USC Viterbi School of Engineering

MORK FAMILY DEPARTMENT OF CHEMICAL ENGINEERING AND MATERIALS SCIENCE

Graduate Seminar

"Studies of Nanoparticle Adhesion to Soft Interfaces and Membranes by using Dissipative Particle Dynamics"

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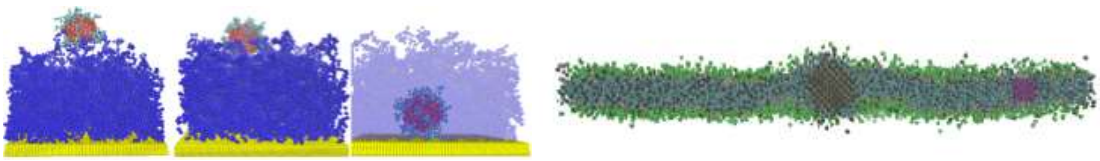
Abstract

Understanding of the physico-chemical mechanisms of nanoparticle (NP) adhesion to soft interfaces, like polymer brushes and lipid membranes, is of paramount importance for the design of novel nanomaterials and biomedical nanotechnologies, as well as for evaluating health threads related to nanoparticle manufacturing. Since the NP adhesion is governed by multiple factors (NP size and shape, surface modification, hydrophobicity and charge) that cannot be easily varied in the experiments, the use of "in-silico" modeling helps guide the experiments and optimize NP structure and surface properties.

We present an original method of "ghost tweezers" (GT) for coarse-grained simulations of NP interactions with complex interfaces [1]. The GT method emulates lab experiments performed to manipulate nanoparticles and biomolecules with optical or magnetic tweezers. It is implemented into the dissipative particle dynamics simulation framework. GT represents a virtual harmonic potential, which tethers NP by a spring at a given distance from the interface. By moving GT with a certain speed, NP is driven to and through the interface, and the average force applied by GT to NP is measured. This force determined in quasi-static simulations is integrated to calculate the free energy landscape of NP-interface interaction and to determine the equilibrium adhesion states and the energy barriers between these states.

The GT method is illustrated on two case study systems: a) interactions of bare and ligand-functionalized NPs with polyisoprene polymer brush in acetone-benzene binary solvent and b) adhesion of a hydrophobic NP to and its translocation through DPPC phospholipid membrane. We analyze different modes of NP adhesion, including partial and full immersion of NP into the polymer brush and internalization of NP by a lipid membrane, depending of NP size, hydrophobicity, and surface modification. The proposed GT method can be further implemented for modeling of nanoparticle behavior in various soft matter and biological systems.

[1] Jianli Cheng, A. Vishnyakov and A.V. Neimark, - Studies of Nanoparticle Adhesion to Grafted Surfaces by the Ghost Tweezers Method,- Journal of Chemical Physics, 2015, V.142, 034705.



Thursday, June 18, 2015
1:00 pm, HED Room 116
The scientific community is cordially invited.