ELECTRON LOCALIZATION IN MOLECULES INTERACTING WITH INTENSE LASER PULSES

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We theoretically study dynamic localization in molecules interacting with intense laser pulses. Mechanism is responsible for the effect of Charge Resonance Enhanced Ionization (CREI) studied for H_2^+ and I_2^+ for over 2 decades within the field of ultrafast intense laser AMO. Here we focus on the multielectron aspects and the attosecond electron dynamics.

Calculations are performed for di- and polyatomic molecules at equilibrium internuclear distances and we discuss multielectron, or more precisely multi-orbital character of the process. CREI has been connected to the dynamic electron localization as well as to the multiple ionization bursts over one laser field cycle. We discuss the similarities and differences between CREI and results for multielectron molecules at equilibrium distances. Results obtained within TDDFT show that as expected if we use laser wavelength tuned to the resonance one could observe resonance enhancement of multiphoton ionization of valence orbitals, analogous to CREI. But calculations also reveal that in contrast to CREI studied for H_2^+ and I_2^+, the resonance one photon transition acts as a trigger for other excitations and leads to enhancement of ionization from multiple inner valence orbitals and the dynamical properties exhibit more complicated behavior than expected from simple '2-level'-H_2^+ picture of CREI.