Convergent close-coupling approach to electron-molecule collisions

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Molecular hydrogen is the simplest neutral molecule, and yet there are still substantial gaps in the literature of accurate cross sections for electron-H_2 collisions. Collisional-radiative models of fusion or astrophysical plasmas containing H_2 require cross sections resolved in electronic, vibrational, and rotational levels, leading to data sets containing in excess of 100,000 transitions. Although a number of theoretical methods for modelling electron-molecule collisions have been available for decades, none are capable of performing the large-scale convergence studies required to ensure the accuracy of the calculated cross sections at all incident energies, and in many cases they make use of approximations which limit the processes which can be studied or the energy regions where the methods are valid.

The molecular convergent close-coupling (MCCC) method has been developed with the aim of producing accurate rovibrationally-resolved elastic, excitation, ionisation, and total cross sections for electrons and positrons scattering on diatomic molecules. The use of prolate spheroidal coordinates allows the target structure to be accurately described over the range of internuclear separations required to account for the nuclear motion.

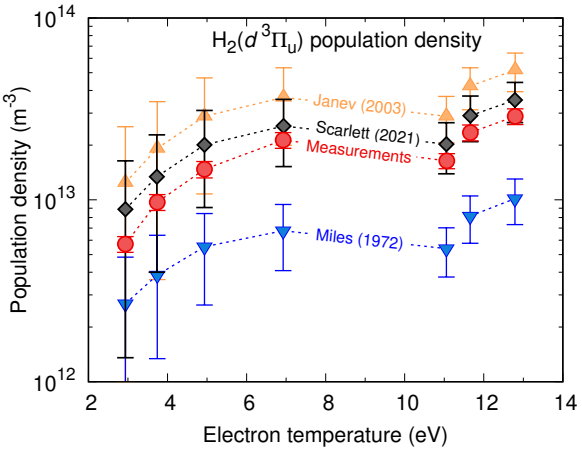

Figure 1. Comparison of measured population densities of the H_2 $d\,^3\Pi_u$ state with predictions from the Yacora CR model [1] using cross sections from the previously recommended data sets of Janev *et al.* [2] and Miles *et al.* [3], as well as the MCCC cross sections [4].

In this presentation we describe the MCCC method and present results for electron scattering on H_2. We will discuss the application of MCCC cross sections in a collisional-radiative model for the triplet system of H_2 (see Figure 1), calculations of dissociation cross sections, and studies of the Fulcher-α band polarisation.

References:
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