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 COMPASS forcefield aims to achieve high accuracy in prediction for a broad range of systems. 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.

An 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.

Recent developments include parameters for the sulfate and sulfonate groups.

To learn more about Materials Studio, go to **accelrys.com/materials-studio**

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