Molecular Orientation of Fluids under Thermal Gradients

Fernando Bresme [C, S]
Imperial College London, Department of Chemistry, London, United Kingdom
f.bresme@imperial.ac.uk

Temperature gradients are responsible for a large number of non-equilibrium effects, which can be used in energy conversion applications, e.g., thermoelectric devices. They provide a free source of energy, but the gradients can be highly dispersed or small, making difficult energy recovery. Hence, there is a current need to explore new approaches for energy conversion. Recent experiments have shown that large/localized temperature gradients can be achieved at the nanoscale / microscale, offering new perspectives for energy recovery. It will be shown how these large gradients can induce novel non-equilibrium effects, *thermo-molecular orientation*, a general effect by which polar and non-polar anisotropic molecules tend to align with the imposed thermal gradient. The combination of computer simulations and non-equilibrium thermodynamics provides a route to extract information on the phenomenological coefficients determining the strength of this effect, and hence predict its magnitude in real systems. The dependence of the effect with molecular architecture and thermodynamic conditions will also be discussed.

[1] F. Bresme, A. Lervik, D. Bedeaux and S. Kjelstrup, "Water polarization under thermal gradients", Phys. Rev. Lett., 101, 020602 (2008).
[2] J. Muscatello, F. Romer, J. Sala, and F. Bresme, Phys. Chem. Chem. Phys 2011.