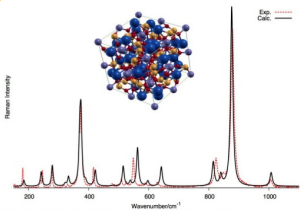
CRYSTAL14 new features in a glimpse

CRYSTAL14 is the last version of the program. It significantly extends its applicability domain, computational performance and predicted properties.

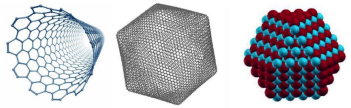


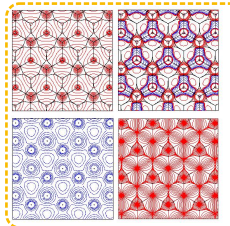
Raman spectrum of Grossular

IR and Raman intensities can be evaluated analitycally through a coupled perturbed scheme. Only a few keywords in the input are sufficient to generate both spectra: FREQCALC, INTENS, INTRAMAN, INTCPHF, END. This requires no scripts, no files to save and copy, no manipulation. Everything is performed by the crystal (or PCRYSTAL, for parallel mode) executable.

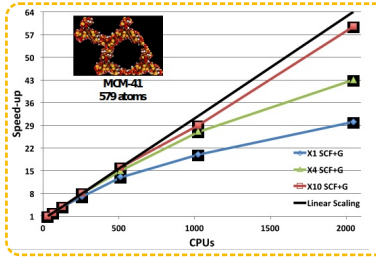
Fully automated (i.e. one keyword, singlerun) algorithms have been implemented in CRYSTAL for computing the elastic, piezoelectric and photoelastic tensors of crystals. From the knowledge of the elastic tensor, for instance, a variety of directional elastic properties of crystals can be derived (bulk, shear and Young moduls, Poisson's ratio and seismic wave velocities, ...). Elastic and piezoelectric tensors can be computed also for low-dimensional 1D and 2D systems (nanotubes, polymers, monolayers, surfaces, etc.). The fully automated calculation of the Equation of State (EOS) of crystals has been revised and new EOSs added (exponential Vinet, logarithmic, Poirier-Tarantola).

CRYSTAL allows to easily build and analyse the structure and properties of a variety of nanostructures, including nanotubes, fullerenelike cages, nanoclusters and nanocrystals.





Bader's topological analysis of the electron charge density of periodic systems can now be automatically performed given that the TOPOND package by C. Gatti has been encoded into the CRYSTAL program. Taking advantage of full parallelization of the algorithms, this analysis can be performed at low cost even for very large systems. Graphical tools are available to plot nice pictures of the electron charge density and its derivatives (see h-BN above).



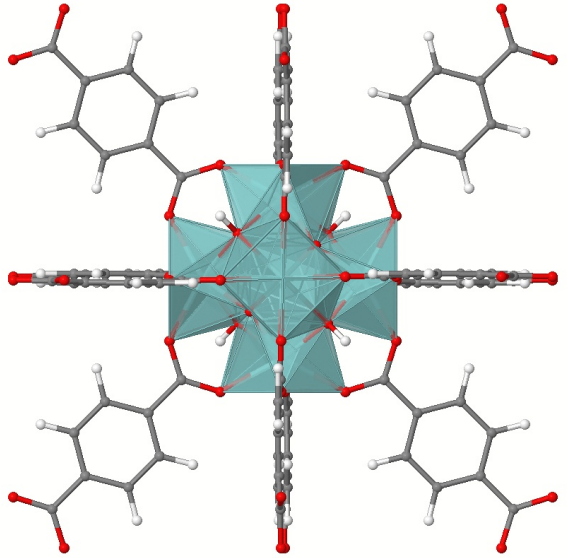
CRYSTAL can be efficiently run both in parallel (P) and massive parallel (MPP) mode. The MPP mode is particularly suitable for studying large systems, drastically improving the speed-up and reducing the requirement for memory.

For more details and further information refer to: Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalleri, S. Casassa, L. Maschio, M. Ferrabone, M. De La Pierre, P. D'Arco, Y. Noel, M. Causa, M. Rerat, B. Kirtman. Int. J. Quantum Chem. 114, 1287 (2014).

CRYSTAL web site: www.crystal.unito.it
Software distribution: www.crystalsolutions.eu
Theoretical Chemistry Group: www.theochem.unito.it
Contacts: **info@crystalsolutions.eu**

CRYSTAL

A powerful and scalable computational tool for solid state chemistry and physics



www.crystal.unito.it

Since 1988 CRYSTAL is used to study the physical and chemical properties of molecules, polymers, nanotubes, surfaces and crystalline solids worldwide.

CRYSTAL is a project leaded by the Theoretical Chemistry Group of the University of Turin - Italy

What is CRYSTAL?

Platforms and distributions

CRYSTAL is distributed according to two basic licences:
- Serial/Parallel Unix/Linux/MacOSx
- Serial Windows

The basic licence for Unix/Linux/MacOSx can be extended by including the Windows binaries, MPP, and CRYSCOR.

Courses

International Schools and Workshops are organised yearly.

A general-purpose program for the study of crystalline solids.

The CRYSTAL program computes the electronic structure of periodic systems within Hartree Fock, density functional (LDA, GGA, mGGA) or various hybrid approximations (global and range-separated hybrids). CRYSTAL lets you perform consistent studies of the physical and chemical properties of crystalline solids (3D), surfaces (2D), polymers (1D) and molecules (0D), like structural features and vibrational properties including IR and Raman intensities, along with magnetic, elastic, piezoelectric, photoelastic and dielectric properties. A unique feature is the extensive exploitation of symmetry to achieve computational efficiency: 230 space groups, 80 two-sided plane groups, 99 rod groups and helical symmetry, 32 crystallographic point groups and molecular point group symmetry (e.g., icosahedral). 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. Restricted (Closed Shell) and Unrestricted (Spin-polarized) calculations can be performed with all-electron and valence-only basis sets with effective core pseudo-potentials.

Main features

Hamiltonians
- Hartree-Fock Theory
- Density Functional Theory
- Numerical-grid based numerical quadrature scheme
- London-type empirical correction for dispersion interactions

Energy derivatives
- Analytical first derivatives with respect to the nuclear coordinates and cell parameters
- Analytical derivatives, up to fourth order, with respect to an applied electric field (CPHF/CPKS)

Basis sets
- Gaussian type function
- All-electron and valence-only with effective core pseudo-potentials
- Predefined and user-specified basis sets supported

Type of calculations
- Single-point energy
- Geometry optimizations
- Harmonic vibrational frequencies including IR and Raman intensities
- Anharmonic frequencies for X-H bonds
- Automated calculation of the elastic tensor of crystalline systems, and piezoelectric and photoelastic tensors
- Automated E vs V calculation for equation of state (3D only)
- Improved tools to model solid solutions

Wave function analysis and properties
- Band structure
- Density of states
- Electron Charge and Spin density
- Atomic multipoles
- Electric field / gradient
- Static/dynamic structure factors
- Electron momentum density and Compton profiles
- Electrostatic potential
- Fermi contact
- Localized Wannier functions
- Mossbauer effect
- Dielectric properties
- Topological analysis of the electron charge density

Sw performances
- Memory management: dynamic allocation
- Full parallelization of the code

Periodic Systems
- Consistent treatment of all periodic systems
- Automated geometry editing

Simmetry
- Symmetry is fully exploited at all steps of the calculation

CRYSCOR extension

A computational tool for the abinitio study of electron correlation in 1D, 2D and 3Dperiodic nonconducting systems, as well as molecules.
- CRYSCOR uses the Hartree-Fock solution provided by the periodic LCAO-code CRYSTAL.
- The local correlation scheme is similiar to that applied in the corresponding molecular techniques, e.g. in the MOLPRO package.
- Two-Electron integrals are efficiently calculated using the density fitting technique and the multipole approximation.
- The Dual Basis set scheme allows for an expansion of the virtual space with respect to that used in the reference HF calculation.

MPP extension

An enhanced massive parallel version of the code is available to allow user to reach an improved scaling in parallel execution on super-computing resources.
- MPP is particularly suitable for studying large systems, drastically improving the speed-up and reducing the requirement for memory.
- An excellent scalability can be obtained when running jobs on approximately NBF/50 cores, where NBF is the number of basis functions.

CRYSTAL-ready solutions

Turn-key solutions to maximize the performance of CRYSTAL.
CRYSTAL-ready solutions deliver CRYSTAL oriented and ready to use systems, able to meet customers specific issues.

Scalabe solutions

CRYSTAL-ready 1401/2 - Entry level systems with 2/4 processors and 20/40 cores. Ideal for individual researchers or small groups.

CRYSTAL-ready 1403 - A small cluster with 4 nodes and a total of 80 cores, expandable. The best combination of price and performance.

CRYSTAL-ready 1404 - The top level system. A NUMA cluster for data centers. Modular, scalable, maximum performance, ease to manage.

Top providers. Hardware are powered by **SGI®**, the trusted leader in HPC. Software are powered by **Aethia**, the Italian HPC software engineering company, exclusive distributor of CRYSTAL.

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CRYSTAL solutions

A joint project between the Theoretical Chemistry Group of University of Turin and Aethia Srl for CRYSTAL codes distribution.