MolMod: A Force Field Database for Molecular Simulation of Fluids

Florian Fleckenstein[1, S], Sebastian Schmitt[1], Hans Hasse[1] and Simon Stephan[1, C]

[1]*Laboratory of Engineering Thermodynamics, RPTU Kaiserslautern, Kaiserslautern, Germany*
simon.stephan@rptu.de

Thermophysical properties of fluids can be predicted routinely today using molecular simulation. The accuracy of these predictions primarily depends on the employed force field. Finding, implementing, and validating force field models is a tedious task. In this contribution, the MolMod database [1,2] is presented. The MolMod database is an open-access web-based database for classical force fields for fluids that can be used in molecular dynamics or Monte Carlo simulations for modeling a large variety of thermophysical properties. The MolMod database contains both component-specific force fields and transferable force fields. In a component-specific force field, the model parameters of a given force field are only valid for a certain component. A transferable force field, on the other hand, is a chemical construction plan that specifies intermolecular and intramolecular interactions between different types of atoms of different chemical groups and can be used for building a force field model for a given component. The extension of the MolMod database to transferable force fields [2] was done based on a data scheme proposed in a recent work of our group [3]. The MolMod database presently comprises about 1,000 component-specific force fields – and is constantly growing. The following transferable force fields are presently available: CHARMM, COMPASS, GROMOS, OPLS-AA, OPLS-UA, Potoff, TAMie, and TraPPE. The MolMod website has a graphical user interface that enables specifying the molecules and provides the references to the original publications of the force fields. The MolMod database provides ready-to-use input files for multiple simulation engines, e.g. LAMMPS [4], GROMACS [5], ms2 [6,7], and ls1 mardyn [8] etc.

References

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