



CASTEP

www.castep.org

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CASTEP is a leading code for calculating the properties of materials from first principles. Using density functional theory, it can simulate a wide range of properties of materials proprieties including energetics, structure at the atomic level, vibrational properties, electronic response properties etc. In particular it has a wide range of spectroscopic features that link directly to experiment, such as infra-red and Raman spectroscopies, NMR, and core level spectra.

Value for Research

CASTEP is a general-purpose materials modelling code with application areas ranging from Energy Materials to Pharmaceuticals. CASTEP is a scalable, robust, and user-focussed package. This has made it ideal for applications such as structure prediction ([AIRSS](#), [Genetic Algorithms](#), [base-line for CCDC “Blind Tests”](#), as a [testbed for the development of tools](#) to bridge the gap between theory and experiment and adoption by communities outside of the traditional theoretical and computational science (e.g. CCP-NC).

Development

The original CASTEP was started by Mike Payne (University of Cambridge) in late 1980s. Written in Fortran77 it became a popular and successful tool. However, by the 90s development had become fragmented with multiple forks of the project and even within individual forks, the barrier to entry was increasingly high with a monolithic codebase. In 1998 the CASTEP Developers Group (CDG) was formed to re-write the code in modular Fortran90 starting with a formal specification document. The re-write was designed around Message Passing Interface (MPI) from the start to take advantage of distributed parallel HPC resources. “New” CASTEP was released in 2000 alongside a user workshop. The principles of embracing changing technology and software standards continues to this day. The CDG and development community have an annual code development workshop aka “codefest” to coordinate effort, discuss future developments, and decide on supported technologies.

Functionality

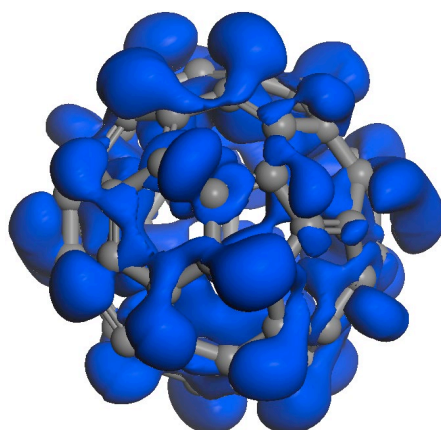
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spectroscopic features that link directly to experiment, such as infra-red and Raman spectroscopies, NMR, and core level spectra.

Research groups can apply for a CASTEP academic source code licence, which is free-of-charge for non-commercial use. STFC (CoSeC) administers academic licences on behalf of Cambridge Enterprise and the CASTEP Developers Group. Note that this academic licence only includes a command-line interface and does not include the BIOVIA Materials Studio graphical interface.

The Future

CASTEP is in active development and is committed to delivering annual releases. New features for the next release include nonlocal Van der Waals Density Functionals. The availability of this method will give CASTEP users the ability to simulate these subtle, long-range effects with the electron density across the entire simulation being taken into account. Our next release focuses on the GPU capabilities of CASTEP, extending the ability to exploit accelerator hardware across more simulation tasks, such as NMR. We aim to provide users with the ability to make effective use of accelerator hardware when available, while preserving the efficiency of traditional CPU use.



LICENCE

Free of charge academic and commercial through Dassault Systèmes BIOVIA Materials Studio

Programming Languages

Fortran 2008 with small amounts of C. Python interface through f90wrap

Repository URL

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