Electron stopping powers in $\text{H}_2$

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Synopsis
Calculations of theoretical mass stopping powers of electrons in $\text{H}_2$ 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 environmental 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 energies. 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 particularly 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 $\text{H}_2$ 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 $\text{e-H}_2$ 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

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

where $N_a$ is the Avogadro number, $\rho$ is the density of the target, $M$ is the molar mass, $\sigma_n$ is the electron impact excitation cross section from the ground state of $\text{H}_2$ with energy $e_0$ to the final state $n$ with energy $e_n$ and $N_f$ is the number of the pseudostates.

In Fig. 1 results for the electron mass STP in $\text{H}_2$ 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 $\text{H}_2$ 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 Muñoz 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.

References

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