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Benchmark Calculations of Atomic Data for Modelling Applications[1]

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In recent years, much progress has been achieved in calculating reliable cross-section datasets for electron scattering from atoms and ions, in particular quasi-one and quasi-two electron systems such as H, He, the alkalis, and the alkaline-earth metals. Until recently, however, accurate calculations of electron collisions with more complex targets, such as the heavy noble gases Ne−Xe, have remained a significant challenge to theory. In this talk, we will illustrate with a few examples how the B-spline R-matrix (BSR) method with non-orthogonal orbitals [1-3] has been able to dramatically improve the quality of theoretical datasets for oscillator strengths [4] as well as electron collisions with numerous targets, including the heavy noble gases [5], and how these data were used successfully in modelling applications [6]. The most recent extension of the method, the B-spline R-matrix with Pseudo-States (BSRMPS) approach, includes a large number of pseudostates in the close-coupling expansion, thereby allowing for the fully non-perturbative treatment of highly correlated processes such as ionization and even ionization with simultaneous excitation [7].

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