Dissociation of H_2^+ in strong inhomogeneous near-fields

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Synopsis We theoretically investigate the dissociation mechanisms in H_2^+ while a inhomogeneous near-field drives the molecular target. By means of numerically solving the time dependent Schrödinger equation (TDSE) we extract the kinetic energy release (KER). For inhomogeneous fields an interesting enhancement and interference structure of the ion signal are observed from the KER in comparison to the standard electric homogeneous fields.

When molecules are subjected to intense laser fields, they absorb one or few photons and dissociate. Upon dissociation, the molecular electronic energy is transformed into the ion kinetic energy release (KER) [1, 2, 3]. The control of dissociation pathways and KER has attracted much attention, where H_2^+ typically serves as a prototype system. Here, we simulate the dissociation of H_2^+ molecule from spatially non-uniform fields, which could be generated by the illumination of metallic nano-structures. We employ the numerical solution of TDSE in reduced dimensions. The field-matter interaction potential is taken as $V_L^s(z,t) = -zE(t)[1+s\kappa(z)]$, where $\kappa(z)$ is a polynomial function representing the inhomogeneous character of the field and s is a switch function [4].

Figs. 1(a)-(b) show the KER spectra of dissociation at relatively weak and strong laser intensities and for spatially inhomogeneous ($s=1$) and homogeneous ($s=0$) laser fields. The initial-state, $v=0$, lies below the threshold for bond-softening (i.e. $v=5$, corresponding to ~ 0.1 eV). Thus, higher v levels allow the molecule to dissociate. A series of peaks in KER in the region $0 \sim 1.5$ eV are primarily originating from the 1ω-crossing. Here, $v=9$ is the threshold for the diabatic 1ω-crossing. Beyond 0.8 eV, *i.e.* for $v>9$, KER again decreases as these levels are non-resonant and prone to vibrational-trapping. The weak signals above 1.5 eV are from above-threshold dissociation (ATD) channels [5]. For the inhomogeneous field, *i.e.* $s=1$, KER slightly increases while largely maintaining its spectral profile, compared with the uniform field, *i.e.* for $s=0$. At higher laser intensities (Fig. 1(b)), the influence of the inhomogeneous field on dissociation is much more pronounced. We see that the adiabatic potential of the $1s\sigma_g$ state is suppressed and the initial level $v=0$ more easily undergoes dissociation. The dissociation probability is strongly enhanced in the energy range $1 \sim 2$ eV, which may originate from the 2ω-crossing. New peaks at roughly 1.5 eV and 2.0 eV for $s=1$ are present and their yields are around a factor of 2-3 higher than those of uniform fields, suggesting that the inhomogeneous field enhances dissociation *via* ATD channels at higher intensities.

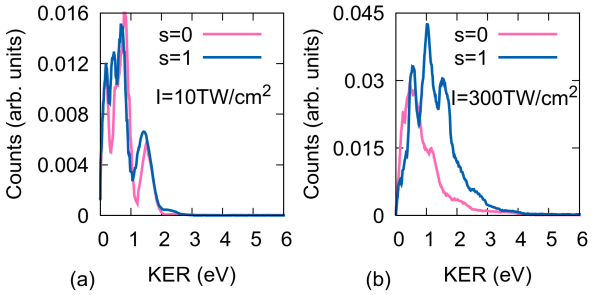

Figure 1. KER spectra of dissociation of H_2^+ for homogeneous ($s=0$) and inhomogeneous ($s=1$) fields, at low (a), and high (b) intensities. A Gaussian-type laser with a single-cycle pulse FWHM and CEP $\phi=0$ is used.

References

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