Time-dependent effective potential for the ultrafast electron dynamics of molecules in intense laser fields: Application to anisotropic ionization of CO

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We developed multiconfigurational methods to deal with multielectron dynamics and reaction/nuclear dynamics of molecules in intense laser fields [1]. One of them is the multiconfiguration time-dependent Hartree-Fock (MCTDHF) method for multielectron dynamics of atoms and molecules, where the many-electron wave function is expressed as a linear combination of Slater determinants for different electron configurations [2]. Effective potentials of natural orbitals are derived on the basis of MCTDHF [3]. The anisotropic near-infrared induced ionization of a CO molecule is analyzed in terms of the effective potentials for natural orbitals [3]. When the laser electric field points to the nucleus O from C, tunnel ionization from the C atom side is enhanced; a hump structure originating from multielectron interaction (electron-electron repulsion) is then formed around $z = -3$ a_0 on the top of the field-induced distorted barrier of the effective potential for the 5σ HOMO, as shown in Figure 1. This hump formation, responsible for the directional anisotropy of tunnel ionization, restrains the influence of the linear Stark effect on the energy shifts of bound states.

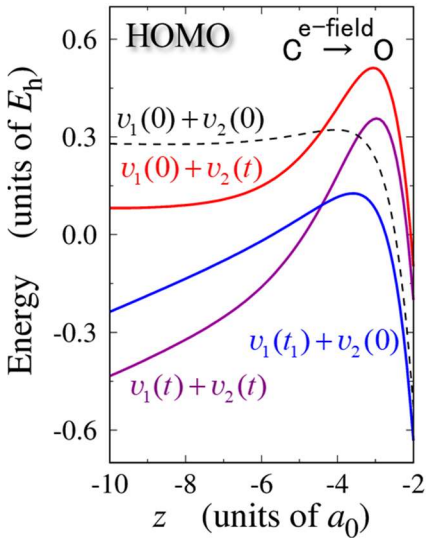

Figure 1: HOMO effective potential $v_1(t)+ v_2(t)$ of CO at t=3/4 cycle of a two-cycle pulse of λ=760 nm (field strength =2.8×10^{10} V/m). $v_1(t)$ and $v_2(t)$ originate from one-body and two-body interactions (the fileld is turned on at t=0). z is the electric coordinate along the C-O axis.

[1] Kato T, Yamanouchi K and Kono H 2018 *Attosecond Molecular Dynamics* eds. Vrakking M J J and Lepine F (Royal Society of Chemistry, Cambridge) pp. 139–182
[2] Kato T and Kono H 2004 *Chem. Phys. Lett.* **392** 533
[3] Ohmura S *et al.* 2018 *J. Phys. B* **51** 034001