Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Colloidal models for anisotropic particles MARTIN GIRARD, MONICA OLVERA DE LA CRUZ, Northwestern Univ — Nanoparticles (NP) self-assembly is often thought as an equivalent to crystallization of atoms, where NP pairs exhibits effective potentials similar to atomic interactions. For the usual spherical NPs, this potential is only dependent on the distance between the particles due to symmetry. Use of anisotropic NPs provide an analog to atomic orbitals, leading to anisotropic effective potentials, which can be used to obtain new crystal lattices.

We express the effective potential of anisotropic NPs as the overlap between two functions, each of which is only dependent on the position and orientation of a single particle. Using a Fourier method, this contribution is expended into spherical harmonics and directly calculated in molecular dynamics simulations, reminiscent of energy calculations in quantum mechanics.

Using the effective potential of two spherical DNA-grafted NPs, we show an approximate method to obtain the Fourier components of an anisotropic shape, as well as the resulting simulations.

Martin Girard
Northwestern Univ

Date submitted: 05 Nov 2015 Electronic form version 1.4