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Non-equilibrium thermodynamics at the nanoscale with the virtual microscope

Thermal gradients and electromagnetic fields are responsible for a wide range of non-equilibrium physical effects (e.g. Soret, Seebeck, Peltier effects), which can be exploited in energy conversion (thermoelectrics), analytical devices, molecular and nanoparticle transport as well as colloidal assembly. We have investigated the non-equilibrium response of molecular fluids and particles to temperature gradients and magnetic fields. The combination of computer simulations and non-equilibrium thermodynamic theories allow us to elucidate the physical behaviour of complex fluids under these external gradients, showing it is richer than anticipated. I will discuss the prospects of non-equilibrium simulation approaches to uncover novel non-equilibrium coupling effects that arise from the interaction of molecular degrees of freedom with thermal gradients, and to predict colloidal assembly phenomena induced by external fields