

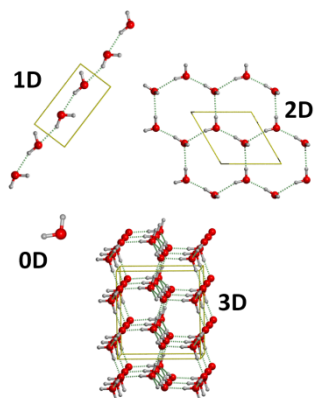


CRYSTAL09

A general-purpose program for the ab-initio study of crystalline solids

The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid HF/DFT approximations. The Bloch functions of the periodic systems are expanded as linear combinations of atom centred Gaussian functions. Powerful screening techniques are used to exploit real space locality.

The code may be used to perform consistent studies of the physical and chemical properties of molecules, polymers, surfaces and crystalline solids: structural features, vibrational properties, electronic structure, magnetic properties, dielectric properties, elastic properties.

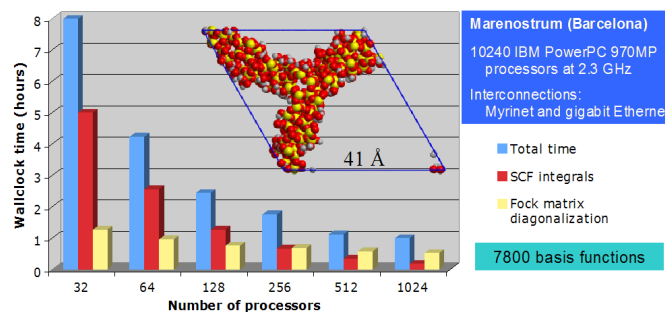


Interfaced to CRYSCOR09 for electronic structure calculations of 1D, - 2D- and 3D- periodic non-conducting systems at the local MP2 level

New features

- Static polarizability and dielectric tensor through a Coupled Perturbed HF/KS scheme
- Phonon dispersion using a direct approach and infrared intensities through a Berry phase approach
- Transition state search
- Constant pressure geometry optimization of cell constants and atomic positions
- Automated calculation of the elastic tensor of crystalline systems
- Automated E vs V calculation for equation of state
- New GGA functionals for solids
- London-type empirical correction for dispersion interactions (Grimme scheme)
- Automatic generation of nanotubes from single-layer systems
- Helical symmetry for polymers
- New tools for initial guess of SCF for d- and f- partly occupied atoms
- New tools for the treatment of solid solutions
- Revised implementation of Electron Momentum Density analysis and Compton profiles
- Enhanced Massive Parallel version (see below)

MCM-41 Computing times



P. Ugliengo, M. Sodupe, F. Musso, I.J. Bush, R. Orlando, R. Dovesi
Realistic Models of Hydroxylated Amorphous Silica Surfaces and MCM-41 Mesoporous Material Simulated by Large-scale Periodic B3LYP Calculations Adv. Mater. 20 (2008) 4579

CRYSTAL web site:

www.crystal.unito.it

Contacts: crystal@unito.it

Demo version and Tutorials

An evaluation version (all functionalities – 20 atoms in the unit cell) is available at the CRYSTAL web site.

A collection of tutorials is also available to guide users from basic calculations to advanced applications

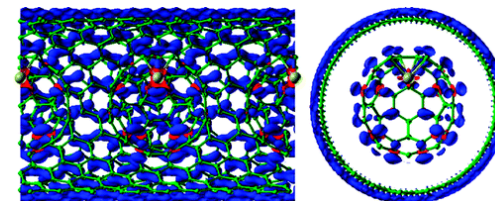
Recent applications

D. Groh, R. Pandey, M.B. Sahariah, E. Amzallag, I. Baraille, M. Rerat
First-principles study of the optical properties of BeO in its ambient and high-pressure phases
 J. Phys. Chem. Solids 70, 789-795 (2009)

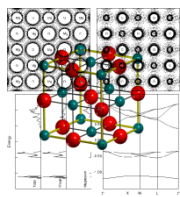
A. Kuzmin, R.A. Evarestov
Quantum mechanics-molecular dynamics approach to the interpretation of x-ray absorption spectra
 J. Phys.: Condes. Matter. 21, article n. 055401 (2009)

F. Cheviré, F. Clabau, O. Larcher, E. Orhan, F. Tessier, R. Marchand
Tunability of the optical properties in the $Y_6(W,Mo)(O,N)_{12}$ system
 Solid State Sci. 11 533-536 (2009)

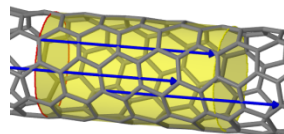
R. Orlando, M. Ferrero, M. Rérat, B. Kirtman, R. Dovesi
Calculation of the static electronic second hyperpolarizability or $\chi(3)$ tensor of three-dimensional periodic compounds with a local basis set
 J. Chem. Phys. 131, article n. 184105 (2009)



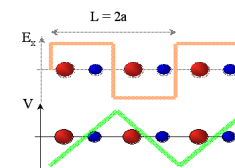
L. Ge, J.H. Jefferson, B. Montanari, N.M. Harrison, D.G. Pettifor, G.A.D. Briggs
Effects of Doping on Electronic Structure and Correlations in Carbon Peapods
 ACS Nano 3, 1069-1076 (2009)



R. Dovesi, B. Civalleri, R. Orlando, C. Roetti, V. R. Saunders
Ab initio quantum simulation in solid state chemistry
 Rev. Comput. Chem. 21, 1-125 (2005)



Y. Noel, Ph. D'Arco, R. Demichelis, C.M. Zicovich-Wilson and R. Dovesi
On the use of symmetry in the ab initio quantum mechanical simulation of nanotubes and related materials.
 J. Comput. Chem. 31, 855-862 (2010)



M. Ferrero, M. Rérat, P. Orlando, R. Dovesi
The calculation of static polarizabilities of periodic compounds. The implementation in the CRYSTAL code for 1D, 2D and 3D systems.
 J. Comput. Chem. 29, 1450-1459 (2008)

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 \(up to order 48\)](#)
 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](#)

Several geometry editing (reduction of symmetry; insertion, displacement, substitution, deletion of atoms)

Type of calculation

Single-point energy calculation

Automated geometry optimization

Uses a quasi-Newton algorithm
 Optimizes in symmetry-adapted cartesian coordinates or in redundant coordinates
 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 G point
 Phonon dispersion using a [direct approach \(efficient supercell scheme\)](#)
 IR intensities through either localized Wannier functions or [Berry phase](#)
[Calculation of the reflectance spectrum](#)
 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 (3D only)

Automated E vs V calculation for equation of state (3D only)

New tools for treatment of solid solutions

Full features

Hamiltonians

Hartree-Fock Theory

Restricted
 Unrestricted

Density Functional Theory

Local [L] and gradient-corrected functionals [G]

Exchange functionals

Slater (LDA) [L]
 von Barth-Hedin (VBH) [L]
 Becke '88 (BECKE) [G]
 Perdew-Wang '91 (PWGGA) [G]
 Perdew-Burke-Ernzerhof (PBE) [G]
[Revised PBE functional for solids \(PBEsol\) \[G\]](#)
[Second-order expansion GGA for solids \(SOGGA\) \[G\]](#)
[Wu-Cohen '06 \(WCGGA\) \[G\]](#)

Correlation functionals

VWN (#5 parameterization) (VWN) [L]
 Perdew-Wang '91 (PWLSD) [L]
 Perdew-Zunger '81 (PZ) [L]
 von Barth-Hedin (VBH) [L]
 Lee-Yang-Parr (LYP) [G]
 Perdew '86 (P86) [G]
 Perdew-Wang '91 (PWGGA) [G]
 Perdew-Burke-Ernzerhof (PBE) [G]
[Revised PBE functional for solids \(PBEsol\) \[G\]](#)
[Wilson-Levy '90 \(WL\) \[G\]](#)

Hybrid HF-DFT functionals

B3PW, B3LYP (using the VWN5 functional), PBE0
 User-defined hybrid functionals

Numerical-grid based numerical quadrature scheme

[London-type empirical correction for dispersion interactions \(Grimme scheme\)](#)

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
 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

Energy derivatives

Analytical first derivatives with respect to the nuclear coordinates and cell parameters

Hartree-Fock and Density Functional methods
 All-electron and Effective Core Potentials

Wave function analysis and properties

Band structure

Density of states

Band projected DOS
 AO projected DOS

All Electron Charge Density - Spin Density

Density maps
 Mulliken population analysis
 Density analytical derivatives

Atomic multipoles

Electric field

Electric field gradient

Structure factors

Electron Momentum Density and Compton profiles ([Enhanced version](#))

Electrostatic potential and its derivatives

Quantum and classical electrostatic potential and its derivatives
 Electrostatic potential maps (2D and 3D)

Fermi contact

Localized Wannier Functions (Boys method)

Dielectric properties

Spontaneous polarization

Berry Phase
 Localized Wannier Functions

Dielectric constant

[New Coupled Perturbed HF\(KS\) scheme](#)
 Finite-field approximation

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 \(MPI\) \(distributed memory\)](#)

New features highlighted in blue