

Compute magnetic resonance properties from first principles

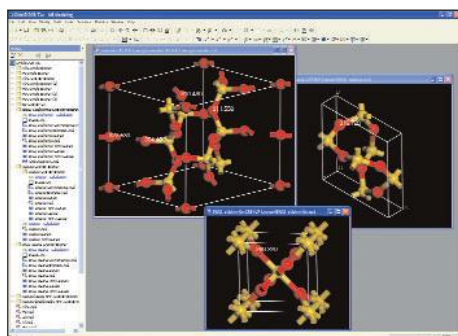
Determine molecular-level structure by comparing a simulated NMR spectrum with experimental data

Compute the NMR shifts of molecules, solids, interfaces, and surfaces for a wide range of materials classes including organic molecules, ceramics, and semiconductors for both molecular and periodic systems

## Materials Studio Datasheet

# NMR CASTEP

NMR CASTEP predicts key magnetic resonance properties of molecules and solid state materials from first principles. Based on density functional theory (DFT), NMR CASTEP enables users to compute NMR chemical shifts and electric field gradient tensors, with unprecedented accuracy. The method can be applied to compute the NMR shifts of molecules, solids, interfaces, and surfaces for a wide range of materials classes including organic molecules, ceramics, and semiconductors. First principle calculations allow researchers to investigate the nature and origin of the magnetic resonance properties of a system without the need for any empirical parameters. NMR CASTEP is thus well suited to research problems in solid state physics, materials science, and chemistry where using computer simulations to perform virtual experiments can lead to tremendous benefits over using experimental NMR techniques alone.



▲ NMR chemical shifts can be predicted for elements in both molecular and solid state systems. This example shows the  $^{17}\text{O}$  shifts for 3 different structures of  $\text{SiO}_2$ : quartz, coesite, and stishovite.

### What does NMR CASTEP do?

NMR CASTEP provides a tool for predicting accurate NMR chemical shift tensors, isotropic shifts, and electric field gradients for any material with tremendous reliability: relative isotropic shifts can be predicted to within a few ppm.

Developed by Cambridge University and the Université de Paris et Marie Curie, NMR CASTEP is the first ab initio NMR method to work for both molecular and periodic systems. The method can be applied

equally well to simulating the NMR chemical shifts of organic molecules, organic crystals, inorganic crystals, or amorphous compounds. By incorporating relativistic effects, the implementation achieves accurate results even for heavy elements.

NMR is often used as an analytical tool to aid in structure prediction. The relative complexity of solid state structures makes this a challenging task. Often, even though the general features of the crystal structure are understood, a detailed analysis of the geometry proves elusive. Using NMR CASTEP it is possible to simulate the NMR spectrum for a series of related structures until a match is discovered between the computed and experimental results. In this way, theory complements experiment, both contributing the determination of the structure.

Using computed chemical shifts, users can perform assignment of the observed NMR spectra. Comparing the accurate results of NMR CASTEP with experiment makes it possible, for example, to assign chemical shifts to atoms unambiguously; to discriminate between crystal polymorphs; or to analyze the degree of disorder in crystalline minerals that lose structure due to radioactive destruction (metamict materials).

NMR CASTEP has been applied to a wide range of research problems including the determination of the structure of icosahedral  $\text{B}_4\text{C}$ ; the assignment of  $^{17}\text{O}$  chemical shifts in zeolites; the comparison of glutamic acid polymorphs; and the structural analysis of aperiodic  $\text{ZrSiO}_4$  through analysis of the  $^{29}\text{Si}$  NMR spectrum. Published results are also available for  $^{77}\text{Se}$  and  $^{125}\text{Te}$ . For further applications, see the list of publications on the Accelrys website.

### The Materials Studio Advantage

NMR CASTEP is operated from within the Materials Studio's MS Modeling software suite. MS Modeling provides a user interface that is easy-to-use and quick to learn, complying with Windows® standards. Materials Visualizer, the core MS Modeling product, runs under Windows 2000 or XP, and it offers a wide range of model building and visualization tools. You

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can rapidly construct models of the systems of interest, select the NMR module, and run an advanced quantum mechanical simulation.

A flexible client-server architecture means that calculations can be run on Windows 2000 or XP, Red Hat Linux (Intel), SGI Irix, or HP Tru64 servers located elsewhere on your network. Results are returned to your PC, where 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.

Output from NMR CASTEP can be instantly displayed in the MS Modeling user interface and shared with colleagues facilitating the analysis and dissemination of results

### How does NMR CASTEP work?

NMR CASTEP has been implemented using the framework provided by the CASTEP<sup>1-3</sup> density functional program. This uses a total energy plane-wave pseudopotential method. Combining the use of pseudopotentials and plane wave basis sets makes it extremely easy to calculate the forces on the atoms. This enables efficient optimization of ionic configurations of molecules, solids, surfaces, and interfaces. The primary reason that CASTEP has become so powerful is the efficiency and accuracy of the numerical methods used to solve the equations determining the electronic state.

NMR CASTEP uses the gauge-including projector augmented-wave (GIPAW) approach<sup>4</sup> to describe the wavefunction in the presence of a magnetic field. Analogous to the GIAO method employed by localized basis approaches<sup>5</sup>, the GIPAW is necessary to maintain translational invariance in the presence of a magnetic field.

The chemical shift tensor,  $\sigma$ , is defined as the ratio between an external magnetic field,  $B_{\text{ext}}$  and the magnetic field induced at the nucleus,  $B_{\text{in}}$ :  $B_{\text{in}} = -\sigma B_{\text{ext}}$ . NMR CASTEP computes  $\sigma$  using density functional perturbation theory<sup>4</sup>. By including relativistic effects<sup>6</sup> the method is accurate even for heavy elements, like Te. Isotropic chemical shifts are simply the trace of  $\sigma$ , and these can be displayed within the MS Modeling user interface.

## Features and capabilities

### Capabilities

- Computation of chemical shift tensor, isotropic chemical shift, and electric field gradients
- Default nuclear quadrupole moments defined for common isotopes. Interface allows users to override default values for the study of exotic nuclei
- Visualization of isotropic shifts and electric field gradients
- NMR CASTEP is based on the CASTEP DFT program. For a full description of the capabilities of CASTEP visit [www.accelrys.com/mstudio/ms\\_modeling/castep.html](http://www.accelrys.com/mstudio/ms_modeling/castep.html).

### System Requirements

NMR CASTEP is an MS Modeling product operated within the Materials Studio® software environment running on Windows 2000 or XP. Calculations are executed by the NMR CASTEP server running on Windows 2000, XP, SGI Irix, Red Hat Linux (Intel), and HP Tru64 operating systems. For detailed hardware and operating system configurations visit [www.accelrys.com/mstudio/sys\\_reqs.html](http://www.accelrys.com/mstudio/sys_reqs.html)

## References

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Accelrys Corporate Headquarters  
10188 Telesis Court, Suite 100  
San Diego, CA 92121  
United States  
Tel: +1 858 799 5000

Accelrys European Headquarters  
334, Cambridge Science Park,  
Cambridge, CB4 0WN, UK  
Tel: +44 1223 228500

Accelrys Asia Headquarters  
Nishi-shimbashi TS Bldg 11F  
Nishi-shimbashi 3-3-1, Minato-ku,  
Tokyo, 105-0003, Japan  
Tel: +81 3 3578 3861