SHOCK17-2017-000243

Abstract for an Invited Paper
for the SHOCK17 Meeting of
the American Physical Society

Next Generation Extended Lagrangian Quantum-based Molecular Dynamics

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A new framework for extended Lagrangian first-principles molecular dynamics simulations is presented, which overcomes shortcomings of regular, direct Born-Oppenheimer molecular dynamics, while maintaining important advantages of the unified extended Lagrangian formulation of density functional theory pioneered by Car and Parrinello three decades ago. The new framework allows, for the first time, energy conserving, linear-scaling Born-Oppenheimer molecular dynamics simulations, which is necessary to study larger and more realistic systems over longer simulation times than previously possible. Expensive, self-consinstent-field optimizations are avoided and normal integration time steps of regular, direct Born-Oppenheimer molecular dynamics can be used. Linear scaling electronic structure theory is presented using a graph-based approach that is ideal for parallel calculations on hybrid computer platforms. For the first time, quantum based Born-Oppenheimer molecular dynamics simulation is becoming a practically feasible approach in simulations of +100,000 atoms—representing a competitive alternative to classical polarizable force field methods.

Refs: J. Chem. Phys. 141, 164123 (2014); A.M.N.; J. Chem. Phys. 144, 234101 (2016); J. Chem. Theor. Comput. 12, 3063 (2016)

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