Séminaire de Chimie Théorique

Salle de Réunion, 3eme Est, bat. A12

Mardi 6 Décembre à 11:00

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Next generation extended Lagrangian first principles molecular dynamics

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-consistent-field optimizations are avoided and normal integration time steps of regular, direct Born-Oppenheimer molecular dynamics can be used. Modern low pre-factor, linear scaling electronic structure theory is presented as well as a graph-based approach that is ideal for parallel calculations on hybrid computer platforms. For the first time, quantum based Born-Oppenheimer molecular dynamics has become a practically feasible approach in simulations with +10,000 atoms and a competitive alternative to classical polarizable force field methods.

Refs:

• A.M.N. Niklasson, “Extended Born-Oppenheimer molecular dynamics”, Phys. Rev. Lett. 100, 123004 (2008);

• M.J. Cawkwell and A.M.N. Niklasson, “Energy conserving, linear scaling Born-Oppenheimer molecular dynamic“, J. Chem. Phys. 137, 134106 (2012); S.M. Mniszewski et. al, “Efficient Parallel Linear Scaling Construction of the Density Matrix for Born-Oppenheimer Molecular Dynamics”, J. Chem. Theory Comput. 11, 4644 (2015);

• A.M.N. Niklasson and M.J. Cawkwell “Generalized extended Lagrangian Born-Oppenheimer molecular dynamics”, J. Chem. Phys. 141, 164123 (2014); A.M.N. Niklasson et. al “Graph-based linear scaling electronic structure theory”, J. Chem. Phys. 144, 234101 (2016).

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