Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Density functional theory for the structure and dynamics of solvent-free nanoparticle–organic hybrid materials HSIU-YU YU, DONALD KOCH, Cornell University — Nanoparticle–organic hybrid materials consist of inorganic nanocores functionalized with oligomeric organic molecules. They exhibit fluid behavior in the absence of solvent with the fluidity provided by the attached oligomers. We present a density-functional theory for the equilibrium structure and transport properties of these materials based on an assumption that the intercore forces are mediated by entropic effects associated with the conformations of the hairs subject to the constraint that the oligomer fluid is incompressible. Because each core particle carries its share of the fluid phase, the structure factor at zero wave number is equal to zero. When the radius of gyration of the oligomers is large compared with the core radius, each core experiences weak interactions with many other cores residing in its neighborhood. Exploiting this limit, the transport properties can be determined in a quasi-analytical manner based on a solution of the non-equilibrium probability density for pairs of particles experiencing a non-pairwise-additive intercore potential.

Hsiu-Yu Yu
Cornell University

Date submitted: 19 Nov 2010 Electronic form version 1.4