

Orientational Effects in a Model Fluid Between Confining Walls and in a Thermal Gradient and/or an External Gravitational Field

Christopher Daub^{C,S}, Per-Olof Åstrand, Joakim Tafjord and Signe Kjelstrup
Department of Chemistry, Norwegian University of Science and Technology, Trondheim, Norway
christopher.daub@ntnu.no

Fernando Bresme
Department of Chemistry, Imperial College London, London, United Kingdom

We investigate the behaviour of fluids confined between two walls and under the influence of either a temperature gradient, an external gravitational field, or both effects concurrently. This set up allows us to consider the impact of liquid-solid interfaces on the molecular orientation and density profile of the fluid. The gravitational field and/or temperature gradient act in concert with the induced density gradient to generate a preferred orientation in molecular fluids consisting of anisotropic molecules. We illustrate this general phenomenon in a number of anisotropic fluids and extend the non-equilibrium thermodynamics theory to encompass these new effects. Comparison of this gravity induced orientational effect with the recently discovered thermo-molecular orientation (TMO) effect has led to new insights into both phenomena.

References

- [1] F. Romer *et al.*, Phys. Rev. Lett. 108, 105901 (2012).
- [2] F. Romer *et al.*, Mol. Simul. 38, 1198 (2013).
- [3] C. D. Daub *et al.*, Phys. Chem. Chem. Phys. 16, 22097 (2014).