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Benchmark Calculations of Electron Impact Electronic Excitation of the Hydrogen Molecule THOMAS MELTZER, JONATHAN TENNYSON, University College London, ZDENEK MASIN, Charles University, MARK ZAMMIT, Los Alamos National Laboratory, LIAM SCARLETT, DMITRY FURSA, IGOR BRAY, Curtin University — Electron collisions with molecules are vital for modelling planetary atmospheres as well as interstellar and industrial plasmas. Reliable data for molecules of interest is extremely sparse and, to date, very few of these molecules have been benchmarked. We present benchmark integrated and differential cross-sections for electron collisions with molecular hydrogen. These calculations are of practical importance, especially for excited electronic states that can be intrinsically difficult to resolve experimentally. We compare the well established *ab initio* R-matrix method with the newly developed Molecular Convergent Close-Coupling (MCCC) approach. Owing to new developments in the UKRMol+ code [1], such as the addition of a mixed B-spline and Gaussian-type orbital continuum, we have been able to push the boundaries of our previous R-matrix calculations to produce accurate cross-sections. Our model uses an R-matrix sphere of 100 Bohr – the largest ever used – to contain the diffuse excited states of H_2, and a large number of outer region channels (1,500 per symmetry). The results show good agreement with the MCCC results [2] and experimental data.
[1] Z. Mašín *et al.*, CPC 249, 107092 (2020).
[2] M. C. Zammit *et al.*, PRA 95, 022708 (2017).

Thomas Meltzer
Charles University

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