Charge-Asymmetric Coulomb Explosion of Diatomic Molecules in Intense Laser Fields

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Much attention has been recently called to the interweaved electronic and nuclear dynamics of a molecule in intense ($\sim 10^{15}$W/cm^2), short pulse ($\sim 10^{-13}$s) laser fields [1]. Of particular interest is the effect of *enhanced ionization*, i.e. ionization rate being much larger than that for the constituent atoms, basically caused by electron localization due to the intra-molecular barrier while the bond distance stretches.

In this talk, we develop a simple model for sequential multiple ionization of diatomic molecules AB in intense laser fields. Modifying the *field-ionization, Coulomb explosion* model by Posthumus *et al.*[2], we incorporate asymmetric charge states $q_{\rm A} \neq q_{\rm B}$ in respective steps, where either the outermost electron localized at the atomic site A, or that at B, is ionized as $(q_{\rm A}-1, q_{\rm B}) \rightarrow (q_{\rm A}, q_{\rm B})$, or as $(q_{\rm A}, q_{\rm B}-1) \rightarrow (q_{\rm A}, q_{\rm B})$. Furthermore, we take account of possible electron dynamics due to the oscillating field: nonadiabatic excitation of a localized electron associated with the inner saddle point, and subsequent field ionization associated with the outer saddle point in both directions according to the oscillating phase. It turns out as a consequence that, for a given net charge $q = q_{\rm A} + q_{\rm B}$, the larger the charge asymmetry $|q_{\rm A} - q_{\rm B}|$, the smaller the bond distance $R_{\rm ion}$ at which ionization occurs.

The present model is shown to account for the behaviors observed in different molecules such as N_2 [3] and NO [4] through the kinetic energy release in Coulomb explosion, as follows. 1) While increasing with q, the distance of ionization oscillates with the even-odd effect in a symmetric pathway ($|q_{\rm A} - q_{\rm B}| = 0$ or 1). 2) Ionization occurs earlier in asymmetric channels than in symmetric ones among competing pathways as $R_{\rm ion}(21 \rightarrow 31) < R_{\rm ion}(21 \rightarrow 22)$.

[1] For example, J.H. Posthumus and J.F. McCann, in *Molecules and Clusters in Intense Laser Fields*, ed. J. Posthumus, Cambridge University Press, 2001, p.27.

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[3] A.Hishikawa, *et al.*, Chem. Phys. **231** (1998) 315.

[4] A. Iwamae, A. Hishikawa, and K. Yamanouchi, J. Phys. B**33** (2000) 223.

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