

Asymmetric Nanoparticles in Thermal Gradients: Soret Effect and Thermomolecular Orientation

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Non-equilibrium effects are of key relevance in both nature and industry. Thermal gradients, in particular, are of significant relevance in the context of colloidal science. Since the early observations of thermodiffusion by Ludwig and Soret [1, 2], other fascinating behaviours have been observed such as uniform rotation of liquid crystals by Lehmann [3] and coupling between electric currents in thermal gradients by Peltier and Seebeck [4]. Aspherical nanoparticles have been shown to exhibit larger thermophoretic drift when aligned with the thermal gradient [5, 6], an observation which highlights the importance of anisotropy in the dynamics out of equilibrium. Using nonequilibrium molecular dynamics simulations, we explore the response of asymmetric nanoparticles dispersed in a dense fluid, subjected to a thermal gradient. The nanoparticles are built with asymmetry in the mass distribution and/or the interaction with the fluid environment. Due to the anisotropies, particles experience transient torques that result in thermomolecular orientation. This effect gives rise to significant changes in the mass dependence of the Soret coefficient with respect to the symmetric case, featuring a maximum instead of a monotonic increase. We show that asymmetric mass distributions and anisotropic particle interactions, properties that can be tuned during the synthesis of heterogeneous nanoparticles, can couple with the imposed thermal field. This study gives insight on the behaviour of nanoparticles under non-equilibrium conditions, and opens new ways of manipulating small colloids using thermal fields.

References:

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