MAR06-2005-000826

Abstract for an Invited Paper
for the MAR06 Meeting of
the American Physical Society

Multiscale Simulation Studies of the Self-Association of Poly(ethylene oxide)-Tethered Fullerenes

GRANT SMITH, University of Utah

I will discuss our multiscale molecular simulation studies of the aggregation of PEO-tethered C-60 fullerenes in water. Our simulations reveal that adjustment of the attachment pattern and molecular weight of the PEO ligands provides exquisite control of the morphology of the self-associating nanostructures formed through a balance of strong fullerene-fullerene attraction, moderately attractive fullerene-PEO interactions and repulsive steric interactions between the PEO ligands. I will also discuss results of our investigations of the influence of external fields (electrical and shear) on the morphology of the self-assembled fullerene nanostructures in bulk aqueous solution as well as results of simulation studies of the self-association of PEO-tethered fullerenes at air-water interfaces.