FHI-aims

Purpose: Electronic Structure Calculations
Latest version: 220117
Licence: ⚠ Must be provided by the user.
Proprietary _ext-link
Website: *http://aimsclub.fhi-berlin.mpg.de/ _ext-link*

The **F**ritz **H**aber **I**nstitute ***ab-initio*** **m**olecular **s**imulations (FHI-aims) is a computer program package for computational materials science based on quantum-mechanical first principles. By using DFT or HF, it allows the resolution of molecular problems or periodical systems, the optimization of structures and the resolution of transport problems.