Open Source
Molecular Dynamics

Features

CP2K is a program to perform simulations of solid state, liquid, molecular and biological systems. It is especially aimed at massively parallel and linear scaling electronic structure methods and state-of-the-art ab-initio molecular dynamics (AIMD) simulations.

CP2K is optimized for the mixed Gaussian and Plane-Waves (GPW) method based on pseudopotentials, but is able to run all-electron or pure plane-wave/Gaussian calculations as well. Features include the following.

Ab-initio electronic structure theory methods using the QUICKSTEP module

- Density-Functional Theory (DFT) energies and forces
- Hartree-Fock (HF) energies and forces
- Moeller-Plesset 2nd order perturbation theory (MP2) energies and forces
- Random Phase Approximation (RPA) energies
- Gas phase or Periodic boundary conditions (PBC)
- Basis sets include various standard Gaussian-Type Orbitals (GTOs), Pseudopotential plane-waves (PW), and a mixed Gaussian and (augmented) plane wave approach (GPW/GAPW)
- PW DFT functionality (energy, forces, stress), including LAPW (all-electron)
- Norm-conserving, seperable Goedecker-Teter-Hutter (GTH) and non-linear core corrected (NLCC) pseudopotentials, or all-electron calculations
- Local Density Approximation (LDA) XC functionals including SVWN3, SVWN5, PW92 and PADE
- Gradient-corrected (GGA) XC functionals including BLYP, BP86, PW91, PBE and HCTH120 as well as the meta-GGA XC functional TPSS
- Hybrid XC functionals with exact Hartree-Fock Exchange (HFX) including B3LYP, PBE0 and MCY3
- Double-hybrid XC functionals including B2PLYP and B2GPPLYP
- Additional XC functionals via LibXC
- Dispersion corrections via DFT-D2 and DFT-D3 pair-potential models
- Non-local van der Waals corrections for XC functionals including B88-vdW, PBE-vdW and B97X-D
- DFT+U (Hubbard) correction
- Density-Fitting for DFT via Bloechl or Density Derived Atomic Point Charges (DDAPC) charges, for HFX via Auxiliary Density Matrix Methods (ADMM) and for MP2/RPA via Resolution-of-identity (RI)
- Sparse matrix and prescreening techniques for linear-scaling Kohn-Sham (KS) matrix computation
- Orbital Transformation (OT) or Direct Inversion of the iterative subspace (DIIS) self-consistent field (SCF) minimizer
- Local Resolution-of-Identity Projector Augmented Wave method (LRIGPW)
- Absolutely Localized Molecular Orbitals SCF (ALMO-SCF) energies for linear scaling of molecular systems
- Excited states via time-dependent density-functional perturbation theory (TDDFPT)

Ab-initio Molecular Dynamics

- Born-Oppenheimer Molecular Dynamics (BOMD)
- Ehrenfest Molecular Dynamics (EMD)
- PS extrapolation of initial wavefunction
- Time-reversible Always Stable Predictor-Corrector (ASPC) integrator
- Approximate Car-Parrinello like Langevin Born-Oppenheimer Molecular Dynamics (Second-Generation Car-Parrinello Molecular Dynamics)

Mixed quantum-classical (QM/MM) simulations

- Real-space multigrid approach for the evaluation of the Coulomb interactions between the QM and the MM part
- Linear-scaling electrostatic coupling treating of periodic boundary conditions
- Adaptive QM/MM

Further features include

- Single-point energies, geometry optimizations and frequency calculations
- Several nudged-elastic band (NEB) algorithms (B-NEB, IT-NEB, CI-NEB, D-NEB) for minimum energy path (MEP) calculations
- Global optimization of geometries
- Solvation via the Self-Consistent Continuum Solvation (SCCS) model
- Semi-Empirical calculations including the AM1, RM1, PM3, MNDO, MNDO-d, PNNL and PM6 parametrizations, density-functional tight-binding (DFTB) and self-consistent-polarization tight-binding (SCP-TB), with or without periodic boundary conditions
- Classical Molecular Dynamics (MD) simulations in microcanonical ensemble (NVE) or canonical ensmble (NVT) with Nose-Hover and canonical sampling through velocity rescaling (CSVR) thermostats
- Metadynamics including well-tempered Metadynamics for Free Energy calculations
- Classical Force-Field (MM) simulations
- Monte-Carlo (MC) KS-DFT simulations
- Static (e.g. spectra) and dynamical (e.g. diffusion) properties
- ATOM code for pseudopotential generation
- Integrated molecular basis set optimization

CP2K does not implement conventional Car-Parrinello Molecular Dynamics (CPMD).

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