Orbitals for classical arbitrary anisotropic colloidal potentials

Martin Girard, Trung Dac Nguyen, and Monica Olvera de la Cruz

Coarse-grained potentials in simulations at the mesoscale are ubiquitous. While there exists various methods to compute effective interactions for spherically symmetric particles, anisotropic interactions are seldom used due to their complexity. Herein we describe a fast calculation method based on Fourier transform of integrals. Using this method we are able to coarse-grain arbitrary anisotropic potentials. We applied the method to Janus particles in screened media and found varied morphologies. One major refinement that we want to bring to the technique is dynamic densities, where the shape of the particle changes when two colloids interact. This is necessary to efficiently simulate very soft colloids such as polymer-coated particles.
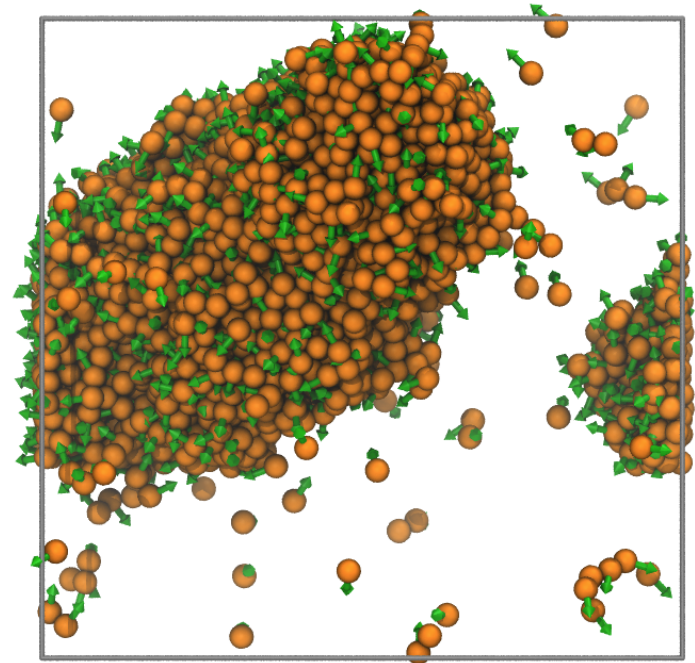
Liquid-like state of the Janus particles, which tends to form elongated droplets

Northwestern