

QM/MM method that links DMol³ with GULP

Fast accurate calculations on large systems

Model localized active site plus its environment

QMERA

QMERA offers modelers a computationally effective approach for combining the accuracy of density functional theory (DFT) quantum mechanics with the speed of a force field calculation. This hybrid approach makes it possible to perform accurate calculations on very large systems using little computer time. It is particularly well-suited for modeling problems in chemical reactivity, where an active site is chemically localized. Researchers can use the method to study problems in nanotubes, nanoclusters, and amorphous material. QMERA can be used to perform virtual experiments, leading to tremendous reduction in costly lab-based experiments as well as shorter developmental cycles. As part of the comprehensive Materials Studio® (MS) software environment, QMERA can be supplemented with sophisticated modeling and analysis tools that help users attain even further insight into their systems of interest.

Overview

Understanding the chemistry of systems with a large number of atoms is essential to improving products and processes in areas such as nanotechnology, pharmaceuticals, petrochemistry, catalysis, and fine and specialty chemicals. In the field of catalysis, for example, it is important to understand how a reaction proceeds at a particular site on a metal surface or in the pore of a zeolite. Similarly, in drug discovery, one would like to understand the reaction paths that lead to a drug being metabolized. These types of systems—with a localized active site surrounded by a large number of atoms that can influence the reactivity—are ideal applications for hybrid quantum mechanical (QM) / molecular mechanical (MM) approaches, which combine the accuracy of quantum mechanics with the speed of a force field calculation.

The QMERA Advantage—Hybrid QM/MM

The QMERA module in Materials Studio performs simulations by combining DFT methods from MS DMol³¹ and force field methods from MS GULP².

QMERA can be used to model systems with hundreds or even thousands of atoms, such as :

- organic molecules
- polymers

- organometallics
- metal oxide clusters
- nanotubes
- nanoclusters
- and more

It can be used to predict a variety of properties for these diverse systems; such as:

- structures
- reaction thermodynamics
- reaction kinetics
- electronic properties

About the DMol³ DFT Program

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, DMol³ has long been one of the fastest methods available for performing calculations, an advantage that becomes apparent especially for larger systems.

About the GULP Force Fields

Materials Studio GULP implements a wide range of potential models, which span both inorganic and organic materials. The potentials include

the shell model, the embedded atom method (EAM) (for metals), and bond order and reactive force fields. GULP also provides van der Waals interactions that can be important in some reactions (e.g. zeolites) and that are not included in DFT, thereby providing an improvement over a purely DFT description of those systems.

Key Uses of QMERA

Heterogeneous and Homogenous Catalysts

QMERA allows the reactivity of heterogeneous and homogeneous catalysts to be screened in extremely fast, but reliable, calculations because it treats only a small portion of the system using DFT. The time needed to complete a geometry optimization with QMERA could be roughly 1/8 of the time needed to do the same calculation with pure DFT, yet the QMERA calculation yields comparable reaction energetics.

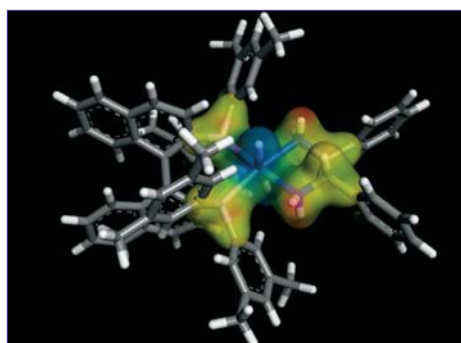


Figure 1. A Ru(H)₂(diphosphine)(diamine) complex modeled by QMERA. QMERA can model this system efficiently, with only a fraction of the atoms treated with quantum mechanics, hence allowing fast, yet accurate, calculations.

Virtual Screening of Candidate Materials

QMERA can be used to perform virtual screening experiments of candidate materials. With this fast hybrid technique, users can quickly screen candidates and subject only the leading candidates to experimental testing, thereby offering a lower cost alternative to performing experimental testing of all possible candidates. QMERA can be used to:

- screen multiple reagents
- propose modifications of a synthetic route
- test nanoclusters of different compositions for catalytic activity
- probe multiple defect sites on a carbon nanotube (see Figure 2)

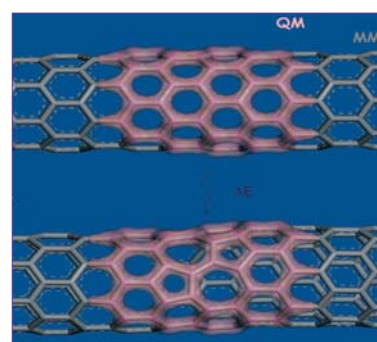


Figure 2. A study of the formation energy of a Stone-Wales defect on a carbon nanotube using QMERA.

How Does QMERA Work?

QMERA is a program that allows combined QM/MM force field calculations to be performed on non-periodic systems by using the ChemShell environment.³ ChemShell is a computational chemistry environment that employs a Tcl interpreter for communication and data handling in hybrid QM/MM calculations, leaving the time-consuming energy evaluations to specialized external codes like MS DMol³ and MS GULP.

The key to success of a mixed QM/MM calculation involves the division of a system into two parts:

- the central “chemically active” QM region
- the surrounding “outer” MM region

Treating the “chemically active” part of the system with quantum mechanics allows the electronic structure and its changes (e.g. bond breaking and formation in a chemical reaction) to be modeled using a minimum of computational resources. The remaining portion of the system is described

using molecular mechanics, with the two regions being allowed to interact. The combination of the speed and efficiency of the MM force field calculations (for the bulk of the system) with the versatility and precision of the QM method (for the important reactive zone) allows reactions in large systems to be studied in a more realistic manner than would be possible using either QM or MM alone.

QMERa provides both mechanical and electronic embedding schemes for treatment of the QM/MM interactions. Dangling covalent bonds between the QM and MM regions are capped with hydrogen “link” atoms, making it possible to treat any type of chemical bond whatsoever. Geometry and transition state optimizations in QMERa can be carried out using a range of minimizers, including a linear-scaling delocalized coordinate algorithm.

What Calculations Can QMERa Perform?

The QMERa module in Materials Studio allows the user to perform hybrid calculations using DFT and force fields. QMERa can currently perform three different tasks:

- Single-point energy calculation
- Geometry optimization
- Transition-state optimization

Each of these calculations can be set up so that it generates specified chemical and physical properties:

- Atomic population analysis (Hirshfeld, Mulliken or electrostatically fitted charges)
- Harmonic vibrational frequencies
- Molecular orbitals (MOs)
- Charge density
- Electrostatic potential

A full list of the force fields and potentials available in GULP is available on the Materials Studio GULP webpage.

The Materials Studio Advantage—Tools to Complement QMERa

QMERa is part of the comprehensive Materials Studio software environment. Materials Studio provides a user-friendly interface that complies with Windows standards, which together with a variety of training options, makes it easy for any user to learn the software with confidence. On top of this, Materials Studio offers a wealth of modeling and simulation tools that can be used to supplement QMERa.

For example, Materials Visualizer—the core of Materials Studio—offers a wide range of model building and visualization tools that allow users to construct models of the systems of interest, easily select the QM region, and run a QM/MM calculation. In particular, researchers in nanotechnology will benefit from the nanotube builder, which can create single walled, multi-walled and bundles of nanotubes, as well as the nanocluster builder, which can create spheres, tetrahedra, and other shapes.

Materials Studio also offers analysis tools that complement QMERa. For example, population analysis control allows users to assign charges and spins and bond orders, while other tools allow users to display 3D renderings of molecular orbitals, charge densities, and electrostatic potentials.

On top of this, a flexible client-server architecture means that calculations can be run on servers located anywhere on a company’s network. Results are returned to a user’s PC, where they may be displayed and analyzed. It is easy to produce high quality graphics of molecular and materials structures, as well as molecular orbitals.

Structures, graphs and other data, such as video clips, can be instantly exchanged with other PC applications, facilitating sharing among colleagues and analysis in spreadsheets and other packages.

System Requirements:

For Materials Studio system requirements see www.accelrys.com/products/materials-studio/system-requirements.html

References

1. Accelrys Materials Studio DMol³ module. Find details at: <http://www.accelrys.com/products/materials-studio/modules/dmol3.html>
2. Accelrys Materials Studio GULP module. Find details at: <http://www.accelrys.com/products/materials-studio/modules/GULP.html>
3. P. Sherwood, A. H. de Vries, M. F. Guest, G. Schreckenbach, C. R. A. Catlow, S. A. French, A. A. Sokol, S. T. Bromley, W. Thiel, A. J. Turner, S. Billeter, F. Terstegen, S. Thiel, J. Kendrick, S. C. Rogers, J. Casci, M. Watson, F. King, E. Karlsen, M. Sjøvoll, A. Fahmi, A. Schäfer and Ch. Lennartz. *J. Mol. Struct. (THEOCHEM)*, **2003**, 632, 1.