The Department of Mechanical Engineering
College of Engineering and Applied Sciences
Stony Brook University

Mechanical Engineering Seminar

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Lecture Title: Design of Smart Drug Delivery Platform Guided by Multiscale Computational Modeling

Thursday, September 28, 2017 at 1:30 PM, Room 173 Light Engineering Building

Abstract

Through nanomedicine, game-changing methods are emerging to deliver drug molecules directly to diseased areas. One of the most promising methods is the targeted delivery of drugs and imaging agents via drug carrier-based platforms. Such drug delivery systems can now be synthesized from a wide range of different materials, made in a number of different shapes, and coated with an array of different organic molecules, including ligands. If optimized, these systems can enhance the efficacy and specificity of delivery compared with those of non-targeted systems. Emerging integrated multiscale experiments, models and simulations have opened the door for endless biomedical applications. Current bottlenecks in design of the drug-carrying particles are the lack of knowledge about: (i) synthesis of delivery vehicle/platform; (ii) microcirculation of drug carriers (nanoparticles) in the blood flow and their subsequent adhesion to vessel wall; (iii) nanoparticle penetration into tumor tissue; and (iv) endocytosis and exocytosis of nanoparticles. In this talk, I will demonstrate a multiscale computational framework, by combining all-atomistic simulation, coarse-grained molecular dynamics and the immersed finite element method, to systematically elucidate the underlying physical mechanisms behind these phenomena. The multiscale computational framework has been demonstrated to successfully capture the self-assembly of drug delivery platform, margination of nanoparticle in the microcirculation, adhesion of nanoparticle to vessel wall under shear flow, as well as the receptor-mediated endocytosis of nanoparticles. All the simulation results have been further corroborated by experimental observations, indicating that the size, shape, surface and stiffness (4S) of nanoparticles are the key design parameters. The present multiscale modeling framework can help us to optimize and design more efficient drug carriers in the near future.

Biography

Dr. Ying Li joined the University of Connecticut in 2015 as an Assistant Professor in the Department of Mechanical Engineering. He received his Ph.D. in 2015 from Northwestern University, focusing on the multiscale modeling of soft matter and related biomedical applications. His current research interests are: multiscale modeling, computational material design, mechanics and physics of soft matter, design of mechanical metamaterials and targeted drug delivery. Dr. Li's achievements in research have been widely recognized by fellowships and awards including Best Paper award from ASME Global Congress on NanoEngineering for Medicine and Biology (2015), International Institute for Nanotechnology Outstanding Researcher Award (2014), Chinese Government Award for Outstanding Students Abroad (2012) and Ryan Fellowship (2011). He has authored and co-authored more than 50 peer-reviewed articles, including Physical Review Letters, Biomaterials, Nanoscale, Macromolecules, Soft Matter, Polymer, Journal of Mechanics and Physics of Solids etc. He has been invited as a reviewer for more than 40 international journals, such as Nature Communications, ACS Nano, Advanced Functional Materials, Carbon, Macromolecules, Journal of Physical Chemistry, ACS Applied Materials & Interfaces, Nanoscale, Chemical Communications and Nanomedicine.

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