

2nd IAEA Technical Meeting on the Collisional-Radiative Properties of Tungsten and Hydrogen in Edge Plasma of Fusion Devices

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Electron collisions with molecular hydrogen and its isotopologues

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Electron-molecule cross sections resolved in the rovibrational levels of the target are required for determining the properties and dynamics of many low-temperature plasmas. We have applied the Molecular Convergent Close-Coupling (MCCC) method to produce a comprehensive set of vibrationally-resolved cross sections for electron collisions with molecular hydrogen and its isotopologues comprised of more than 60,000 entries. This complete collision data set is available to the research community via the dedicated MCCC database (mccc-db.org). For H₂ the data set includes transitions from all bound vibrational levels of the ground electronic state to all vibrational levels of 18 excited electronic states (all states in the $n = 2, 3$ shells) with similar datasets for each of the isotopologues. We are working on producing a vibrationally resolved set of cross sections for scattering on the electronically excited $c^3\Pi_u$, $a^3\Sigma_g^+$, $B^1\Sigma_u^+$, $C^1\Pi_u$, and $EF^1\Sigma_g^+$ states of all H₂ isotopologues with first results (not vibrationally-resolved) already available. Recent calculations have also been performed for vibrationally-resolved ionisation of the $n = 1-2$ states, as well as fully rovibrationally-resolved transitions within the ground state and between the ground and $n = 2$ states. An overview of the available MCCC dataset will be presented, and examples of its utilisation in fusion and astrophysical plasma modelling will be given.

Primary author: SCARLETT, Liam

Co-authors: FURSA, Dmitry (Curtin University); BRAY, Igor (Curtin University); Dr ZAMMIT, Mark (Los Alamos National Laboratory)

Presenter: SCARLETT, Liam

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