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H_2 : a simple molecule with complex dynamics

Adam Kirrander,[1]

[1] *PTCL, Oxford University, United Kingdom*

adamk@physchem.ox.ac.uk

The hydrogen molecule may be the simplest of molecules, but its highly complex and non-adiabatic dynamics is far from simple. Due to the low mass of the nuclei, separation into electronic, vibrational and rotational energy becomes difficult for excited states and the energy levels are much better described as mixed rovibronic levels. Furthermore, highly excited rovibronic levels couple to the ionisation and dissociation continua. These states have a limited lifetime, which gives them an inherent line width in spectral measurements.
We apply Multichannel Quantum Defect Theory (MQDT) and R-matrix theory to calculate and interpret preionised and predissociated hydrogen spectra. Furthermore, we show how to obtain branching ratios for the dissociative reactions. These branching ratios are highly relevant to astrophysical processes in diffuse interstellar clouds. Finally, we intend to emphasise how our theoretical treatment gives a physically intuitive understanding of the dynamics of highly excited molecules in general.