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Molecular data for hydrogen plasmas

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Low-temperature hydrogen plasmas are ubiquitous throughout the Universe. They exist in fusion plasmas, solar atmospheres, planetary atmospheres, primordial gas clouds, and determined much of the chemistry of the early Universe. To accurately model these plasmas requires a vast amount of atomic and molecular collision data.
Recently we have embarked on the projects of calculating *ab initio* electron- and photon-molecule data of important diatomics. In this talk, I will present our results on the hydrogen molecule H_2, its ion H_2^+, the isotopologues, and discuss possible implications of these new results.
To model electron-molecule collisions we have developed the molecular convergent close-coupling method [1-3]. Results from these studies are the first of their kind: calculating cross sections of all electronically driven processes and explicitly demonstrating convergence of the cross sections over a broad range of impact energies. Generally, the results are in good agreement with experiments, however, for some major processes large discrepancies are seen with generally "accepted" and used data.
For the photon-molecule project, we have recently developed our own code with the goal of calculating comprehensive opacity tables that are accurate across the entire range of temperature space, from molecular dominated opacities through to ion dominated opacities. Recently we calculated state-resolved photodissociation cross sections of H_2^+ [4] via the electronically excited states, and investigated isotopic effects. We also explored radiative association via excited states. We close by briefly discussing how the radiative association cross sections computed here may be of use in modeling the formation of anti-hydrogen molecular ions.
[1] M. C. Zammit *et al. Phys. Rev. Lett.* **116**, 233201 (2016)
[2] M. C. Zammit *et al. Phys. Rev. A* **95**, 022708 (2017)
[3] M. C. Zammit *et al. Phys. Rev. A* **90**, 022711 (2014)
[4] M. C. Zammit *et al. Astrophys. J.* **851**, 64 (2017)