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Electron impact dissociation of molecular hydrogen and its isotopologues

Content

Dissociation processes play significant roles in the modeling of hydrogenic plasmas. An accurate description of dissociation processes requires a comprehensive set of electron-impact excitation cross sections that are fully resolved in transitions between vibrational levels of the ground and excited electronic states. Such data set has recently been produced by the Curtin University research group using the Molecular Convergent Close-Coupling (MCCC) method for molecular hydrogen and all isotopologues, and contains more than 60,000 entries [1]. This complete collision data set is available to the research community via the LXCat database and the dedicated MCCC database (mccc-db.org).

The MCCC cross section dataset was used to determine cross sections of dissociation into neutral fragments for electron scattering on the ground and vibrationally excited states of molecular hydrogen and isotopologues [2]. The radiative cascade from the excited bound vibrational levels can lead to dissociation via the vibrational continuum of lower electronic states. For triplet states, the radiative cascade terminates on the dissociative $b\ ^3\Sigma_u^+$ state. For singlet states, it terminates on the ground state leading to a population of the bound vibrational levels and dissociation via the ground state vibrational continuum. We have produced a comprehensive set of cross sections for vibrational excitations and dissociation of molecular hydrogen and isotopologues via electron-impact excitation and radiative cascade [3].

Electron-impact dissociation proceeds almost exclusively via excitation of the dissociative $b\ ^3\Sigma_u^+$ state in low-temperature plasmas. The latest measurements for dissociation of the ground vibrational level of H_2 are in excellent agreement with MCCC calculations [4]. However, in the absence of similar measurements for vibrationally-excited or isotopically substituted H_2, cross sections for dissociation of these species must be determined by theory alone. We have recently [5] identified large discrepancies (up to a factor of three) between MCCC cross sections and the recommended and widely used R-matrix cross sections [6] for dissociation of vibrationally-excited H_2, D_2, T_2, HD, HT, and DT, with disagreement in both the isotope effect and dependence on an initial vibrational level. The source of the discrepancies and the consequences for plasma models which have incorporated the previously recommended data will be discussed.

We have conducted a Monte-Carlo simulation of electron beam propagation in a gas of molecular hydrogen [7]. Ab-initio estimates have been obtained for energy deposition parameters and dissociation probabilities due to the primary and secondary electrons. The uncertainty of the collisions cross section dataset leads to uncertainties of the derived collision data. We have developed a computational framework for propagating uncertainties for such derived collision data using the Total Monte-Carlo method.

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