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High-Precision Cross Sections for Electron-Atom Collisions in Laser and Lighting Applications[1]

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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 recently 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]. This method allows us to generate target descriptions of unprecedented accuracy in collision calculations. Example results [5-7] 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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