Molecular Simulations of Thermodynamic Properties Using Accurate Quantum-Chemical *Ab Initio* Potentials

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Accurate data on thermodynamic properties of fluids are particularly important for the design and dimensioning of efficient and energy-saving industrial installations. For many properties experimental measurements of high accuracy are possible today. However, in the case of harmful, dangerous, and corrosive fluids or for extreme temperature and pressure regions, the use of theoretical methods and computer simulations is reasonable and essential. Different models for the description of interactions between atoms and molecules can be utilized in molecular simulations. Most commonly used are so-called effective pair potentials, which are adjusted to experimental data. The reliability of such potentials depends strongly on the quality of the applied experimental data; their extrapolation abilities to extreme temperature and pressure regions are questionable. The use of quantum chemical calculations enables an alternative approach where interaction energies are calculated without application of experimental data, i.e. *ab initio*. Such highly precise potential functions enable the calculation of thermodynamic properties with high accuracy. In this work molecular dynamics and Monte Carlo simulations of argon as a model substance have been carried out with the molecular simulation code *ms2* [1]. Different pair potentials have been used including an effective Lennard-Jones potential and an *ab initio* potential from our research group [2]. The *pρT*-results are compared with the most accurate experimental data as well as with an *ab initio* EOS that explicitly includes nonadditive three-body interactions [3].

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