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Molecular Dynamics Simulation of Colloidal Nanoparticle Forces
KRISTEN FICHTHORN, Penn State University, YONG QIN, Penn State University — An improved understanding of the forces between colloidal nanoparticles could lead to new strategies for achieving their selective assembly for a variety of different applications. We employ molecular dynamics simulations to study the interplay between solvation and van der Waals forces for model colloidal nanoparticles. We consider the influence of nanoparticle size, shape, and surface roughness, as well as solvent type (Lennard-Jones vs. n-decane) and solvent-solid interaction (solvophobic vs. solvophilic). We find that solvation forces can be comparable to van der Waals attraction and, thus, they can play an important role in determining the stability of colloidal suspensions. Surface roughness causes nanoparticles to rotate so they approach one another via paths of minimum free energy. This rotation causes crystalline (icosahedral) nanoparticles to approach one another via alternating face-face and vertex-vertex conformations, suggesting that solvation forces can control nanoparticle alignment during assembly. Finally, our simulations of solvophobic nanoparticles in n- decane yield insight into how the drying transition is influenced by the relative sizes of the solvent molecules and nanoparticles.

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