

Abstract Submitted
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Ultrafast molecular photoionization using a complete Multiconfiguration Time-dependent Hartree Fock Approach¹ KEITH V. LAWLER, DANIEL J. HAXTON, C. WILLIAM MCCURDY — A MCTDHF method treating electrons and nuclei on the same dynamical footing has been implemented using prolate spheroidal coordinates for the electrons. Many-electron diatomics in fields are treated in full dimensionality. Ionization of diatomics by short pulses is described by combining exterior complex scaling (ECS) and the projected flux method of analyzing the N -electron time-dependent MCTDHF wavefunction $ket\Psi(t)$. The photoionization cross section from a short pulse calculation is

$$\sigma(E) = \frac{2\pi\alpha\omega_{fi}}{|F_{pulse}(E)|^2} \int_0^T dt \int_0^T dt' \langle\Psi(t')|i(\hat{H}_{ECS} - \hat{H}_{ECS}^\dagger)|\Psi(t)\rangle e^{iE(t-t')} \quad (1)$$

where H is nonhermitian only on the complex of the ECS contour. The pulse ends at $t = 0$, and $F_{pulse}(E)$ is its Fourier transform. By projecting the N -electron time-dependent wave function onto an electronic state of the $(N - 1)$ -electron cation, we calculate excitation ionization cross sections. This approach is applied to channel-specific single photoionization of H_2 , He_2 , and N_2 including correlation among all electrons.

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