MII Seminar Series

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Prof. Shengfeng Cheng

"Molecular Dynamics Modeling of Polymers"

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Abstract:
Molecular Dynamics (MD) simulations are increasingly applied to understand the structure, dynamics, and mechanics of polymers. In this seminar he will provide a survey of recent research activities in his group on modeling synthetic and biological polymers with either atomistic or coarse-grained (CG) simulations. On the synthetic polymer side, the topics include atomistic modeling of polyimides focusing on the computation of Tg and dielectric constant, CG modeling of the rheological properties of polyimides with branching, CG modeling of the interpolyelectrolyte complexes, polyelectrolyte-coated nanoparticles and their interactions and self-assembly, and nanoparticle-brush composites. On the biopolymer side, their effort is mainly devoted to a special supramolecular polymer named microtubules that are made of tubulin proteins and serve as a crucial component of the cytoskeleton. Prof. Cheng has developed an intuition-based CG model that can be used to study the self-assembly and nanomechanics of microtubules. Recently his team has made progress to connect this CG model to the known atomistic structure of tubulin proteins, including the direct computation of tubulin bond energies. They also demonstrate that a similar CG model can be applied to actin-filaments. His research endeavors in other areas of soft matter physics, including bubble physics, evaporation, friction, adhesion, and crumpling, will also be briefly covered.

Bio:
Shengfeng Cheng joined the Department of Physics at Virginia Tech as an assistant professor in August 2013. He is also an affiliated member of the Macromolecules and Interfaces Institute. He obtained his Ph.D. from Johns Hopkins University in 2010 and then joined Sandia National Laboratories as a postdoctoral appointee. Before coming to the United States, he attended Nanjing University in China and graduated with a Master of Science in 2003. In his career, he has worked on physics of aperiodic structures, friction, crumpling, and spreading. His current research interests center on theory and molecular modeling of soft matter systems including polymers and nanocomposites. His hobbies include soccer and weiqi (a board game popular in east Asia).

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