Molecular Model Database of the Boltzmann–Zuse Society for Computational Molecular Engineering

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The openly accessible molecular model database (MolMod DB) of the Boltzmann–Zuse Society for Computational Molecular Engineering contains materials relations (force fields) for over 150 low-molecular fluids, meant for molecular modelling and simulation with molecular dynamics (MD) and Monte Carlo (MC) solvers [1].

The molecular models in the database have been published in about 30 articles over the past 20 years, which are associated with the respective entries and can be followed on the MolMod DB web front end. The database provides a wide range of search functionalities, e.g., for substances (names and CAS numbers) and model classes. Input files for several common environments can be downloaded via the web front end, including the file formats used by the molecular simulation codes ms2 [2], GROMACS [3], LAMMPS [4], and ls1 mardyn [5].

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