Computer simulations of colloidal particles at liquid interfaces

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ABSTRACT

Colloidal particles are known to be very efficient stabilizers for fluid interfaces with applications in the food and cosmetics industry, enhanced oil recovery, drug delivery or waste water management. However, the impact of the particles on the interface stability depends on a number of parameters such as the particle shape, the contact angle on the particle surface, the particle-particle interactions, or the underlying hydrodynamics.

Computer simulations aiming at a thorough understanding of particle stabilized interfaces are generally required to include all these underlying processes. After reviewing some approaches to tackle particle stabilized interfaces, we introduce our combined multicomponent lattice Boltzmann and molecular dynamics method together with its massively parallel implementation. The applicability of the method is demonstrated by reporting on simulations of fluid interfaces stabilized by spherical, anisotropic, or even fully deformable colloidal particles. We focus on the forces involved in the adsorption of single or few particles to a flat or curved interface and the formation of particle stabilized emulsions such as bijels or Pickering emulsions. We demonstrate that ellipsoidal particles are more efficient stabilizers than spherical particles. The anisotropic shape leads to a wealth of additional timescales in the formation of emulsions and has a strong impact on the final structure and average droplet size due to local particle reordering.

We close with an outlook on open problems in the field, future applications as well as limitations and possible improvements of available algorithms.

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