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Imaging Molecular Orbitals with Ultrashort Intense Laser Pulses
ANDRE D. BANDRAUK[1], Universite de Sherbrooke, GERARD LAGMAGO KAMTA[2], McGill University, MOLECULAR IMAGING TEAM — Exact 3-D numerical solutions of the time-dependent Schroedinger equation, TDSE, for the one-electron H2+ molecule in the Born Oppenheimer (fixed nuclei) approximation have been obtained to calculate the angular dependence of ionization rates as a function of internuclear distance in the presence of ultrashort (5 fs) intense (I 10^{14} W/cm^2) 800 nm laser pulses. It is shown that the ionization rates reproduce well the molecular orbital symmetries and structures near equilibrium whereas at larger internuclear distances where CREI (Charge Resonance Enhanced Ionization) occurs considerable deviation of orbital structure occurs due to "off-axis" tunnelling ionization. The results show that intense low frequency ultrashort pulses can image molecular orbitals provided molecules can be properly aligned.

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