

CHT-15-199

Effect of amphiphilicity on the interfacial thermal motion of Janus particles

Abstract

The thermal motion of nanometer-sized Janus particles at the interface between two immiscible fluids is studied via molecular dynamics simulations. Spherical nanoparticles composed of two sides with different affinity to fluid phases are considered, and their diffusivity is evaluated as a function of size and surface chemistry. As the amphiphilicity increases, we observe that the in-plane interfacial diffusivity decreases. Similarly, rotational diffusion of Janus particles is reduced compared to their homogeneous counterparts. Detailed analysis of the fluid structure around the particles reveals that this is mainly due to the formation of a dense adsorption layer around more amphiphilic particles, which leads to increased resistance acting against nanoparticle motion and in-plane rotation. The numerical method is validated by simulating the diffusion of homogeneous particles in a bulk fluid and comparing the translational and rotational diffusivity with the Stokes-Einstein(-Debye) correlations. Our results may have implications in understanding the transport of molecules and particles with anisotropic surface properties attached to soft interfaces including cell membranes.