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Translational and rotational diffusion of Janus nanoparticles at liquid interfaces HOSSEIN REZVANTALAB, SHAHAB SHOJAEI-ZADEH, Rutgers University — We use molecular dynamics simulations to understand the thermal motion of nanometer-sized Janus particles at the interface between two immiscible fluids. We consider spherical nanoparticles composed of two sides with different affinity to fluid phases, and evaluate their dynamics and changes in fluid structure as a function of particle size and surface chemistry. We show that as the amphiphilicity increases upon enhancing the wetting of each side with its favored fluid, the in-plane diffusivity at the interface becomes slower. Detail analysis of the fluid structure reveals that this is mainly due to formation of a denser adsorption layer around more amphiphilic particles, which leads to increased drag acting against nanoparticle motion. Similarly, the rotational thermal motion of Janus particles is reduced compared to their homogeneous counterparts as a result of the higher resistance of neighboring fluid species against rotation. We also incorporate the influence of fluid density and surface tension on the interfacial dynamics of such Janus nanoparticles. Our findings may have implications in understanding the adsorption mechanism of drugs and protein molecules with anisotropic surface properties to biological interfaces including cell membranes.

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