BIOVIA MATERIALS STUDIO DMOL³

DATASHEET

BIOVIA Materials Studio DMoL³ is a modeling program that uses density functional theory (DFT) to simulate chemical processes and predict properties of materials both rapidly and accurately. Because Materials Studio DMoL³ can predict processes in gas phase, solution, and solid environments, it is broadly applicable to research problems in chemistry, pharmaceuticals, materials science, and chemical engineering, as well as solid state physics. Researchers can use the program to investigate the nature and origin of the chemical, electronic, and structural properties of a system without the need for any experimental input. Use Materials Studio DMoL³ to perform virtual experiments, leading to tremendous savings in costly experiments and shorter developmental cycles.

WHAT DOES MATERIALS STUDIO DMOL³ DO?

Researchers in chemistry, pharmaceuticals, and materials science may be tasked with a number of challenging goals like the development of new compounds, such as a more efficient catalyst or a more effective medicine; or they may need to improve a manufacturing process by determining a more efficient synthesis pathway; or they may be faced with simply understanding and describing fundamental processes,

The geometry and highest occupied molecular orbitals (HOMO) of two structures optimized in Materials Studio DMol³. The top structure is caprolactone, a monomer use in the production of artificial skin. The lower structure is Al(OH)3, which can initiate ring opening. Materials Studio DMol³ can be used to predict the mechanisms of ring opening and polymerization.

explaining why one particular material is better than another. Modeling can address all of these challenges, provided that the method is fast and accurate. Materials Studio DMoL³ is just such a method.
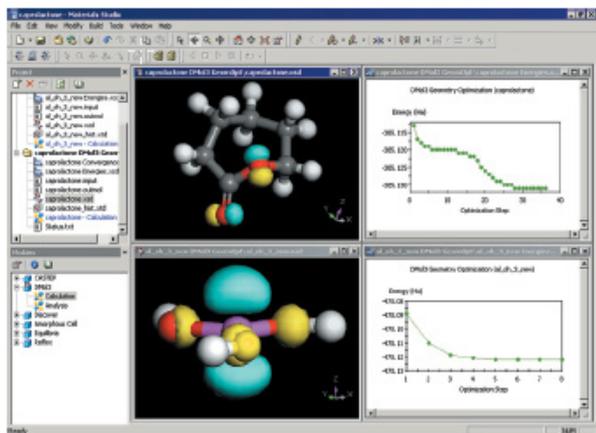
Materials Studio DMoL³ is a DFT program with a long track record of successful commercial applications. With its unique approach to solving quantum mechanical equations, Materials Studio DMoL³ has long been one of the fastest methods available for performing calculations, an advantage that becomes apparent especially for larger systems, those with over 500 atoms.

With its ability to model both molecular and solid state problems, the application provides a way to study the broadest possible range of problems in a single package. The method is equally well suited to performing a conformational analysis of a small molecule as it is to modeling catalysis on a metal surface.

The program can be used in areas such as pharmaceutical drug discovery to model ligand binding or in drug development to understand crystal polymorphs. Use Materials Studio DMoL³ to design new metallocene catalysts for polymerization, or to understand the mechanism of supported metal catalysts. You can even use Materials Studio DMoL³ to predict band gaps and design new solid state materials.

Materials Studio DMoL³ has been applied to such diverse research problems as homogeneous catalysis, heterogeneous catalysis, semiconductors, molecular reactivity, and combustion technology. Example applications include the study of the process of chemical vapor deposition, understanding the action of automotive catalysts, explaining the mechanism of polymerization reactions, and investigating combustion techniques under extreme conditions.

Materials Studio DMoL³'s emphasis is on speed – without compromising quantum mechanical accuracy. An efficient geometry optimization algorithm lets you predict minimum energy structures rapidly. A transition state search employing a combination of LST/QST algorithms facilitates the evaluation of energy barriers. Reaction rates for use in BIOVIA Materials Studio Cantera chemical dynamics calculations can also be generated using the DMoL³ Reaction Kinetics task. Using parallel versions of the Materials Studio DMoL³ code, large problems can be tackled.

THE MATERIALS STUDIO ADVANTAGE

Materials Studio DMoL[3] is part of the Materials Studio® software environment. Materials Studio provides a user-friendly interface, complying with Windows® standards. Materials Studio Visualizer, the core of Materials Studio, offers a wide range of model building and visualization tools that allow you to construct rapidly models of the systems of interest, easily select Materials Studio DMoL[3], and run an advanced quantum mechanics calculation. The simple user interface together with BIOVIA's training programs ensure that even new users will be able to use the program with confidence.
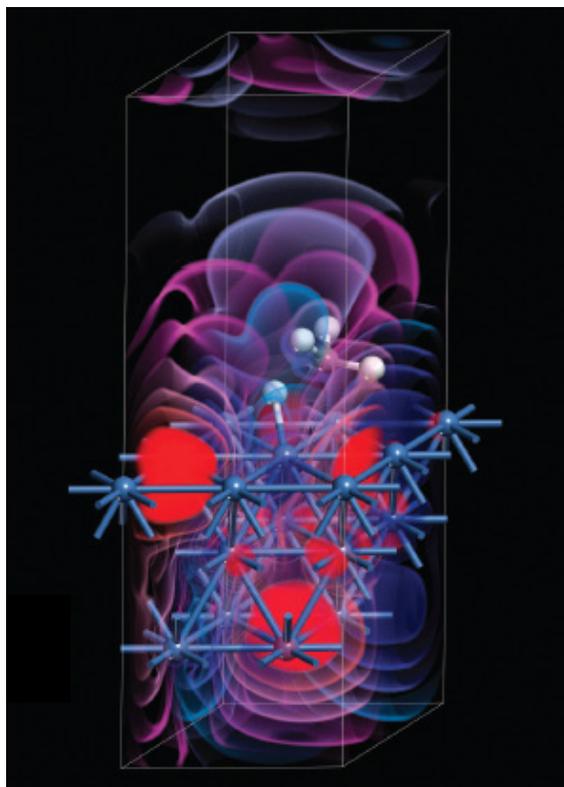
Dissociation of methane on a nickel(III) surface calculated with Materials Studio DMol[3]. The highest occupied molecular orbital is displayed together with the dissociation products chemisorbed on the the metal surface.

A flexible client-server architecture means that calculations can be run on servers located anywhere 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. Structures, graphs, and other data such as video clips produced from Materials Studio DMoL[3] output can be instantly exchanged with other PC applications, assisting you when sharing them with colleagues or when analyzing them using spreadsheets and other packages.

Spreadsheet-like setup allows the method to be applied in a high-throughput environment, performing multiple, repetitive calculations easily, and storing the results in a table. Subsequent statistical analysis can reveal hidden structure-property relationships that can be easily exploited to design new materials or explain behavior on the molecular level.

HOW DOES BIOVIA MATERIALS STUDIO DMOL[3] WORK?

Materials Studio DMoL[3] achieves its speed and accuracy by using numerical functions on an atom-centered grid as its atomic basis.[1,2] The atomic basis functions are obtained from solving the DFT equations for individual atoms and are hence quite accurate. The high quality of these basis sets minimizes basis set superposition effects and allows an improved description of molecular polarizabilities.[3]

The electron density in Materials Studio DMoL[3] is expanded in terms of multipolar, atomic-centered partial densities. This provides a compact yet highly accurate representation of the density, and allows for a good scaling with growing system size. Consequently the evaluation of the Coulomb potential scales linearly with the size of the system. The Hamiltonian matrix elements are calculated by using a sophisticated numerical integration algorithm that also scales linearly.

The algorithms in Materials Studio DMoL[3] allow for very efficient parallelization of the numerical integration procedure. Materials Studio DMoL[3] can perform both All Electron or pseudo-potential calculations. Accurate DFT semi-local pseudo-potentials (DSPP)[4] or the more conventional Effective Core Potentials (ECP)[5,6] can be used.

Geometry and transition state optimizations are performed using delocalized internal coordinates, both for molecular[7] as well as for periodic[8] calculations. This includes the ability to impose Cartesian geometry constraints while performing the optimization in internal coordinates. A transition state search scheme has been implemented which based on a combination of traditional LST/ QST methods[9]. This new robust and fast scheme[10] allows rapid location of transition states.

Solvent effects are included using the COSMO model to simulate a continuum. Uniquely, this model includes periodic cases[11] making it possible to model polymer solvation or heterogeneous catalysis in solution.

FEATURES AND CAPABILITIES

Calculation Tasks

- Restricted and unrestricted DFT calculations
- Geometry optimization
- Transition state search using a combined LST/QST/ Conjugate Gradient approach
- Transition state optimization using eigenvector following
- Determination and graphical display of the complete reaction path
- Frequency calculations using full or partial Hessians
- Solvation via COSMO[11]

Functionals

- Local DFT functionals: PWC, VWN
- GGA-DFT functionals: PW91, BLYP, BP, BOP, PBE, VWN-BP, RPBE, and HCTH
- Harris functional for fast calculations.
- Tkachenko-Scheffler parameters for dispersion corrected DFT for PBESOL, RPBE, and PW91 exchange-correlation functionals
- Hartree-Fock exact exchange (for non-periodic systems)

Basis Sets

- Numerical AO basis sets: Minimal, DN, DND, DNP, TNP
- All electron or core potentials: relativistic effective core potentials, effective core pseudo-potentials, DFT semi-core pseudo-potentials.
- Scalar relativistic all electron calculations

Restart and Job Control Options

- Choose number of CPUs
- Specify server machine
- Monitor output and status reports including text or graphs of energy and gradient during geometry optimization
- Live updates of the geometry
- Halt jobs on remote server via BIOVIA Studio Materials Visualizer

Properties

- Band structure
- Bond order analysis
- Electron work function
- Electrostatic moments
- Fukui indices
- Heats of formation, free energy, enthalpy, entropy, heat capacity, ZPVE
- Mulliken, Hirshfeld, and ESP charges
- Nuclear electric field gradients
- UV/Vis spectra, excited states, polarizability and hyperpolarizability 12
- Vibrational Analysis (with partial Hessian support)
- Empirical Hardness

Graphical Displays with Materials Studio Visualizer

- 3-D contours and 2-D slices
- Animation of normal modes
- Fermi surface
- Fukui functions
- Molecular orbitals, charge, spin & deformation densities
- Overlay multiple plots and color surfaces by property maps

Miscellaneous Options

- Multiple k-points
- Real space cut-off
- Full point-group and space-group symmetry
- Multiple options for accelerating SCF convergence: DIIS, density mixing, smearing.
- Separate spin states for Basis Set Superposition Error (BSSE) corrections

To learn more about Materials Studio, go to 3dsbiovia.com/materials-studio

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