VIBRATIONAL EXCITATION OF H_2 MEDIATED BY THE $^2\Sigma_g$ FESHBACH RESONANCE

Eliane M. de Oliveira, Márcio T. do N. Varella and Marco A. P. Lima

Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, UNICAMP, 13083-970, Campinas, São Paulo, Brazil

In low−energy electron scattering by polyatomic molecules, the coupling between electronic and vibrational degrees of freedom plays an important role when the incident particle is temporarily captured in the neighborhood of the molecule (resonance). This phenomenon is strongly responsible for the formation of reactive species (ions) in discharge environments (cold plasmas).

Hydrogen molecule has a number of nearby low-lying electronic states. In particular, there are experimental data on excitation to the lowest excited states, all of which have vertical excitation thresholds in the range 10-13eV. These studies yield a wealth of data including features which have been associated with several series of resonances [1]. While considerable effort has been devoted to the $^2\Sigma_u$ shape resonance in elastic e^-−H_2 collisions, reported theoretical data for core-excited and Feshbach resonances are sparse. Hydrogen may be viewed as a prototype system presenting the essential dynamical features and difficulties found in more complex molecules.

In this work, we study vibrational excitation and dissociation of H_2 mediated by the $^2\Sigma_g$ Feshbach resonance. Electron collisions are described with the Schwinger multichannel method (SMC) [2] in combination with a time-dependent formulation of the Local-Complex-Potential (or Boomerang) model [3] to account for the nuclear dynamics. We explore the e^-–H_2 $^2\Sigma_g$ resonance associated with the $a^3\Sigma_g^+$ parent state of H_2 and its influence on the elastic and $X^1\Sigma_g^+ \rightarrow b^3\Sigma_u^+$ excitation cross section. To the best of our knowlege, a systematic *ab initio* study of this resonance has never been carried out. In Fig. 1 we show the resonance position (upper panel) and width (lower panel) as a function of the interatomic distance (R). The upper panel also shows the potential energy curves for the electronic states of interest, obtained with restricted Hartree-Fock and improved-virtual-orbital SCF wave functions.

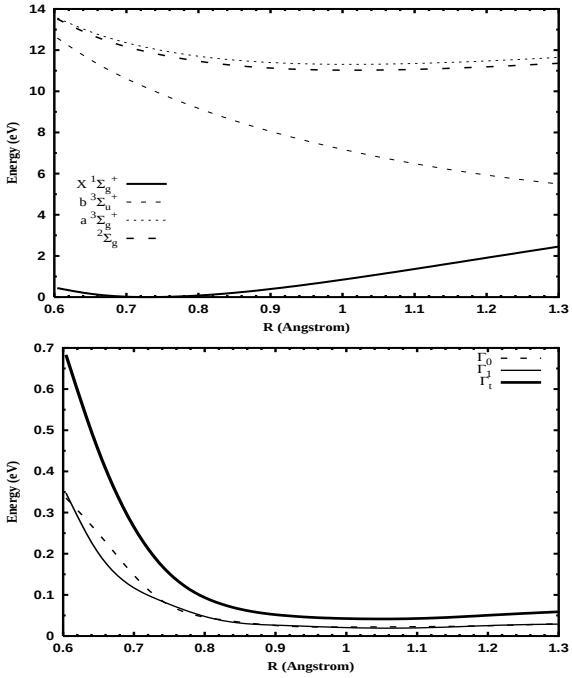

Fig. 1. Upper panel: Potential energy curves of H_2 and H_2^- ($^2\Sigma_g^+$). Lower panel: Resonances width of H_2^- ($^2\Sigma_g^+$) as a function of the internuclear distance.

References

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