

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Modeling the Self- and Directed-assembly of Viruses on Surfaces

DANIEL SULLIVAN, Colorado School of Mines, GEORGE GILMER, Lawrence Livermore National Laboratory, CRISTIAN CIOBANU, Colorado School of Mines — The exploitation of naturally self-assembling viruses has received much attention recently in regards to fabrication of nanomaterials and devices. Formation of dense viral mono- and multilayers as well as viral immobilization via chemospecific surface functionalization can be studied by modeling viruses as colloidal particles. We use a modified Lennard-Jones (LJ) potential, characterizing each colloid as an integrated collection of LJ particles, to describe intercolloidal and colloid-surface interactions. By carefully selecting the LJ interaction parameters and performing molecular dynamics simulations, we are able to replicate experimentally observed behavior of viruses on both strongly and weakly interacting surfaces in our surrogate colloidal system. Kinetic properties of the computational system are monitored and we find them to be in good agreement with predictions based on experimental data. We provide a basis for further investigation into the capabilities and limitations of modeling self-assembly of viral systems of technical interest using classical molecular dynamics.

Daniel Sullivan
Colorado School of Mines

Date submitted: 22 Dec 2010

Electronic form version 1.4