Molecular hydrogen collision data

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Collisions between particles on the molecular scale are ubiquitous in the universe. Technologies and sciences that rely on electron collision data include electric lighting, fusion technology, materials research, climate science, astrophysics, radiotherapy and plasma cancer therapy.

Although collision physics is of technological and scientific interest, accurate and efficient scattering models are not easily utilised or do not exist. Currently convergence studies are rarely perfomed for electron-molecule scattering and hence there is a lack of accurate comprehensive theoretical collision data even for the major scattering processes. Adequate and systematic account of large close-coupling (target state) and projectile partial-wave expansions is the most difficult challenge for theoretical techniques, and yet is the strength of the molecular convergent close-coupling (CCC) method.

Recently we applied the CCC method to electron scattering from the hydrogen molecule H_2 [1] and its hot (vibrationally excited) ion H_2^+ [2]. Convergence of the major scattering processes has been explicitly demonstrated in the fixed-nuclei approximation. For H_2^+, collision data was obtained for each vibrational state of the molecule and cross sections were then weighted according to the Frank-Condon (FC) distribution to compare with experiments. As a demonstration of the method we present electron-impact ionisation cross sections of the respective molecules in Fig. 1. The CCC results are the first available *ab initio* results over a broad energy range and they are in excellent agreement with experiment.

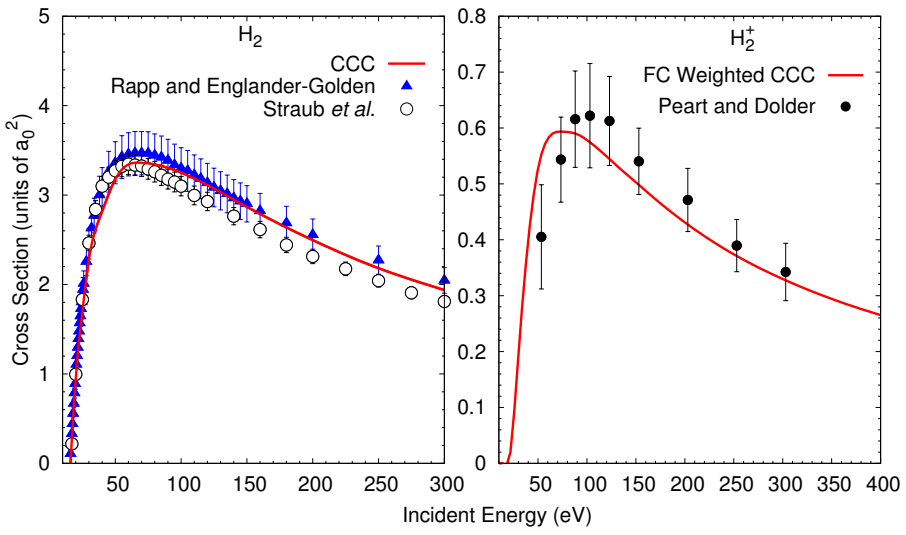

Figure 1: *Ionisation cross sections of electron scattering from molecular hydrogen H_2 and its hot (vibrationally excited) ion H_2^+. Convergent close-coupling (CCC) results are compared with experimental measurements [3, 4, 5].*

References

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