Molecular convergent close-coupling calculations for the ionisation of H_2 and its isotopologues

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The molecular convergent close-coupling (MCCC) method was used to calculate cross sections for total ionisation of H_2 and its isotopologues, starting from vibrational levels in the $X\ ^1\Sigma_g^+$, $B\ ^1\Sigma_u^+$, $C\ ^1\Pi_u$, $EF\ ^1\Sigma_g^+$, $a\ ^3\Sigma_g^+$ and $c\ ^3\Pi_u$ electronic states. Electron collisions with H_2 and its isotopologues play an important role in governing the dynamics of various low-temperature plasmas relevant in fusion and astrophysical applications. We compare our calculations with those of Wünderlich [1] and find generally good agreement.

The cross sections for total ionisation of H_2 from the $v = 0$ vibrational level in the $X\ ^1\Sigma_g^+$, $B\ ^1\Sigma_u^+$, $C\ ^1\Pi_u$, $EF\ ^1\Sigma_g^+$, $a\ ^3\Sigma_g^+$ and $c\ ^3\Pi_u$ electronic states are shown in Figure 1 and are compared with calculations by Wünderlich [1] obtained using the semi-classical Gryzinski method. Generally, we find good agreement with Wünderlich [1] at high energies but not in the intermediate energy range, as expected. There are several experiments [2, 3] for ionisation of the ground state $X\ ^1\Sigma_g^+(v = 0)$ where we find good agreement. However, there are no experimental data for excited states.

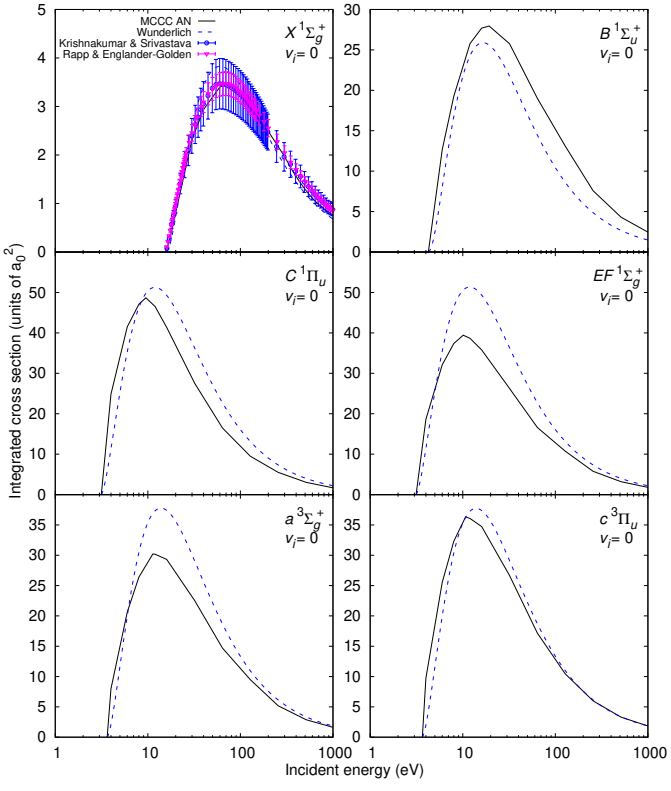

Figure 1: Cross sections for electron-impact ionisation of various electronic states of H_2 in the $v = 0$ vibrational level. All panels include comparison with Wünderlich [1]. Measurements by Krishnakumar & Srivastava [3] and Rapp & Englander-Golden [2] are included for $X\ ^1\Sigma_g^+$.

[1] D. Wünderlich, At. Data Nucl. Data Tables **140**, 101424 (2021)

[2] D. Rapp and P. Englander-Golden, J. Chem. Phys. 43, 1464 (1965).

[3] E. Krishnakumar and S. K. Srivastava, J. Phys. B: At., Mol. Opt. Phys. 27, L251 (1994).