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Adiabatic-nuclei calculations of electron and positron scattering from molecular hydrogen and its ion[1]

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We report the extension of the convergent close-coupling (CCC) method for electron-molecule scattering [1] to the adiabatic-nuclei (AN) formulation which allows us to study the effects of nuclei motion and electron-impact dissociation processes. For H_2^+ and its isotopologues [2] we have modeled collisions with hot (vibrationally excited) molecules and compared with available experimental data for dissociative ionization, proton production, and the dissociative products kinetic energy release distributions. For H_2 we have performed AN calculations of positron scattering with emphasis on establishing convergent low-energy total and vibrational $0 \rightarrow 1$ excitation cross sections. To study electron collisions with H_2 we have developed a spheroidal coordinate formulation of the CCC method that allows for an accurate description of the target wave functions to large inter-nuclei distances. Excitation cross sections for vibrationally resolved transitions between low-lying H_2 states have been calculated and used to determine vibrational excitation of the H_2 ground state via excitation of electronically excited singlet states and radiative cascade. [1] Zammit et al., J. Phys. B **50**, 123001 (2017). [2] Zammit et al., Phys. Rev. A **90** 022711 (2014)

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