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Extended Lagrangian Born-Oppenheimer Molecular Dynamics: quantum mecahnical molecular dynamics for extended time and length scales[1] ANDERS NIKLASSON, MARC CAWKWELL, Los Alamos National Laboratory — Born-Oppenheimer molecular dynamics (BOMD) based on density functional theory offers a very accurate quantum mechanical approach to atomistic simulations that is more reliable and general compared to classical MD. Unfortunately, BOMD simulations are often limited by a high computational cost or by problems such as unbalanced phase space trajectories, numerical instabilities and a systematic long-term energy drift. These problems become particularly severe in combination with reduced complexity or linear scaling algorithms that are necessary for the study of large systems. We have recently taken some steps toward a new generation of first principles MD, which combines some of the best features of regular BOMD and Car-Parrinello MD, while avoiding their most serious shortcomings. The new dynamics is given in terms of an extended Lagrangian (XL), where auxiliary extended electronic degrees of freedom are added to the nuclear part. Our framework enables accurate geometric integration of both the nuclear and electronic degrees of freedom that provide a time-reversible and energy conserving dynamics on the ground state BO potential energy surface that is stable also under approximate SCF convergence. XL-BOMD provides a surprisingly simple and general framework for atomistic simulations

[1]DOE, BES Office of Sicence and LDRD-DR

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