Abstract Submitted
for the DFD10 Meeting of
The American Physical Society

Molecular dynamics simulations of Janus nanoparticle assembly at interfaces WEIKANG CHEN, JOEL KOPLIK, ILONA KRETZSCHMAR, CCNY — We study the formation of clusters of nano-sized Janus particles (having surface regions with different interactions) at a liquid-vapor interface using molecular dynamics simulations. The individual particles are modeled as rigid spherical sections of an atomic lattice, with short ranged atom-atom interactions chosen to selectively attract subregions of the particle surface, and with a solid-liquid interaction favoring a 90 degree contact angle at the liquid interface. The simulations automatically incorporate the competition between Brownian motion, fluid convection and molecular attraction, as well as evaporation of the liquid if desired. We study the distribution and shape of the clusters found in equilibrium, and the structures resulting when the solvent evaporates.

Joel Koplik
CCNY

Date submitted: 05 Aug 2010 Electronic form version 1.4