State-of-the-art force field for condensed phase materials and isolated molecules

Accurate prediction of structural, conformational, vibrational, and themophysical properties

Applicable to a wide range of materials chemistries and systems including interfaces and mixtures

MS Modeling Datasheet

COMPASS

COMPASS is a powerful forcefield that supports atomistic simulations of condensed phase materials. COMPASS stands for Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies. It is the first *ab initio* forcefield that has been parameterized and validated using condensed-phase properties in addition to various *ab initio* and empirical data for molecules in isolation. Consequently, this forcefield enables accurate and simultaneous prediction of structural, conformational, vibrational, and thermophysical properties, that exist for a broad range of molecules in isolation and in condensed phases, and under a wide range of conditions of temperature and pressure.

The latest enhancements to the COMPASS force field have concentrated on parameterization of more than 45 inorganic oxide materials and mixed systems, including interfaces of organic and inorganic materials.

COMPASS: Leading-Edge Science

COMPASS development aims to achieve high accuracy in prediction. The goal is to be able to predict properties of molecules, both in isolation and in the condensed phase, with an accuracy comparable with experiment. It is an *ab initio* forcefield because most parameters are initially derived based on *ab initio* data. Following this step, parameters are optimized to yield good agreement with experimental data. In particular, thermophysical data for molecular liquids and crystals are used to refine the nonbond parameters by using molecular dynamics simulations.

Another objective of COMPASS development is to systematically extend the coverage so that it will eventually include most of the common organic and inorganic materials that are of interest to the materials researcher. Currently, the coverage includes the most common organics, inorganic small molecules, polymers, some metal ions, metal oxides, and metals. All of the parameters in COMPASS are derived in a consistent manner so that, in principle, one can study very different systems including interfaces and mixtures.

Applying COMPASS

COMPASS is applied through the Discover simulation product, running within MS Modeling in the Materials Studio® software environment. The software is operated through your PC, running under Windows® NT4, 2000, or XP. Calculations may be performed on Windows NT4, 2000, or XP, Red Hat Linux (Intel), SGI™ Irix®, or HP Tru64 servers.

References

1. Sun, H. and Rigby, D., "Polysiloxanes: *Ab Initio* Force Field and Structural, Conformational and Thermophysical Properties," *Spectrochimica Acta*, **1997**, *A153*, 1301-1323.
2. Rigby, D., Sun, H., and Eichinger, B. E., "Computer Simulations of Poly(ethylene oxide): Force Field, PVT Diagram and Cyclization Behavior," *Polymer International*, **1997**, *44*, 311-330.
3. Sun, H., "COMPASS: An *Ab Initio* Force Field Optimized for Condensed-Phase Application-Overview with Details on Alkane and Benzene Compounds," *J. Phys. Chem.*, **1998**, *B102*, 7338-7364.
4. Sun, H., Ren, P., and Fried, J. R., "The COMPASS Force Field: Parameterization and Validation for Phosphazenes," *Comput. Theor. Polymer Sci.*, **1998**, *8*, 229-246.
5. Bunte, S. W. and Sun, H., "Molecular Modeling of Energetic Materials: The Parameterization and Validation of Nitrate Esters in the COMPASS Force Field," *J. Phys. Chem.*, **2000**, *B104*, 2477-2489.
6. Sun, H., "The COMPASS Force Field: Parameterization for Small Molecule Gases," **2000**, in press.

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