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Computation of Raman Spectra from Density Matrix Linear Response Theory in Extended Lagrangian Born-Oppenheimer Molecular Dynamics ANDERS NIKLASSON, JOSHUA COE, MARC CAWKWELL, Los Alamos National Laboratory — Linear response calculations based on density matrix perturbation theory [A. M. N. Niklasson and M. Challacombe, *Phys. Rev. Lett.* **92**, 193001 (2004)] have been developed within a self-consistent tight-binding method for extended Lagrangian Born-Oppenheimer molecular dynamics [A. M. N. Niklasson, *Phys. Rev. Lett.*, **100**, 123004 (2008)]. Besides the nuclear coordinates, extended auxiliary electronic degrees of freedom are added to the regular Born-Oppenheimer Lagrangian, both for the electronic ground state and response densities. This formalism enables highly efficient, on-the-fly, analytic computations of the polarizability autocorrelation functions and the Raman spectra during energy conserving Born-Oppenheimer molecular dynamics trajectories. We will illustrate these capabilities via time-resolved Raman spectra computed during explicit, reactive molecular dynamics simulations of the shock compression of methane, benzene, tert-butylacetylene. Comparisons will be made with experimental results where possible.

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