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Interfacial transport and orientation of Janus nanoparticles under shear flow HOSSEIN REZVANTALAB, SHAHAB SHOJAEI-ZADEH, Rutgers University — We investigate the configuration of Janus nanoparticles adsorbed at liquid-fluid interfaces in presence of shear flow. The interfacial behavior of nanoparticles with different size and shape is followed using Molecular Dynamics simulations. We create Janus nanoparticles by tuning the affinity of the atoms on each side of the particle with the two fluids, and model the shear as a symmetric Couette flow. We demonstrate the existence of a steady-state orientation for particles at the interface, which is governed by the balance between the shear-induced torque and the resistance due to capillary forces. There is a threshold shear rate above which the nanoparticle starts to rotate out of its energetically favorable upright orientation. This threshold is found to be higher for more amphiphilic particles due to the stronger interfacial tension resisting against the shear-induced disturbance. Moreover, the geometry plays a significant role in defining the range of attainable orientations. Janus cylinders with high aspect ratio show a sudden shift in orientation which does not drastically change with increasing shear rate, while thin discs require a larger threshold shear but can achieve a wider range of orientations. Our analysis of a fluid flow that reorients suspended nanoparticles can also give insight into the hemodynamics of blood flow and the interaction of anisotropic drug carriers with cell membranes.

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