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Strong Field dissociative ionization of the D_2^+

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Synopsis Strong field dissociative ionization of the D_2^+ molecule in the multiphoton regime is investigated employing *ab initio* calculations for fixed molecular axis orientations. The resulting joint (photoelectron and nuclear kinetic) energy spectra are explored. The number of photons absorbed in each multiphoton peak of these spectra is determined analyzing the angular distribution of the photoelectrons, while the exact path followed by D_2^+ is identified studying the time evolution of the nuclear wave packets.

Despite being the simplest molecular system, the complete dynamical description of the D_2^+ considering all electronic and nuclear degrees of freedom is not a trivial task. Present-day theoretical approaches employed for the investigation of photoionization usually solve the problem in reduced dimensions, and commonly neglect the rotation of the molecule. Our previous studies on the photodissociation of D_2^+ [1, 2] showed the importance of the molecular rotation as the resulting light induced conical intersections (LICIs) influenced strongly the dynamical properties of the molecule.

In this work we incorporate the ionization in our two-state (ground and first excited) model [1, 2] previously developed for the description of photodissociation by considering a third ionized state corresponding to a well defined asymptotic momentum $\vec{k}$. For this three-level system the 1D nuclear Schrödinger equation is solved numerically and the KER spectra is extracted from the final population of the ionized state. The combined ionization and dissociation spectrum is obtained by performing individual calculations for several ionization channels (i.e. continuum electron momenta $\vec{k}$).

Here we report our results obtained for the dissociative ionization of D_2^+ in the multiphoton regime. Although our long term goal is to describe the dynamics in the LICI picture, the present results were obtained for fixed molecular axis orientations. In accordance with previous investigations, the dominant features of the joint energy spectra (JES) were multiphoton peaks (see Figure 1.) [3]. Our model allowed us to analyze the angular distribution of the photoelectrons for each point of the JES. Employing a partial wave analysis we were able to determine the number of absorbed photons in each multiphoton peak as indicated on the transverse energy conservation lines of Figure 1.

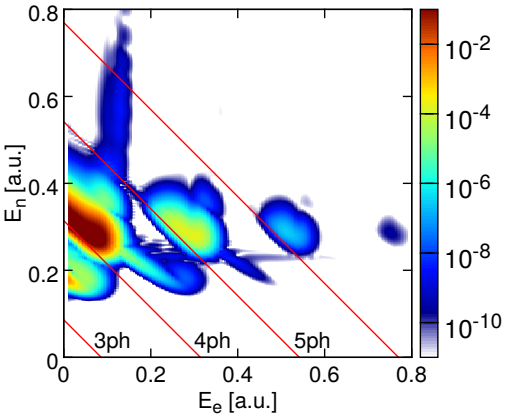

Figure 1. Joint energy spectrum (JES) for D_2^+ as a function of electron (E_e) and nuclear (E_n) kinetic energy. The D_2^+ was irradiated with a 10 fs long laser pulse with $\lambda = 200$ nm and $I_0 = 3 \times 10^{13}$W/cm^2.

In order to better understand the undergoing processes we also investigated the time-dependent nuclear wave packet density. Taking into account also the topology of the electronic potential energy surfaces we were able to identify the time moment and location (i.e. internuclear separation) where the population transfer between the considered potential energy surfaces occurred [4].

References

[1] G. J. Halász *et al.* 2013 *J. Phys. Chem. A* **117** 8528
[2] G. J. Halász *et al.* 2013 *Phys. Rev. A* **88** 043413
[3] A. Tóth *et al.* 2016 *J. Phys. Chem. A* **120** 9411
[4] A. Tóth *et al.* 2017 *Chem. Phys. Lett.* Accepted for publication

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