MS Modeling Datasheet

DMol^3

Premier density functional theory program for gas phase, solvent, and solid state simulations

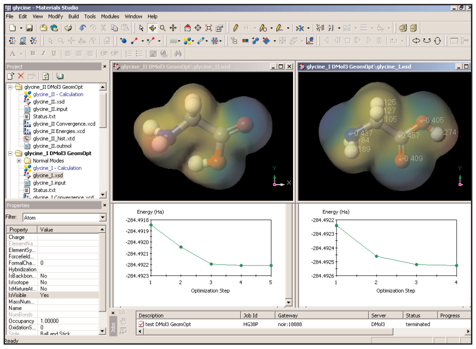
Reliable prediction of electronic structure, reaction energetics, thermochemical, electronic, and optical properites

Well suited to research problems in chemisty, materials science, chemical engineering, and solid-state physics

DMol^3 is a unique density functional theory (DFT) quantum mechanical code that allows users to study problems in the chemical and pharmaceutical industry as well as in materials science with high accuracy and reliability. DMol^3 can simulate processes in gas phase, solvent, surface, and solid environments, which makes it well suited to research problems in chemistry, materials science, chemical engineering, and solid state physics.

DMol^3 is a premier, robust DFT program with a long track record of successful commercial applications. DMol^3 has a unique approach to electrostatics, and and is an efficient optimizer. DMol^3 has long been one of the fastest methods available for performing molecular DFT calculations, especially for large molecules. It now extends this approach to solid-state problems via a high-performance internal coordinate optimizer that can treat the full range of solid-state systems. The DMol^3 code delivers the first robust, general-purpose internal coordinate optimization scheme for periodic systems. 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 works for both molecular and periodic systems, and is significantly faster than traditional methods. Using parallel versions of the DMol^3 code, large problems can be tackled.

DMol^3 has been enhanced, in some cases improving performance by up to a factor of 3-4, depending upon the system studied and the hardware system used. This makes DMol^3 one of the fastest ab initio codes in the world. The added Handy-Tozer functionality enables the simulation of hydrogen bonded systems and accurate molecular structures and thermodynamic data can be obtained. DMol^3 is an important tool that can find many industrial applications, for example in the pharmaceuticals industry and the study of catalysts.



Properties

Filter: Atom

Property	Value
Charge	
ElementNa...	
ElementSy...	
Forcefield...	
FormalCha...	0
Hybridization	
IsBackbon...	No
IsIsotope	No
IsMixtureAt...	No
IsVisible	Yes
MassNum...	
Name	
NumBonds	
Occupancy	1.00000
OxidationS...	0
Style	Ball and Stick

Description	Job Id	Gateway	Server	Status	Progress
☑ test DMol3 GeomOpt	HG38P	noir:18888	DMol3	terminated	

▲ *The geometry of two conformations of glycine optimized in DMol^3. DMol^3 predicts glycine_I to be lower in energy by about 1.0 kcal/mol. The chart documents are updated as the calculation proceeds indicating the energy after each optimization step. The molecular electrostatic potentials of glycine_I and glycine_II are displayed. These give indications of where a reaction would take place.*

The transition state toolbox contains the powerful transition state confirmation method Nudged Elastic Bands (NEB). NEB enables scientists to verify that the transition state obtained by the LST/QST technique is the one linking the reactants and the products.

DMol^3 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.

The Materials Studio Advantage

DMol^3 is an MS Modeling product and is operated from 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 DMol^3 with two mouse clicks, and run an advanced quantum mechanics calculation.

A flexible client-server architecture means that cal-

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culations can be run on Windows NT, 2000 or XP, Linux, running on Intel 32 bit compatible systems, IRIX, and 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. Find more specific information in the 'System Details' section of this datasheet.

Structures, graphs, and other data such as video clips produced from 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.

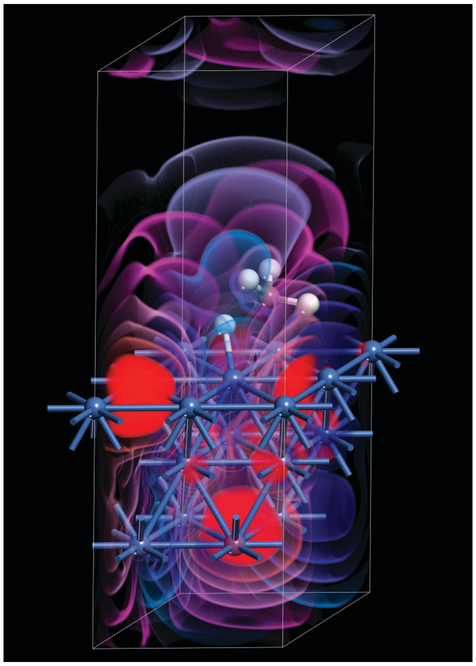
How Does DMol^3 work?

DMol^3 uses numerical functions on an atomcentered grid as its atomic basis[1,2]. The atomic basis functions are obtained from solving the DFT equations for individual atoms and are stored as sets of cubic spline. The high quality of these basis sets minimizes superposition effects and, consequently, dissociation of molecules, for example, is accurately described. The long-range tail of the basis set exhibits correct charge distribution, and allows an improved description of molecular polarizabilities[3].

The electron density in 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. The multipolar representation of the electron density is used to evaluate Coulomb potential via the solution of Poisson's equation. Thus, calculation of the Coulomb potential, in principle a costly step, is replaced by fast evaluation of potential on each center, an operation which 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 DMol^3 allow for very efficient parallelization of the numerical integration procedure.

DMol^3 can perform both All Electron (or All Electron Relativistic for heavy elements), or pseudo-potential calculations. The later is an alternative to all electron calculations where either the newly developed DFT semi-local pseudo-potentials (DSPP)[4] or Effective Core Potentials (ECP)[5,6] can be used. Currently, DSPPs and ECPs are provided beginning with element number 21, Sc.



▲ *Dissociation of methane on a nickel(III) surface calculated with DMol^3. The highest occupied molecular orbital is displayed together with the dissociation products chemisorbed on the the metal surface.*

Users are encouraged to use DSPPs rather than ECPs. The former have been developed specifically for DMol^3 calculations whereas the latter are for Hartree-Fock potentials.

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 new transition state search scheme has been implemented which uses a combination of traditional LST/QST methods[9] and a subsequent refinement using a conjugate gradient method[10,11]. This new robust and fast scheme[12] allows transition state optimization without the added expense of computing a second derivative matrix, as required by traditional transition state searching algorithms.

Finally, the NEB method is a robust technique to validate a transition state by connecting it to the proper reactant and product. NEB can be used to investigate PES containing several energy minima and maxima for both molecules and solids.

Consequently, NEB allows users to effectively answer the question, “Does this TS really connect my presumed reactant with the presumed product or does it connect alternative minima?”

DMol^3 is accessed via two separate licenses (DMol^3 Molecular and DMol^3 Solid State). Their features and capabilities are listed below.

Features and Capabilities

Features marked with an asterisk (*) can not be accessed via the user interface, but are available by modifying the input file.

Calculation Tasks

- Restricted and unrestricted DFT calculations
- Geometry and energy predictions
- Transition state search using a combined LST/QST/Conjugate Gradient approach
- Transition state optimization using eigenvector following
- Graphical display of the reaction path with the reaction pre-viewer of the Materials Visualizer
- Optimization with robust delocalized internal coordinates
- Frequency calculations using full or partial Hessians
- Animation of normal modes using the Materials Visualizer
- Transition state confirmation using the NEB method.

Functionals

- Local DFT functionals: PWC, VWN
- GGA-DFT functionals: PW91, BLYP, BP, BOP, PBE, VWN-BP, RPBE, and HCTH
- Harris functional for fast calculations.

Basis Sets

- Numerical AO basis sets: Minimal, DN, DND, and DNP
- Relativistic effective core potentials and scalar relativistic all electron, effective core pseudo-potentials, all electron relativistic and DFT semi-core pseudo-potentials.

Restart and Job Control Options

- SCF restart via vector or density*
- Optimization and Frequency calculation restart*
- 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
- Kill jobs on remote server via Materials Visualizer.

Properties

- UV/VIS spectra (molecules only)
- Mulliken, Hirshfeld, and ESP charges
- Electrostatic moments
- Fukui indices
- Nuclear electric field gradients
- Bond order analysis
- Heats of formation, free energy, enthalpy, entropy, heat capacity, ZPVE
- Solvation via COSMO[13,14]*
- Visualization of molecular orbitals, charge, spin & deformation densities using the Materials Visualizer
- Visualization of Fukui functions using the Materials Visualizer
- Generating 3-D contours and 2-D slices using the Materials Visualizer
- Overlay multiple plots and color surfaces by property maps using Materials Visualizer.

Miscellaneous Options

- Multiple k-points (solid state only)
- Real space cut-off
- Use of symmetry
- Various SCF options: DIIS, density mixing, smearing.

References

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