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Time-Dependent Electron Localization Functions, TDELF's, for Molecular Ionization and Harmonic Generation in Intense Laser Pulses[1]

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— The nonlinear nonperturbative response of N2,CO2,OCS,CS2 are studied numerically by solutions of Kohn-Sham (KS) orbital equations in the presence of few cycle intense I>10^{14} W/cm^2, 800nm laser pulses. It is found generally that ionization rates depend on different functionals and ionization also occurs from inner-shell KS orbitals .This is sensitive to laser-molecule orientation as predicted earlier [1]. Ionization rate maxima correspond to the alignment of maximum KS orbital densities with the laser polarization instead of orbital ionization potentials,Ip. These results are corroborated through time analysis of TDELF's where ionization occurs from lone pair or bond regions of the corresponding molecule at various times during the pulses. Time frequency analysis of Harmonic Generation spectra allow for identification of recollision times of ionized electrons with the parent ion.

[1] EF Penka, AD Bandrauk, Phys Rev A81, 023411(2010); 84, 035412(2011).

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