Electron stopping powers in H_2

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Synopsis Calculations of theoretical mass stopping powers of electons in H_2 have been performed in the energy range of 0 to 300 eV. Generally good agreement with experiment is found.

An important parameter of interest in medical and enviromental applications is the electron stopping power (STP). Accurate evaluation of the electron STP in molecules requires a complete set of electron impact cross sections for all important reaction channels including excitation, ionisation and dissociation. Calculations of the STP have been performed for a number of molecules using Born-Bethe theory with results available from the NIST database [1]. The Born-Bethe results for the STP are expected to be accurate at high incident electron eneregies. However, measurements of the STP for a number of diatomic molecules [2] revealed discrepancies with the Born-Bethe results even at very high energies (5000 eV). Calculations are particular difficult for intermediate energies (10-500 eV) where reliable set of cross sections is largely unavailable.

In this report we present calculations of electron STP for the H_2 molecule performed using the convergent close-coupling method (CCC). We have recently obtained a comprehensive set of electron-impact excitation, elastic, ionisation and total cross sections for e-H_2 scattering over wide energy range (0.1-300 eV) [3, 4]. Here we use the results of the CCC calculations to obtain the electron mass STP using the following relation

$$-\frac{1}{\rho}\frac{dE}{dx} = \frac{N_a}{M}\sum_{n=1}^{N_T}(e_n - e_0)\sigma_n(E_i),\qquad (1)$$

where N_a is the Avogadro number, ρ is the density of the target, M is the molar mass, σ_n is the electron impact excitation cross section from the ground state of H_2 with energy e_0 to the final state n with energy e_n and N_T is the number of the pseudostates.

In Fig. 1 results for the electron mass STP in H_2 are presented for a number of models to establish convergence and elucidate the importance of various reaction channels. The smallest model CC(92) includes only 92 pseudostates describing the bound states of the H_2 molecule. The largest model CCC(492) has in addition a large number of

pseudostates modeling coupling to ionisation channels. The large difference between the CCC(492) and CC(92) models indicate the particular importance of the ionisation channels for STP calculations. Results of the CCC(259) and CCC(427) models demonstrate a very good rate of convergence of our results. Comparison with measurements of Muńoz *et al.* [5] shows generally a good agreement. Both theory and experiment show the maximum at 75 eV. The experiment is somewhat higher than the CCC value below 50 eV. We find this is related to the way the experimental STP values were obtained from the measured average excitation energy and the total and elastic cross sections utilised.
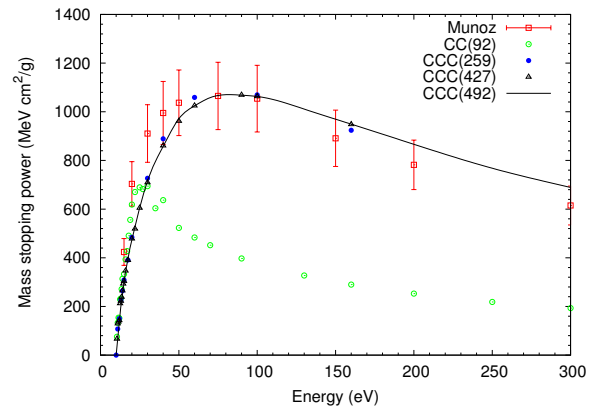
Figure 1. Mass stopping power for electron scattering on the ground state of molecular hydrogen. The CCC results are produced from the calculations descibed in Ref. [4]. Experimental data are due to Muńoz *et al.* [5].

References

[1] Stopping power and range tables for electrons. http://physics.nist.gov/PhysRefData/Star/Text/method.html

[2] J. C. Oller *et al.* 2006 *Chem. Phys. Let.* **421** 432

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

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

[5] A. Muńoz *et al.* 2007 *Chem. Phys. Let.* **433** 2614

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