8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Coarse-Grained Molecular Dynamics Simulations of Nano-Particle Internalization into Bilayer Membranes

***Sulin Zhang[1], Ju Li[2], George Lykotrafitis[3], and Subra Suresh [3]**

[1] Department of Engineering Science and Mechanics, The Pennsylvania State University
212 EES Bldg, University Park, PA 16802, USA
suz10@psu.edu

[2] Department of Materials Science and Engineering, University of Pennsylvania, 223 LRSM, 3231 Walnut Street
Philadelphia, PA 19104, USA
liju@seas.upenn.edu

[3] Affiliation
Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139
gelyko@mit.edu
ssuresh@mit.edu

Key Words: *Nano-particles, Cell, Endocytosis, Coarse-grained Molecular Dynamics*

ABSTRACT

Owing to their small size, ligand-coated nano-particles (NPs) can efficiently be directed to and subsequently internalized by type-specific cells, thereby enabling promising biomedical applications including disease diagnosis, tumor cell tracking and recognition, and site-specific gene/drug delivery. We here present coarse-grained molecular dynamic (CGMD) simulations of receptor-mediated endocytosis of NPs. The coarse-grained model for bilayer membranes established herein is computationally highly efficient, yet captures the fundamental thermodynamic properties including bending rigidity and viscosity of bilayer membranes. Our simulations show that the degree of wrapping of NPs and the geometrical transition of the bilayer membrane are dependent on the particle size and NP-membrane adhesion energies. For multiple NPs interacting with cell, we show wrapping and internalization of NPs are governed by curvature-mediated interactions. The simulations indicate that the competition for receptors among NPs governs the uptake rate, exhibiting a source-limited process. The CGMD model not only provides an efficient computational tool for bilayer membranes, but also enhances the fundamental understanding of the energetics and kinetics of endo/exocytosis.