

数学与系统科学研究院

计算数学所学术报告

报告人: **Prof. Wonpil Im**

(Lehigh University, US)

报告题目:

**Ion Channel Brownian Dynamics:
Approximate, Yet Still Useful Approach**

邀请人: 卢本卓研究员

报告时间: 2018年4月26日(周四)

下午 15:00--16:00

报告地点: 数学院南楼N714 会议室

报告摘要:

In this talk, I will first introduce three well-known computational approaches to study ion channel conductance and selectivity: molecular dynamics (MD), Brownian dynamics (BD), and Poisson-Nernst-Planck (PNP) electrodiffusion theory. By using OmpF porin, an outer membrane protein in *Escherichia coli* as a model system,

these approaches are compared in terms of equilibrium ion distribution, and how underlying microscopic parameters needed for BD and PNP can be obtained from MD is discussed. In addition, the non-equilibrium BD and PNP results of OmpF, such as ion conductance and selectivity (reversal potential), are also compared. By using the voltage-dependent anion channel (VDAC) in the outer membrane of mitochondria as a model system, both equilibrium and non-equilibrium results of MD and BD are discussed with an emphasis on the efficacy of BD in studying ion channel. Finally, various applications of BD through a web-based graphical user interface in CHARMM-GUI (www.charmm-gui.org) are illustrated.

Brief BIO:

Wonpil Im received in bachelor's and master's degrees from Hanyang University in Seoul. He then earned his Ph.D. in Biochemistry from Cornell University. He did his post-doctoral research at the Scripps Research Institute in La Jolla, California. In 2005, he was hired as an assistant professor in the Center for Computational Biology and Department of Molecular Biosciences at the University of Kansas, Lawrence. In 2011, he was promoted to associate professor and then professor in 2015. In 2016, he joined the Faculty in Departments of Biological Sciences and Bioengineering at Lehigh University, and he has been named the Presidential Endowed Chair in Health - Science and Engineering. Wonpil was recently awarded the Friedrich Wilhelm Bessel Research Award from the Humboldt Foundation and was named a KIAS Scholar from the Korea Institute for Advanced Study. Prior to Lehigh, he was awarded the Alfred P. Sloan Research Fellowship (2007), ACS HP Outstanding Junior Faculty Award (2011), J. Michael Young Undergrad Advisor Award (2011), Meredith Docking Scholar (2013), and University Scholarly Achievement Award (2015).

Research in his lab is focused on the applications of theoretical/computational methods to chemical and physical problems in biology and material sciences. In particular, he is interested in modeling and simulations of biological membranes and associated proteins, glycoconjugates, and protein-ligand (drug) interactions. In addition, his lab has been developing CHARMM-GUI for the biomolecular modeling and simulation community.

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