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Time Reversible Linear Scaling ab initio Molecular Dynamics C.J. TYMCZAK, Texas Southern University and Los Alamos National Laboratory, ANDERS NIKLASSON, MATT CHALLACOMBE, Los Alamos National Laboratory — We present a time-reversible Born-Oppenheimer molecular dynamics scheme, based on self-consistent Hartree-Fock or density functional theory, where both the nuclear and the electronic degrees of freedom are propagated in time. We show how a time-reversible adiabatic propagation of the electronic degrees of freedom is possible despite the non-linearity and incompleteness of the self-consistent field procedure. With a time-reversible lossless propagation the simulated dynamics is stabilized with respect to a systematic long-term energy drift and the number of self-consistency cycles can be kept low (often only 2-4 cycles per nuclear time step) thanks to a good initial guess given by the adiabatic propagation of the electronic degrees of freedom. The proposed molecular dynamics scheme therefore combines a low computational cost with a physically correct time-reversible representation of the dynamics, which preserves a detailed balance between propagation forwards and backwards in time.

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