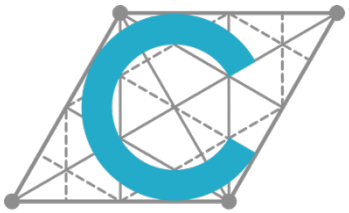
CoSeC SOFTWARE SPOTLIGHT



CRYSTAL

www.crystal.unito.it

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CRYSTAL is an ab initio electronic structure program, concentrating on density functional theory (DFT) for periodic systems. Unusually, the software uses a Gaussian Basis set.

Value for Research

CRYSTAL is a general-purpose DFT theory code, approximately solving the Schrödinger equation, one of the fundamental equations of nature. As such it has found a very wide and varied use, and examples include examining the fundamentals of chemical bonding in solids; catalysis; surface adsorption; properties of materials in batteries; carbon sequestration; electrical conductivity and associated thermoelectric properties; doping; magnetic properties and novel material prediction.

Development

CRYSTAL is the result of a long-standing collaboration between what was originally SERC Daresbury Laboratory and the Theoretical Chemistry Group at the University of Turin, Italy, the latter who visited Daresbury in the early 1980s to develop the software with their expert in Gaussian Basis sets, Vic Saunders. They had developed a semi-empirical code to study the electronic structure of periodic systems but needed Vic to produce an *ab initio* code. The result was CRYSTAL88 and many follow up releases, the latest of which is CRYSTAL23. The team at Turin has driven the scientific side of CRYSTAL's development, while members of Scientific Computing (SC) have performed the computational work e.g. Turin has implemented spin orbit coupling and methods to automatically optimise basis sets, whilst SC have concentrated on the optimisation and parallelisation of the code.

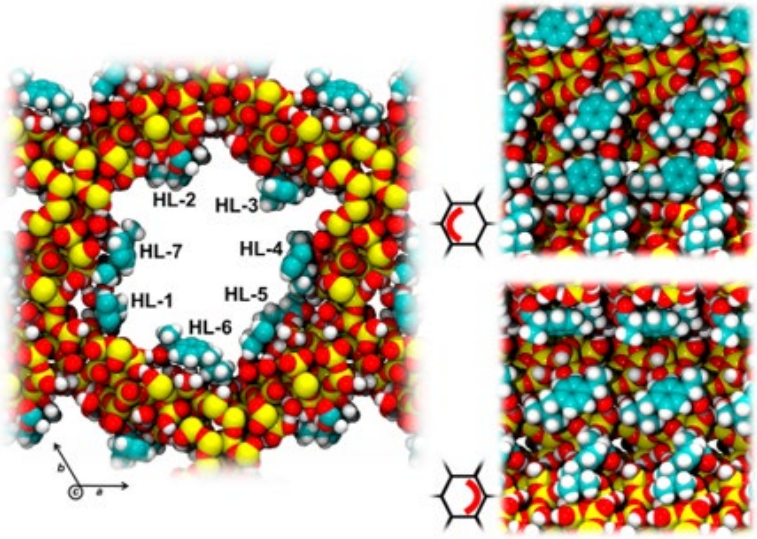
Functionality

CRYSTAL solves the electronic structure of periodic systems at the DFT level. it can exploit full space group symmetry, and as it uses a local, Gaussian basis set calculations that involve exact exchange are not prohibitively expensive. It features a wide set of methodologies and can calculate many properties of the system from the solutions of Kohn-Sham equations. Functionality includes calculations on molecules, polymers, slabs and CRYSTALs; full use of crystallographic symmetry; a variety of Hamiltonians; efficient parallelisation using MPI and OpenMP; geometry optimisation with analytic

forces; Coupled-Perturbed-Kohn-Sham calculations; vibrational analysis, including anharmonicity; and calculation of a wide variety of properties of the system.

The Future

CRYSTAL is being actively developed. At SC, the team are focusing on extending the parallel versions of the code so that they can exploit multiple GPU accelerators. This includes further focus on the linear algebra and the ability to map a single k point to multiple GPUs, which thanks to the library ELPA, has now been achieved. The team will also work on implementing the two electron integrals required for the Kohn-Sham Hamiltonian, as well as DFT exchange and correlation terms – which in turn, has incidentally sped up the CPU version of the code through back porting the vectorised GPU code.



From: Large-Scale B3LYP Simulations of Ibuprofen Adsorbed in MCM-41 Mesoporous Silica as Drug Delivery System, *J. Phys. Chem. C*. 2014;118(46):26737-26749. doi:10.1021/jp507364h
Description: B3LYP-D* structure of the High Loading model, i.e., MCM-41 with seven ibuprofen molecules adsorbed in its pore. (left) View along c axis. (right) Lateral view cut to show the two halves of the pore.

LICENCE	Programming Language	Repository URL
UK based https://www.crystalsolutions.eu/prod/crystal-cryscor/academic-uk/38-crystal23-for-unixlinuxintel-mac-os-x.html https://www.crystalsolutions.eu/crystal-cryscor.html	Fortran 2008, C++, Python3, ScaLapack, ELPA	Closed source