

Control of electron localization in the dissociation of H_2^+ using orthogonally polarized two-color sequential laser pulses

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Synopsis Orthogonally polarized two-color sequential laser pulses are used to control the electron localization in the dissociation of H_2^+ . The first single attosecond pulse, whose polarization axis is perpendicular to the molecular axis, excites H_2^+ from $1s\sigma_g$ to $2p\sigma_u$, and the time-delayed infrared pulse, whose polarization axis is parallel to the molecular axis, steers the electron between two nuclei. The simulation of the time-dependent Schrödinger equation predicts the control degree of the electron localization can be up to 90% with the current laser technology. To the best of our knowledge, we first reveal that the new mechanism for this asymmetric localization is due to the mixture of $2p\pi_g$ and $2p\pi_u$, instead of $1s\sigma_g$ and $2p\sigma_u$ in the previous studies.

The electron localization in the dissociation of H_2^+ is a fundamental problem in the ultrafast physics. The understanding of the electron localization is based on the quantum interference of $1s\sigma_g$ and $2p\sigma_u$ states: the relative phase between these two states decides which nucleus has the larger probabilities to capture the electron, and the relative probability of the two states decides the asymmetric degree.

In this article, we raise a new strategy to control the electron localization using orthogonally polarized two-color pulses. The polarization axis of the first ultraviolet (UV) pulse is perpendicular to the molecular axis. The time-delayed infrared (IR) laser pulse, whose polarization axis is parallel to the molecular axis, steers the electron between two nuclei during the dissociation. Different from before, where only the two lowest molecular orbits are involved, more states participate in this dynamics. This strategy can be practiced with the current laser technology, and can be applied to many big molecules.

We solve the time-dependent Schrödinger equation in the Cartesian coordinate (atomic units, $e=m=\hbar=1$ are used unless indicated otherwise) [1]:

$$i \frac{\partial}{\partial t} \psi(x, z, R; t) = [H_0 + H_I] \psi(x, z, R; t),$$

where H_0 is the field-free Hamiltonian:

$$H_0 = -\frac{1}{2M} \frac{\partial^2}{\partial R^2} - \frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \frac{\partial^2}{\partial z^2} + \frac{1}{R} - \sum_{\pm} \frac{1}{\sqrt{x^2 + (z \pm R/2)^2 + s}}$$

and H_I is the coupling between the electron and

the external fields:

$$H_I = xE_{uv}(t) + zE_{IR}(t),$$

where M is the reduced nuclear mass and $M=918$. The soft core parameter $s=0.64$.

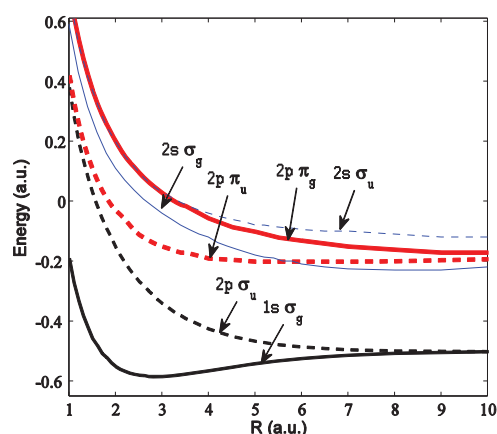


Figure 1. The potential curves of several quantum states within the Born-Oppenheimer approximation.

Fig.1 shows the several potential curves. The attosecond pulse excites the molecule from $1s\sigma_g$ to $2p\pi_u$, followed by the mixture of $2p\pi_u$ and $2p\pi_g$ induced by the infrared laser-molecule dipole coupling. By changing the time delay between the attosecond pulse and femtosecond pulse, or tuning the carrier envelop phase of the infrared laser pulse, the electron localization can be controlled effectively.

References

- [1] Feng He 2012, Phys.Rev.A 86, 063415.

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