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All-active-electron nonadiabatic time-dependent calculations on diatomics using MCTDHF[1] DANIEL HAXTON, THOMAS RESCIGNO, Lawrence Berkeley National Laboratory, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Laboratory — Calculations on energies, properties, and excitations of various diatomic molecules in a non-Born-Oppenheimer framework are presented. These calculations use the multiconfiguration time-dependent Hartree-Fock (MCTDHF) method and are performed in the nonorthogonal coordinate system of prolate spheroidal coordinates for the electrons, and the bond length R. An interpolating polynomial basis is used in the electronic and nuclear degrees of freedom, and the wavefunction is expanded in terms of slater determinants of electronic orbitals times the full primitive basis in R. Ionization is accounted for by complex scaling of the radial prolate spheriodal variable; dissociation may be similarly treated. We present calculations aimed towards describing pump-probe experiments within an all-active-electron framework, in which we prepare ground states, excite with a pulse and then extract spectral information via further propagation of the wavefunction.

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Daniel Haxton
Lawrence Berkeley National Laboratory

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