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Ab initio Monte Carlo simulations of neon and argon

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Gibbs ensemble Monte Carlo simulations of neon and argon with *ab initio* pair potentials were performed. This approach is called ‘global simulation’ since quantum mechanical calculations and simulations are performed in order to obtain thermodynamic data without use of any results of experimental measurements.

During the simulations, the densities of the coexisting phases, their pair correlation functions, the vapour pressure and the enthalpy and entropy of vapourization were calculated from just above the triple point to close to the critical point. The influence of the potential choice (*ab initio* potentials, a simple and a more complex empirical potential have been compared) and of the addition of the Axilrod–Teller three-body potential on the above mentioned properties were investigated.

Phase equilibria calculated with the pair potentials studied show only a rather crude agreement with the experimental phase equilibria, but the inclusion of Axilrod–Teller three-body interaction to the potential leads to a very good agreement for all studied quantities for neon as well as for argon. For neon our simulation results for density and vapour pressure have an accuracy similar to the best presently available experimental data. It may be ventured that our simulations can supply reliable thermodynamic data of neon where no experimental data are available.

Confirmed by the good results of the calculation of phase equilibria, we studied another application of global simulations. We used simulation results to extend an equation of state for the near-critical region to higher pressure. Now the range of applicability of this equation of state is enlarged by the use of quantum mechanics and simulation.