Electron scattering from molecular hydrogen

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Synopsis A comprehensive set of excitation cross sections for electron collisions with molecular hydrogen have been produced. Convergence of the cross sections has been established to be better than 11%.

We have recently extended the convergent close-coupling (CCC) method to model electron and positron collisions with molecules [1, 2, 3, 4, 5, 6]. For these types of collisions it is our aim to provide a comprehensive set of cross sections that are demonstratively convergent and valid over a wide range of incident energies.

Molecular hydrogen is the simplest neutral molecule. For theorists the H_2 molecule is a natural starting point for developing and testing computational techniques. A large number of theoretical methods have been applied to study e-H_2 collisions in the past, however modern large-scale close-coupling techniques have not yet been applied to the problem (with the exception of R-matrix with pseudo-state and time-dependent close-coupling methods applied to calculation of ionisation). The largest and most detailed calculations are more than ten years old. They included no more than the first nine states of H_2 therefore neglecting coupling to the high lying excited states and ionisation channels. No convergence studies have been performed for e-H_2 scattering to date and the accuracy of the calculated cross sections is largely uncertain.

This unsatisfactory situation is surprising given the importance of the H_2 molecule in fundamental science and applications. Molecular hydrogen is the most abundant molecule in the Universe, particularly in interstellar space and in the atmospheres of gas giants and the outermost planets in our Solar System. It is present at the edge region of fusion devices and widely used in plasma processing. A comprehensive dataset of e-H_2 collision data is in great demand for modelling various astrophysical and technological plasmas. It is our aim to provide such data.

We present results of large-scale fixed-nuclei close-coupling calculations of electron scattering from the ground state of H_2 [3,4] for incident electron energies from 10 to 300 eV. The calculations have been performed using a single-centre implementation of the CCC method. We have established convergence of the close-coupling expansion by increasing the size of the calculations from nine to 491 states. A partial wave expansion of the projectile electron wave function has been performed to the maximum angular momentum value Lp=8 and total angular momentum projection Mtot=8. Higher partial waves have been accounted for using a Born top-up procedure. Overall, the uncertainty of the CCC cross sections is better than 11%. Differential and angle integrated cross sections will be presented for a number of excited states ($b\ ^3\Sigma_u^+$, $a\ ^3\Sigma_g^+$, $c\ ^3\Pi_u$, $B\ ^1\Sigma_u^+$, $E,F\ ^1\Sigma_g^+$, $C\ ^1\Pi_u$, $e\ ^3\Sigma_u^+$, $h\ ^3\Sigma_g^+$, $d\ ^3\Pi_u$, $B'\ ^1\Sigma_u^+$, $D\ ^1\Pi_u$, $B''\ ^1\Sigma_u^+$, $D'\ ^1\Pi_u$) together with total and total ionization cross sections.

As an example, we present in Fig. 1 the electron-impact excitation cross section for the $b\ ^3\Sigma_u^+$ state.

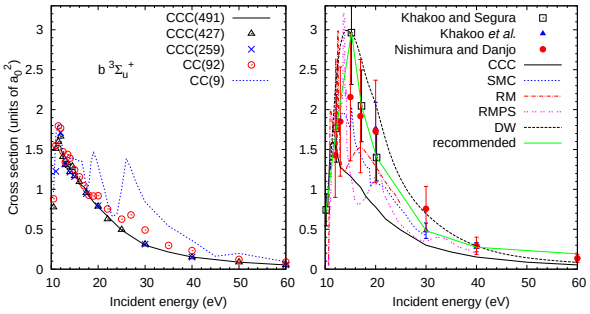

Figure 1. Electron impact excitation cross section of the $b\ ^3\Sigma_u^+$ state of H_2. The left panel presents convergence studies for the CCC models and the right panel presents the comparison with experiment and previous calculations, see Ref. [6] for details.

References

[1] M. C. Zammit *et al.* 2013 *Phys. Rev. A* **87** 020701 (R)

[2] M. C. Zammit *et al.* 2013 *Phys. Rev. A* **95** 022707

[3] M. C. Zammit *et al.* 2013 *Phys. Rev. A* **88** 062709

[4] M. C. Zammit *et al.* 2014 *Phys. Rev. A* **90** 022711

[5] M. C. Zammit *et al.* 2016 *Phys. Rev. Lett.* **116** 233201

[6] M. C. Zammit *et al.* 2017 *Phys. Rev. A* **95** 022708

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