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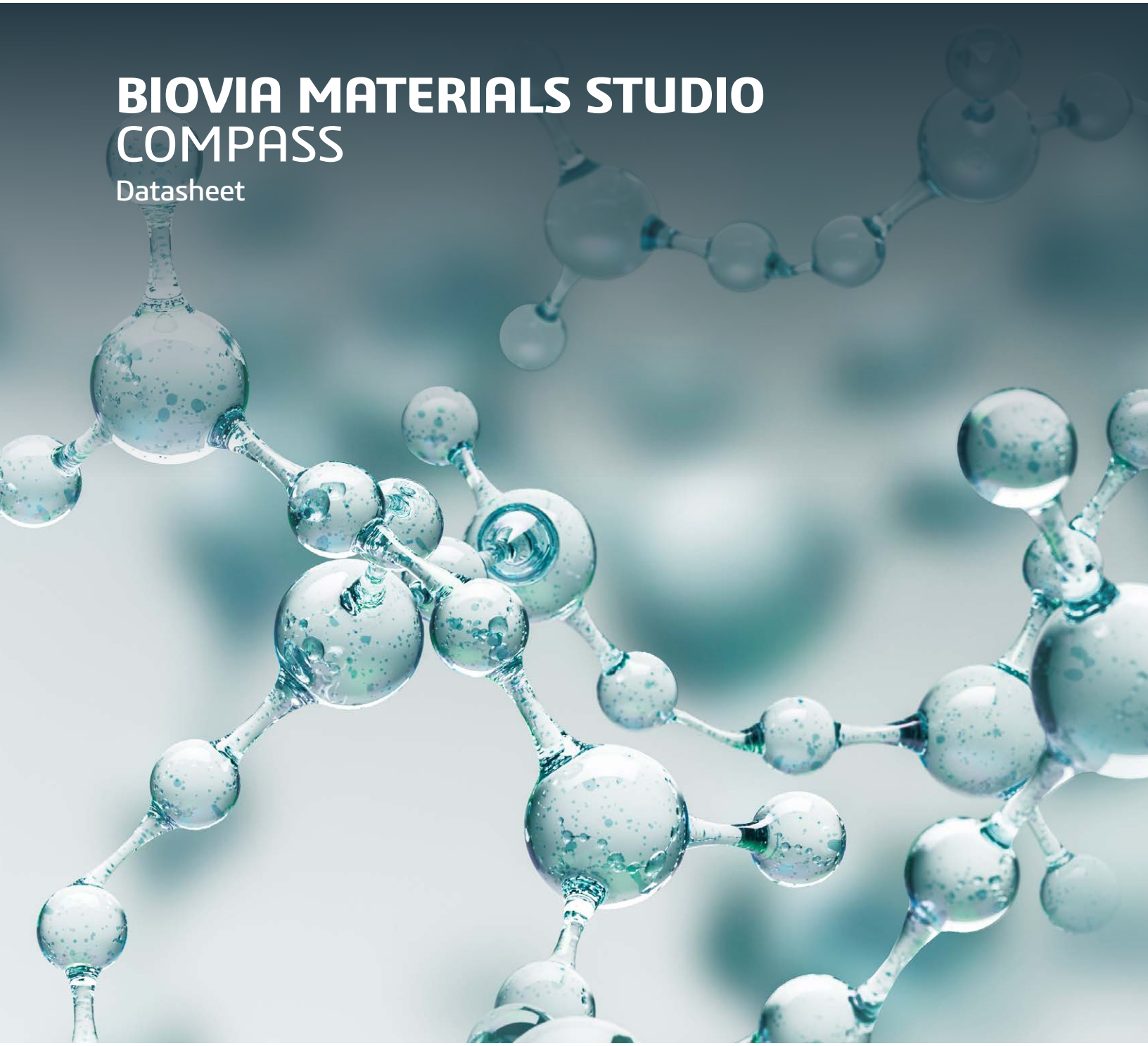
BIOVIA MATERIALS STUDIO
COMPASS

Datasheet



DASSAULT SYSTEMES

BIOVIA Materials Studio COMPASS is a powerful forcefield that supports atomistic simulations of condensed phase materials. Materials Studio 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 Materials Studio 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 experiments. 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 nonbonded parameters by using molecular dynamics simulations.

Another objective of Materials Studio COMPASS development is to systematically extend the coverage so that it includes most of the common organic and inorganic materials that are of interest to the materials researchers. In the latest version of the parameters, COMPASS III [8], the coverage includes the most common organics including drug-like molecules, inorganic small molecules, polymers, some metal ions, metal oxides, metals, solvents including ionic liquids. Many materials specific applications such as lithium ion batteries are also specifically parameterized..

All of the parameters in Materials Studio COMPASS are derived in a consistent manner (as described in reference [8]). so that, in principle, one can often study complex systems containing mixed materials classes.

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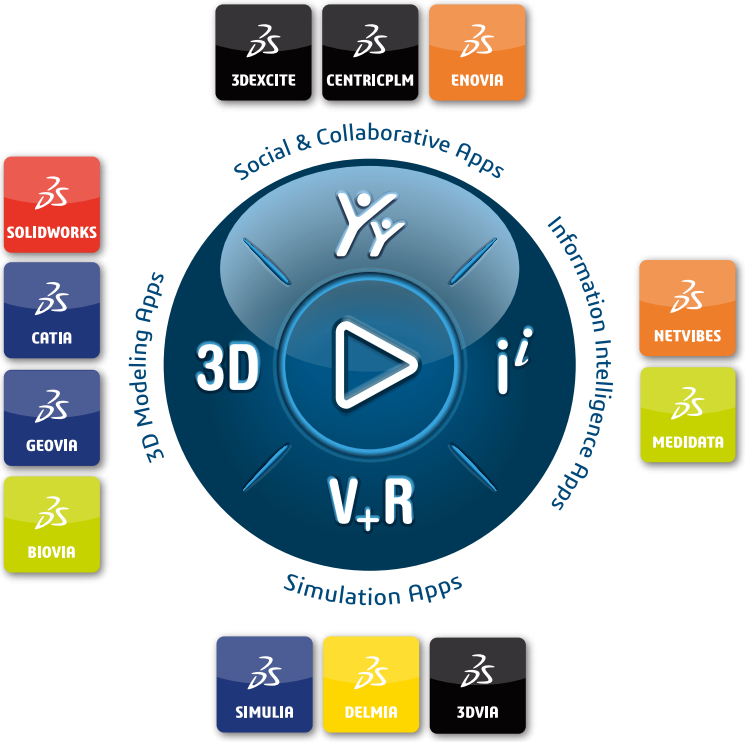

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