Evaluation of the Rescattering Processes for the Ionization and Dissociation of D_2^+ ions in the Fragmentation of D_2 by intense laser pulses

X. M. Tong, Z. X. Zhao and C. D. Lin
Kansas State University, Department of Physics, Manhattan, KS 66506, USA

The ionization and fragmentation of simple molecules by intense laser pulses has been studied extensively in the past two decades. For the simplest diatomic molecule, H_2^+ or D_2^+, theoretical studies have identified fragmentation mechanisms such as bond softening, bond hardening and charge resonance enhancement ionization (CREI) at internuclear separations larger than the equilibrium value. It is widely assumed that double ionization of D_2 is a two-step process where D_2 was first ionized by the laser pulse. As the D_2^+ ion is launched in a vibrational wavepacket and expands, it can be further excited or ionized, resulting in fragments of D and/or D^+ with different kinetic energies. The kinetic energies characterize the internuclear separations where the dissociation or ionization occur.

In a recent experiment, Staudte et al [1] measured the momentum distribution of the deuteron pairs at high energies and identified the rescattering mechanism as responsible for the production of these ions. Similarly, the rescattering mechanism has also been identified from measuring the D^+ momentum distribution in the experiment of Niikura et al. [2] In this contribution we present our analysis of the rescattering process.

In the simulation, we assumed that D_2 is first ionized near the peak of the laser pulse. By removing an electron from D_2, it weakens the force binding the two deuterons and therefore launches a vibrational wavepacket $\chi(R,t=0)$ which is taken to be the ground vibrational state of D_2. This wavepacket propagates in the ground electronic potential (σ_g). The ionization of the first electron is assumed to be described by the ADK model which has been properly modified for diatomic molecules. The electron is assumed to be launched from the z-axis (direction of linear polarization) with a Gaussian transverse velocity distribution according to the ADK model. With these initial conditions, we follow the motion of this first electron classically in the combined laser field and the Coulomb field of the D_2^+ ion. From the classical equation of motion we look for the distance of closest approach and the corresponding "rescattering time" t_r. From which we further calculate the equivalent asymptotic scattering energy and impact parameter of a "free" electron by the D_2^+ ion and use the excitation cross sections at different internuclear separations from the literature. To simplify the analysis, we choose laser intensity such that direct ionization of D_2^+ from the σ_g ground state is not possible. Instead, D_2^+ can be excited by the impact of the rescattered electron to the σ_u or π_u states. Depending on the laser intensity, the D_2^+ can follow the excited electronic potential curves such that it ends up to be $D + D^+$, or it can be further ionized by the laser and ends up as two deuterons. The kinetic energies of the fragments give information about the time of the rescattering processes and the time of the ionization processes. By choosing proper laser intensity the analysis of the fragment kinetic energies allows the determination of the temporal resolution of the collision at the attosecond level and the spatial resolution of deuterons at the sub-Angstrom level. The details of the simulation will be presented.

Reference:
[1] A. Staudte et al., Phys. Rev. A65, 020703 (2002).
[2] H. Niikura et al, Nature, 417, 917 (2002