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Dissociative photoionization of H_2

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Introduction

Absorption of photons with energy above the 18.1eV in H_2 molecule leads to emission of an electron and dissociation of the molecule according to the equation $H_2 + h\nu \rightarrow H + H^+ + e^-$. This is called dissociative ionization and the process we are interested in. The doubly excited states (DES) of H_2 are embedded in this ionization continuum. The DES are both dissociative and autoionizing.

Recent theoretical work [1] has suggested that higher DES, the so called Q_3, Q_4,. . . states, could contribute significantly to the measured proton kinetic energy distribution (KED) spectrum at high photon energies. Where, the notation Q_i indicates DES lying above the i and below the i+1 ionization thresholds. We have investigated the contributions of DES to the dissociative ionization in the proton KED spectra by combining high-energy resolution experiments with accurate theoretical calculations [2].

Experiment

The experiment was performed using a 24-m spherical grating monochromator with a 200-lines/mm grating installed at BL 3B. The polarization of monochromatized light was estimated to be ~80%. An effusive gas nozzle was used to feed a flow of hydrogen molecules interacting perpendicularly the photon beam. The kinetic energy of proton was analyzed by a hemispherical electrostatic energy analyzer [3]. The analyzer and gas nozzle were rotated around the photon beam. The KED spectra were measured at 0° and 90° with respect to the light polarization vector.

Results and Discussin

Fig. 1 shows the proton KED spectra obtained at 0° (left) and at 90° (right) with the theoretical cross sections. The experimental results have been normalized to the theoretical cross-sections at a photon energy of 39 eV.

In the spectra of 0°, peak E is the signature of the autoionizing Q_1 and Q_2 states of $^1\Sigma^+_u$ symmetry. It can be seen that the intensity of peak E decreases with photon energy, in good agreement with the theory. The theoretical results show that, between 36 and 39 eV, a substantial part of the peak D intensity of 0° is due to the Q_3 and to a lesser extent Q_4 DES. While for the peak D obtained at 90°, the Q_3 and Q_4 states barely contribute to the peak intensities. In the experimental spectrum at 36 eV, there is an additional peak F in both of 0°and 90°, which is explained in terms of the interference between direct ionization and autoionization while the molecule dissociates. In the results at 90°, the peaks A, B and C are mainly due to the lowest Q_2 DES of $^1\Pi_u$ symmetry as shown below 36 eV [4]. However, between 36 and 39eV, contributions from higher Q_2 states are quite significant to these peaks.

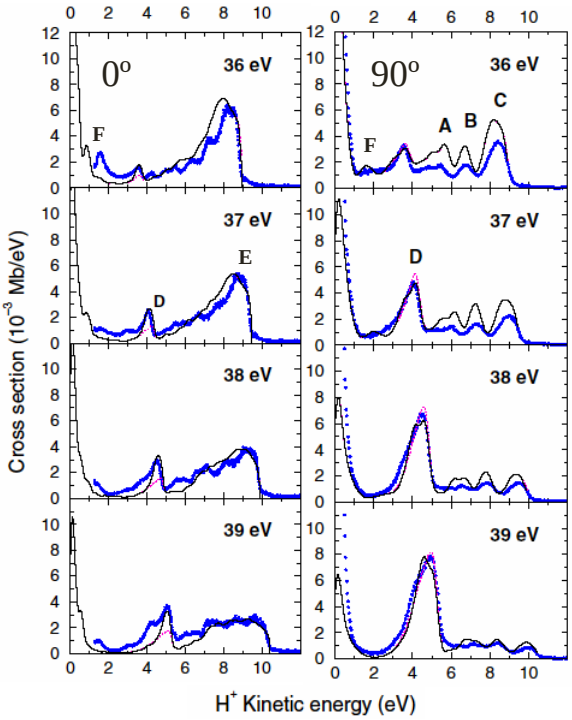

Fig. 1. Proton KED spectra of H_2 in the photon energy range 36-39 eV. Dots: experiment; full black curves: theory; dotted red curves: calculated background excluding Q_3 and Q_4 DES.

References

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