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Mesoscale Modeling of Marangoni Convection in Evaporating Colloidal Droplets[1] MINGFEI ZHAO, XIN YONG, Binghamton Univ — In this work, we develop a three-dimensional free-energy-based multiphase lattice Boltzmann-Brownian dynamics model with thermal effects for elucidating particle dynamics in evaporating nanoparticle-laden droplets in the presence of Marangoni convection. The introduction of thermal effects enables the development of the 3D internal flow structures due to concomitant inhomogeneous evaporation at the droplet surface and thermal conduction inside the droplet. In particular, the model is capable of capturing thermal Marangoni flow along the surface of droplets and its interplay with the internal flow. We calculate the temperature field separately and consider the thermal effect as a forcing term in the lattice Boltzmann model. We first model non-evaporating droplets loaded with nanoparticles and the effects of temperature field on the flow structure. By implementing evaporation, we probe the self-assembly of nanoparticles inside the droplets or at the liquid-vapor interface. We analyze the microstructure of nanoparticle assemblies through radial distribution functions and structure factors. Our findings provide critical insights into the dynamics of nanoparticle self-assembly in evaporating fluid mass with Marangoni convection.

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Mingfei Zhao
Binghamton Univ

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