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A ligand phase transition on nanorods and its effect on their surface forces[1] ASAPH WIDMER-COOPER, University of Sydney, PHILLIP GEISSLER, U.C. Berkeley — Synthesizing nanometer-scale objects with controlled optical and electronic properties is now a relatively straightforward task, however organizing such objects into extended structures that could revolutionize technology remains a challenge, especially for anisotropic particles. Nanorods behave like liquid crystals in solution and can assemble into structures with the rods oriented perpendicular with respect to a substrate upon drying, assemblies that could potentially be used to print nanostructured solar cells and photoelectrochemical devices. Achieving complete control of this process, however, requires detailed understanding of the rod-rod and rod-surface interactions. Like most nanoparticles, CdS nanorods are passivated with ligands to stabilize them from random aggregation in solution. Using molecular dynamics simulations with explicit ligands and solvent we investigate the structure of phosphonic acid ligands on CdS nanorods as a function of temperature and show that they can undergo an ordering transition close to room temperature. We calculate the potential of mean force between the rods and show that this changes the rod-rod interaction from purely repulsive to attractive. This should have a significant effect on their self-assembly behavior.

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Asaph Widmer-Cooper
University of Sydney

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