MS Modeling Datasheet

CASTEP

CASTEP is an *ab initio* quantum mechanical program employing density functional theory (DFT) to simulate the properties of solids, interfaces, and surfaces for a wide range of materials classes such as ceramics, semiconductors, and metals. First principle calculations allow researchers to investigate the nature and origin of the electronic, optical, and structural properties of a system without the need for any experimental input, with the exception of the atomic number of mass of the constituent atoms. CASTEP is thus well suited to research problems in solid state physics, materials science, chemistry, and chemical engineering. In these areas, researchers can employ computer simulations to perform virtual experiments, which can lead to tremendous savings in costly experiments and shorter developmental cycles.

What Does CASTEP Do?

Originally developed in the Theory of Condensed Matter Group at Cambridge University, UK, CASTEP (Cambridge Sequential Total Energy Package) is a suite of programs that provides advanced quantum mechanical calculations for chemicals and materials research. CASTEP has been rewritten in Fortran90, an object oriented programming language. This will allow for rapid deployment of new technology and drastically cut the development time typically needed to introduce new methods and tools within CASTEP.

A new transition state search employing a combination of LST/QST algorithms with subsequent conjugate gradient methods greatly facilitates the optimization of the transition state structure. This robust and easy-to-use scheme offers significant speed-up as compared to traditional methods.

The elastic constants task uses the finite deformation technique in order to obtain a full 6x6 tensor of the elastic constants for a periodic structure of any symmetry. CASTEP automatically generates the set of distorted structures that is required by symmetry to produce

the full set of elastic constants. The linear response functionality in CASTEP calculates phonon frequencies within the linear response formalism and it allows the prediction of several thermodynamic properties such as free energy and heat capacity. Moreover, the ability to make thermodynamical properties prediction of solid-state systems is valuable since it enables the simulation of many condensed matter properties such as the phase stability of structural modifications.

Based on total energy pseudopotential methods, CASTEP takes the number and type of atoms in a system and predicts properties such as lattice constants, molecular geometry, elastic constants, bandstructures, density-of-states, charge densities and wave functions, and optical properties. The pseudopotential plane-wave technology underlying CASTEP is well validated, with hundreds of scientific publications written each year showing new applications of the code. Efficient parallel versions of the code are also available for large systems requiring hundreds of atoms.

CASTEP has been applied to a wide range of research problems such as surface chemistry, physi- and chemisorption, heterogeneous catalysis, defects in semiconductors, grain boundaries, stacking faults, nanotechnology, molecular crystals, polymorphic studies, diffusion mechanisms, and molecular dynamics of liquids.
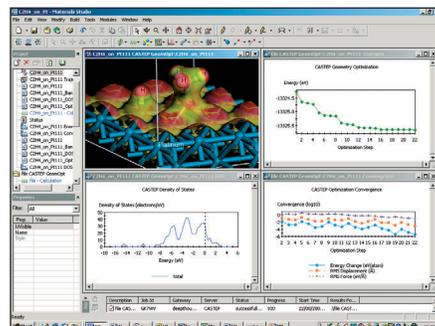
The Materials Studio Advantage

CASTEP is an MS Modeling product operated within the Materials Studio® software environment. Materials Studio provides a user-friendly interface, complying with Windows® standards. Materials Visualizer, the core MS Modeling product, offers a wide range of model building and visualization tools that allow you to rapidly construct models of the systems of interest, select the CASTEP module with two mouse clicks, and run an advanced quantum mechanical calculation.

A flexible client-server architecture means that calculations can be run on servers located elsewhere on your network. Results are returned to your PC, where

MATERIALS STUDIO

they may be displayed and analyzed. You can easily produce high quality graphics of molecular and materials structures, molecular orbitals, electrostatic potentials, or charge densities. Structures, graphs, and other data such as video clips produced from CASTEP output can be instantly exchanged with other PC applications, assisting you when sharing them with colleagues or when analyzing your results using spreadsheets and other packages.

How Does CASTEP work?

CASTEP[1-3] uses a total energy plane-wave pseudopoten-

▲ C_2H_4 absorption on a Pt(111) surface showing the electrostatic potential projected on the electronic density isosurface. Density of states, energy evolution, and energy convergence graphs are also shown.

tial method. In the mathematical model of the material, CASTEP replaces ionic potentials with effective potentials acting only on the valence electrons in the system. Electronic wavefunctions are expanded through a plane-wave basis set, and exchange and correlation effects in electron-electron interactions can be included within either the local density (LDA) or generalized gradient (GGA) approximations. Combining the use of pseudopotentials and plane wave basis sets makes it extremely easy to calculate the forces on the atoms, enabling efficient optimization of ionic configurations of molecules, solids, surfaces, and interfaces. The primary reason that CASTEP has become so powerful is the numerical methods used to solve the equations determining the electronic state.

A new transition state search scheme has been implemented, which uses a combination of traditional LST/QST methods[4] and a subsequent refinement using a conjugate gradient method[5,6]. This new robust and fast scheme[7] allows transition state optimization without the added

expense of computing a second derivative matrix, as required by traditional transition state searching algorithms.

The Future

Over the last ten years, there has been staggering progress in the application of QM techniques to materials science. Ten years from now, these codes will be widely and routinely used, accessible from the desktop personal computers of thousands of scientists. CASTEP is uniquely positioned to drive this development. It is the only code in its class available as commercial-quality software, supported by a worldwide team of scientists, maintained in regular high-quality software releases, and seamlessly integrated with a comprehensive range of model-building and simulation tools.

Features and Capabilities

Calculation tasks

· Calculation of total energies, forces, and stresses
· Geometry relaxations (ionic degrees of freedom and cell parameters) with or without internal and external constraints
· Molecular dynamics using NVE, NVT, and Langevin dynamics
· Transition state search based on the linear and quadratic synchronous transit methodology (LST/QST)
· Calculation of elastic constants based on the finite deformation technique
· Calculation of phonon frequencies within the linear response formalism.

Capabilities

· Automatic, intelligent selection of key parameters (basis sets, FFT mesh, k-points, convergence criteria, ...)
· Choice of local and non-local functionals for approximating exchange and correlation effects
· Ultra soft and norm-conserving pseudopotentials for the entire periodic table
· Visualization of band structures, local and partial density of states
· Calculation of frequency dependent electronic dielectric

function and optical properties

· Transition state search using a combined LST/QST/Conjugate gradient approach.

Job control and restart options

· Choice of data distribution strategy for parallelization: k, G, or k+G

· Choose number of CPU's

· Specify server machine

· Monitor output and status reports including text or graphs of energy and gradient during geometry optimization

· Live updates of the model geometry and job status

· Kill jobs on remote server via the Materials Visualizer

· SCF, MD, and optimization restarts.

Properties

· UV/VIS spectra

· Mulliken population and charge analysis

· Bond-order analysis

· Visualization of the charge, spin, and deformation densities using the Materials Visualizer

· Generating 3-D contours and 2-D slices of volumetric properties using the Materials Visualizer

· Overlay multiple plots and color surfaces by property maps using the Materials Visualizer

· Computation of static elastic constants

· Phonon dispersion

· Total and projected phonon density of states

· Thermodynamic properties in quasiharmonic approximations (free energy, enthalpy, entropy, heat capacity, Debye temperature).

Miscellaneous Options

· Multiple k-points

· Real or reciprocal space pseudopotential representation

· Full use of symmetry of the system

· Various SCF options: DIIS, density mixing, smearing.

References

1. Milman, V., Winkler, V., White, J. A., Pickard, C. J, Payne, M. C., Akhmatskaya, E. V., and R. H. Nobes, *Int. Quant. Chem*., **2000**, *77*, 895.

2. Payne, M. C. , Teter, M. P., Allan, D. C, Arias, T. A., and Joannopoulos, J. D., *Rev. Mod. Phys*., **1992**, *64*, 1045.

3. M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, M. C. Payne, J. *Phys.: Cond. Matt.*, 2002, 14, 2717.

4. Halgren, T. A. and Lipscomb, W. N., *Chem. Phys. Lett.,* **1997***, 49*, 225.

5. Bell, S. and Crighton, J. S., *J. Chem. Phys.,* **1984**, *80,* 2464.

6. Fischer, S. and Karplus, M., *Chem. Phys. Lett*., **1992**, *194,* 252.

7. N. Govind, M. Petersen, G. Fitzgerald, D. King-Smith, and J. Andzelm, Computational Materials Science28, 250 (2003)