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Lagrangian Time-Reversible Born-Oppenheimer Molecular Dynamics ANDERS NIKLASSON, Theoretical Division Los Alamos National Laboratory — A Lagrangian generalization of time-reversible Born-Oppenheimer molecular dynamics [Niklasson et al., Phys. Rev. Lett., vol.97, 123001 (2006)] is proposed. The new formulation enables highly efficient symplectic or geometric integrations of both the nuclear and the electronic degrees of freedom that are stable and energy conserving even under incomplete self-consistency convergence. It is demonstrated how the accuracy is improved by over an order of magnitude compared to previous formulations at the same level of computational cost. The proposed Lagrangian includes extended electronic degrees of freedom as auxiliary dynamical variables in addition to the nuclear coordinates and momenta. While the nuclear degrees of freedom propagate on the Born-Oppenheimer potential energy surface, the extended auxiliary electronic degrees of freedom evolve as a harmonic oscillator centered around the adiabatic propagation of the self-consistent ground state (http://arxiv.org/abs/0711.3466).

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