshold regime, which is often dominated by resonance structure.

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