Understanding Nano Environmental Health and Safety through Multiscale Modeling

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Abstract: Engineered nanomaterials (ENMs) have tremendous potential to produce beneficial technological impact in numerous sectors in society. Safety assessment is, of course, of paramount importance. However, the myriad variations of ENM properties makes the identification of specific features driving toxicity challenging. At the same time, reducing animal tests by introducing alternative and/or predictive in vitro and in silico methods has become a priority. It is important to embrace these new advances in the safety assessment of ENMs. In this talk, I will highlight two aspects related to safety assessment of ENMs. One is the blood circulation of ENMs. We have recently developed an efficiency numerical method to study the blood circulation behaviors of ENMs through large scale fluid-structure interaction simulations. The blood plasma can be resolved by the highly parallelized Lattice-Boltzmann method. And the deformation of red blood cells and ENMs can be solved by the coarse-grained lattice model. The immersed boundary method has been applied to couple the fluid flow with immersed molecular structures. Such an efficient numerical method can help to understand the vascular dynamics of ENMs under the influence of their size, shape, stiffness and surface properties, as well as local physiological conditions. On the other aspect, we have studied the interactions between ENMs and cells through large scale molecular dynamics. By using all-atom and coarse-grained molecular dynamics simulations, we have systematically explored how the size, shape, stiffness and surface functionalization will affect the cellular uptake pathways of ENMs. All the simulation tools and results can be further applied to advance the hazard and risk assessment of ENMs. This, in turn, would greatly promote the safe and sustainable use of ENMs and effectively boost ENM-driven innovations.

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 70 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 reviewer for more than 50 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. He currently serves as the Topic Editor of MDPI-Polymers, an international leading journal in polymer field.