Simulation in Chemistry

General information

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Techniques

1. Stochastic Simulation
2. Molecular Dynamics
3. Quantum Chemistry
4. Edition & Visualization

About

This document provides an overview of computational simulation techniques commonly used in condensed matter physics, chemistry, and materials science. It also provides a lists the programs, software packages, or frameworks employed for such simulations.

Stochastic

Programs

- Melquiades (GPL)
- DL-Monte (BSD)
- Cassandra (GPL)
- GOMC (MIT)
- Dice (GPL)

Dynamics

Programs

- Gromacs (LGPL)
- Lammps (GPL)
- CP2K (GPL)
- Tinker (Tinker license)

Quantum

Programs

- CP2K (GPL)
- ORCA (Academic)
- MOPAC (LGPL)
- Quantum Espresso (GPL)
- Octopus (GPL)
- XTB (LGPL)
- DFTB (LGPL)

Edit

Programs

- Molden (Molden license)
- Travis (GPL)
- Gabedit (Gabedit license)
- Jmol (LGPL)
- Avogadro (GPL)
- VMD (VMD license)
- Molekel (GPL)
- EasyHibrid (Open)