# A Database for Molecular Models for the Simulation of Thermodynamic Properties of Fluids

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A database is presented that contains molecular force field models of over 150 pure fluids [1]. The database development was conducted under the auspices of the Boltzmann-Zuse Society of Computational Molecular Engineering (BZS) and it focusses on validated models developed by its members in the last 20 years. Most technically-relevant small and medium sized molecules are included. They are described by rigid multi-centre Lennard-Jones interaction sites combined with electrostatic interactions. Also ion models are included. The models were developed in a consistent way and are known to describe vapor-liquid equilibrium data (saturated densities, vapor pressure, enthalpy of vaporization) well, as such data was used in the parameterization. In many cases, also predictions of other properties, like transport and interfacial properties, were tested and found to be in good agreement with experimental data. Many of the molecular models were also successfully tested for mixtures using combination rules like those of Lorentz and Berthelot.

The database contains full specifications of the molecular models including references to the corresponding original literature. It provides a wide range of search functionalities and offers downloads of input files for several molecular simulation codes, like LAMMPS [2], GROMACS [3], ms2 [4], and ls1 mardyn [5]. Since these molecular simulation codes are based on different approaches to realize for example multipole interactions, the geometry definition or the rigidity of molecules, on the fly conversion routines are the core of the database. This enables researchers to include the molecular models easily in their individual work flows.

References

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