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Computer Simulation study of polyhedral nanoparticle self-assembly at interfaces. VIKRAM THAPAR, UNMUKT GUPTA, FERNANDO ESCOBEDO, Cornell University — The self-assembly of polyhedral particles confined to a fluid-fluid interface is studied using Monte Carlo simulations. Several polyhedral shapes are studied, which are selected from a family of truncated cubes which include cubes, cuboctahedra, and octahedra. First we studied the case of hard particles pinned to the interface by restricting their movement in the direction perpendicular to it while allowing their free rotations. Our results suggest that the known solid phases and mesophases of these shapes in the 3D bulk are "translated" into variants in 2D space. These insights on 2D entropic self-assembly of polyhedral particles is a first step toward understanding the self-assembly of particles at fluid-fluid interfaces, which is driven by a complex interplay of entropic and enthalpic forces. As a second step we hence studied the particle-surface and particle-particle interactions associated with a fluid-fluid interface using both continuum and polybead models to assess the role of enthalpic interactions in determining the particle orientation behavior with respect to interface. We find that the thickness of the interface can introduce non-trivial effects on the preferential particle orientations.

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