

Abstract Submitted
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Atom-Atom Scattering with TDDFT - Beyond the Born-Oppenheimer Approximation.¹ RYAN M. HATCHER, ALAN R. TACKETT, MATTHEW J. BECK, SOKRATES T. PANTELIDES, Vanderbilt University — We report results of calculations of atom-atom scattering going beyond the Born-Oppenheimer (B-O) approximation. We use time-dependent density functional theory with an adiabatic approximation to the scalar exchange-correlation potential in the local-density approximation. We use pseudopotentials, keeping the nearest approach larger than the core radius. The ions are treated as classical particles while the electrons have full freedom to evolve off their instantaneous ground state. If radiative energy loss is not included, energy is conserved; part of the initial ion kinetic energy is transferred to electrons and stays there after separation, a clear sign of effects beyond the B-O approximation. Results of treating radiative losses at two levels of approximation will be discussed. Further results of ongoing calculations of scattering of a Si atom by a solid Si matrix will be described.

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