CRYSTAL

Purpose: Electronic Structure Calculations
Latest version: 17
Licence: ⚠ Must be provided by the user.
Proprietary _ext-link
Website: *http://www.crystal.unito.it/ _ext-link*

CRYSTAL performs ab initio calculations of the ground state energy, energy gradient, electronic wave function and properties of periodic systems. Hartree-Fock or KohnSham Hamiltonians can be used.