## Vapor-liquid Interfacial Properties of the Lennard-Jones Truncated and Shifted Fluid: A Comparative Study by Molecular Simulation, DFT, and DGT

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Vapor-liquid interfacial properties such as surface tension and adsorption play an important role in many processes. Unfortunately, there are presently no experimental methods that yield direct information on the interfacial region like density profiles. Such data can presently only be obtained with computational methods, namely by molecular simulations, density gradient theory (DGT), and density functional theory (DFT). We consider the molecular simulation data as reference, against which the results from the other two methods are compared. For a rigorous comparison, the equation of state (EOS) on which DGT and DFT are based must be consistent with the force field that is used in the molecular simulations. In this contribution we compare results from molecular simulations, DGT, and DFT for the Lennard-Jones fluid truncated and shifted at 2.5 s. In a first step, an EOS is developed for this fluid. It is based on perturbation theory and called the Perturbed Truncated and Shifted (PeTS) EOS. The results from the Pets EOS are in very good agreement with molecular simulation data for both stable and metastable states. The Pets EOS is developed into a functional, called Pets-i, where i stands for interface. The DGT influence parameter is determined from the simulation data on the interfacial tension and shows no temperature dependence. Density profiles, pressure profiles, interfacial thickness, and interfacial tension obtained with all three methods are compared and are always in good agreement. The molecular simulation and the DFT data show density fluctuations in the interfacial region which are analyzed in the Fourier space. The wavelength of these fluctuations in both methods agrees almost perfectly, while the amplitude shows some differences. These density fluctuations on the liquid side of the vapor-liquid interface result from an oscillatory layering structure.