

226c Computational Study of Self Assembly of Nanoparticles with Anisotropic Interactions

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Self assembly of nanoparticles into one-dimensional, two-dimensional or three-dimensional assemblies has been of substantial interest due to their collective optical, electrical and magnetic properties. We developed a simplified particle-based model that properly includes the anisotropic interparticle interactions arising from the nanoparticle shape as well as electrostatic and directional van der Waals interactions. We applied this model to a system of ligand-stabilized semiconductor nanoparticles in solution, and carried out molecular simulations that successfully predict the two-dimensional assembly found in experiments. Our simulations demonstrate that nanoparticles with anisotropic interactions can be viewed as patchy particles that may serve as programmable building blocks for desired nanoparticle assemblies.