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Shear-induced orientation of Janus nanoparticles at liquid interfaces

Abstract

We investigate the dynamics of single Janus nanoparticles adsorbed at a liquid interface under shear using molecular dynamics simulations. Janus nanoparticles of spherical, cylindrical, and disc-shaped geometry are created by tuning the affinity of the atoms on each side of the particle with the interacting fluids. We demonstrate the existence of a steady-state orientation for these geometries at the interface, which is governed by a balance between the shear-induced and capillary-induced torques. There exists a shear rate above which the nanoparticle rotates out of its energetically favorable orientation. This unlocking threshold is higher for more amphiphilic particles due to the stronger capillary forces along the contact line resisting against the shear-induced torque. Moreover, the unlocked particles undergo two types of dynamics: 1) a smooth tilting over a relaxation period approaching a steady configuration, or 2) oscillatory rotations damping toward equilibrium. We construct phase diagrams characterizing the orientational dynamics of nanoparticles based on their geometry and surface chemistry as well as the applied shear rate. These results can be used for directed-assembly of anisotropic particles at liquid interfaces.