Dynamic Effects on the Photoinduced and Ionization-Induced Reactions

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Abstract:

In recent years, molecular behaviors in an intense laser field has attracted much attention. When a molecule is ionized in a strong laser field, chemical bonds are broken by a Coulomb explosion due to the repulsion between positive charges within the molecule. For example, it has been reported that H_3^+ is produced from the dications of methanol, ethane, allene and so on. These molecules vertically ionized become a high-energy state. An excess energy obtained by the vertical ionization is converted to a molecular motion to initiate the reaction. Although the molecule once reaches an equilibrium structure along the energy surface of the ionized state, the molecule overcomes the energy barrier for the subsequent reaction, if the excess energy is sufficient. According to previous studies, a roaming of the H_2 molecule commences first, followed by decomposition reactions to produce H^+ and H_2^+ in addition to H_3^+, which shows that there exist multiple channels from an equilibrium structure. Such ionization-induced reactions are similar to photoinduced reactions where molecules vertically excited to a high-energy state according to the Franck–Condon principle obtain an excess energy to drive the reaction and there are multiple channels at the conical intersection of the internal conversion. We have clarified the dynamic effects on the selection of channel in the ionization-induced reactions as well as the photoinduced reactions.[1,2]

Refernces

[1] T. Matsubara, *Bull. Chem. Soc. Jpn.*, 94, 1720-1727 (2021).

[2] T. Matsubara, *Phys. Chem. Chem. Phys.,* 24, 17303-17313 (2022).