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Nanoparticles in Complex Fluids, at Interfaces, in Polymers: Topology Matters

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One versatile way to control the assembly and integration of nanoparticles is to tether organic molecules with specific functionalized groups to their surface. The tethers modify both inter particle interactions and their interaction with their surroundings, without disrupting the nanoparticles' unique properties. While it is often assumed that uniformly coating spherical nanoparticles with short organic ligands will lead to symmetric hybrids, using explicit-atom molecular dynamics simulations of model nanoparticles, we discovered that the hybrids exhibit a large variety of non-symmetric coatings, driving new pathways to control assemblies. These configurations of the coating stem from the high curvatures of small particles and comparable size tethers. In solution geometric factors dictate the symmetry of the hybrid and its stability, where the chain end-group coding and the solvent play only a secondary role. At water-vapor interface the anisotropic nanoparticle coatings seen in bulk solvents are enhanced. The coatings become significantly asymmetric and assume distinctive orientation with respect to the liquid interface. The asymmetry and degree of orientation depend strongly on the free volume provided by the geometry and the end group, as well as the solvent properties. At an interface asymmetric hybrids align with the surface to minimize free energy. These asymmetric coatings and oriented hybrids are expected to drive new self-assemblies symmetries in the bulk and at surfaces. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.