CRYSTAL14 Program Features

CRYSTAL

- Features
- Theoretical background
- How to cite

SOFTWARE

- How to get a copy
- Download
- License fee
- Platforms

DOCS & SETS

- Documentation
- Interfaces
  - CRYSCOR

Full Features

New features with respect to CRYSTAL09 are in *italics* and red

Hamiltonians

- **Hartree-Fock Theory**
  - Restricted
  - Unrestricted
- **Density Functional Theory**
  - Semilocal functionals: local [L], gradient-corrected [G] and *meta-GGA (tau-dependent) [T]*
  - Hybrid HF-DFT functionals
    - Global hybrids: B3PW, B3LYP (using the VWN5 functional), PBE0 and more
    - *Range-separated hybrids:*
      - *Screened-Coulomb (SC): HSE06, HSEsol*
      - *Long-range Corrected (LC): LC-wPBE, LC-wPBEsol, wB97, wB97-X*
  - *Minnesota semilocal and hybrid functionals:*
    - *M05 family: M05, M05-2X*
    - *M06 family: M06, M06-2X, M06-HF, M06-L*
  - *Double hybrid functionals: B2-PLYP, mPW2-PLYP, B2GP-PLYP*
  - User-defined hybrid functionals
- Numerical-grid based numerical quadrature scheme
- London-type empirical correction for dispersion interactions (DFT-D2 scheme)

Energy derivatives

- **Analytical first derivatives with respect to the nuclear coordinates and cell parameters**
  - Hartree-Fock and Density Functional methods (LDA, GGA, mGGA, global- and range-separated hybrids)
  - All-electron and Effective Core Potentials
- *Analytical derivatives, up to fourth order, with respect to an applied electric field (CPHF/CPKS)*
  - *Dielectric tensor*
  - *(Hyper)-polarizabilities*

Type of calculation

- **Single-point energy calculation**
- **Geometry optimizations**
  - Uses a quasi-Newton algorithm
  - Optimizes in symmetry-adapted cartesian coordinates
  - Optimizes in redundant coordinates
    - New internal coordinates handling and algorithm for back-transformation
  - Full geometry optimization (cell parameters and atom coordinates)
  - Freezes atoms during optimization
  - Constant volume or pressure constrained geometry optimization (3D only)
  - Transition state search
- **Harmonic vibrational frequencies**
  - Harmonic vibrational frequencies at Gamma point
  - Phonon dispersion using a direct approach (efficient supercell scheme)
  - *Phonon band structure and DOSs*
  - *Calculation of Atomic Displacement Parameters and Debye-Waller factors*
  - IR intensities through localized Wannier functions and Berry Phase
  - *IR and Raman intensities through CPHF/CPKS analytical approach*
  - *Simulated reflectance, IR and Raman spectra*
  - Exploration of the energy and geometry along selected normal modes
- **Anharmonic frequencies for X-H bonds**
- **Automated calculation of the elastic tensor of crystalline systems**
  - *Generalized to 2D and 1D systems*
  - *Calculation of directional seismic wave velocities*
  - *Calculation of isotropic polycrystalline aggregates elastic properties via Voigt-Reuss-Hill scheme*
- **Automated E vs V calculation for equation of state (3D only)**
  - *New EoSs: Vinet, Poirer-Tarantola and polynomial*

- *Automated calculation of pressure dependence of volume and bulk modulus*

- ***Automated calculation of piezoelectric and photoelastic tensors***
  - *Direct and converse piezoelectricity (using the Berry phase approach)*
  - *Elasto-optic tensor through the CPHF/CPKS scheme*
  - *Electric field frequency dependence of photoelastic properties*

- ***Improved tools to model solid solutions***
  - *Generation of configurations*
  - *Automated algorithm for computing the energy (with or without geometry optimization) of selected configurations*

Basis set

- **Gaussian type functions basis sets**
  - s, p, d, and f GTFs
  - Standard Pople Basis Sets
    - STO-nG n=2-6 (H-Xe), 3-21G (H-Xe), 6-21G (H-Ar)
    - polarization and diffuse function extensions
  - *Internal library of basis sets with a simplified input*
  - User-specified basis sets supported

- **Pseudopotential Basis Sets**
  - Available sets are:
    - Hay-Wadt large core
    - Hay-Wadt small core
  - User-defined pseudopotential basis sets supported

Periodic systems

- **Periodicity**
  - Consistent treatment of all periodic systems
  - 3D - Crystalline solids (230 space groups)
  - 2D - Films and surfaces (80 layer groups)
  - 1D - Polymers
    - space group derived symmetry (75 rod groups)
    - helical symmetry (up to order 48)
  - *1D - Nanotubes (with any number of symmetry operators)*
  - 0D - Molecules (32 point groups)

- **Automated geometry editing**

- 3D to 2D - slab parallel to a selected crystalline face (hkl)
- 3D to 0D - cluster from a perfect crystal (H saturated)
- 3D to 0D - extraction of molecules from a molecular crystal
- 3D to n3D - supercell creation
- 2D to 1D - building nanotubes from a single-layer slab model
- *2D to 0D - building fullerene-like structures from a single-layer slab model*
- *3D to 1D, 0D - building nanorods and nanoparticles from a perfect crystal*
- *2D to 0D - construction of Wulff's polyhedron from surface energies*
- Several geometry manipulations (reduction of symmetry; insertion, displacement, substitution, deletion of atoms)

Wave function analysis and properties

- **Band structure**
- **Density of states**
  - Band projected DOSS
  - AO projected DOSS
- **All Electron Charge Density - Spin Density**
  - Density maps
  - Mulliken population analysis
  - Density analytical derivatives
- **Atomic multipoles**
- **Electric field**
- **Electric field gradient**
- **Static structure factors and *dynamic structure factors including the Debye-Waller factor***
- **Electron Momentum Density and Compton profiles**
  - *Electron momentum density maps*
  - *Automated anisotropy maps*
  - *Partitioning according to Wannier functions*
- **Electrostatic potential and its derivatives**
  - Quantum and classical electrostatic potential and its derivatives
  - Electrostatic potential maps
- **Fermi contact**
- **Localized Wannier Functions (Boys method)**
- ***Mossbauer effect (isotropic effect and quadrupolar interaction)***
- **Dielectric properties**
  - Spontaneous polarization

        - Berry Phase
        - Localized Wannier Functions
    - Dielectric constant
        - Coupled Perturbed HF(KS) scheme
        - Finite-field approximation
    - *High-order static electric susceptibilities (2nd and 3rd order)*
- ***Topological analysis of the electron charge density via the TOPOND package, fully integrated in the program***

Software performance

- **Memory management: dynamic allocation**
- **Full parallelization of the code**
    - parallel SCF and gradients for both HF and DFT methods
    - Replicated data version (MPI)
    - Massive parallel version (MPI) (distributed memory) *(Improved version: lower memory usage and better scaling)*
    - *Parallel (replicated data) version of the "properties" module*
    - *New parallelization strategy on IRREPs*
- ***Enhanced exploitation of the point-group symmetry***

Interfaces

- *Internal interface to CRYSCOR (serial version)* for electronic structure calculations of 1D,- 2D- and 3D-periodic non-conducting systems at the L-MP2 correlated level and Double-Hybrids
- *Internal interface to TOPOND* for topological analysis of the charge density