A Journey into Quantum Molecular Dynamics and DFT

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Outline

Methods for Electronic Dynamics

By Propagation Algorithm

Born-Oppenheimer Molecular Dynamics (BOMD)

Car-Parrinello Molecular Dynamics (CPMD)

Ehrenfest Molecular Dynamics

Methods for Electronic Dynamics

By Level of Electronic Theory

Density Functional Theory (DFT-MD)

Wavefunction Theory (WFT-MD)

Hartree-Fock (HF-MD)

Post-Hartree-Fock (MP2-MD, CCSD-MD)

Semi-empirical Methods (SE-MD)

Methods for Non-Adiabatic Dynamics

Trajectory Surface Hopping (TSH)

Multi-Configuration Time-Dependent Hartree (MCTDH)

Methods Including Nuclear Quantum Effects

Path Integral Molecular Dynamics (PIMD)

- Centroid Molecular Dynamics (CMD)
- Ring Polymer Molecular Dynamics (RPMD)

Wave Packet Propagation

Hybrid Methods

Quantum Mechanics / Molecular Mechanics (QM/MM)