

数学与系统科学研究院

计算数学所学术报告

报告人: **Dr. Longzhu Shen**

(*Yale University*)

报告题目:

**Predictive Toxicology and Safer
Chemical Design**

邀请人: 卢本卓 研究员

报告时间: 2016 年 8 月 16 日 (周二)

下午 15:00-16:00

报告地点: 数学院南楼七层

702 会议室

Abstract:

Green chemistry aims at seeking sustainable solutions for chemical products and processes. Chemicals and chemical products with specific functional needs have touched almost every corner of our life. However, the complex entanglement between chemistry and biology spaces sometimes defies the reductive mode of thinking. Unintended biological consequences may occur upon exposure to certain chemicals. Toxicity is a concern with many chemicals currently in commerce, and with new chemicals that are introduced each year. The standard approach to testing chemicals is to run studies in laboratory animals, but because of the expense of these studies and concerns for animal welfare, few chemicals besides pharmaceuticals and pesticides are fully tested. Over the last decade there have been significant developments in the field of computational toxicology which combines in vitro tests and computational models. The ultimate goal of this field is to build predictive toxicity models and infer safer chemical design. The success of this field is anchored on three key factors, ie. construction of a design variable space with encapsulation of mechanistic toxicology information, an effective predictive model that connects the design variables and toxicity outcomes and a mathematical scheme to present the complete solution in the design variable space. As a pioneer investigation, I'd like to present to you a coalesced effort between mechanistic toxicology, computational chemistry and statistical learning in addressing the three-fold of goals at one once.

Bios :

Dr. Longzhu Shen obtained his Ph.D. degree at Carnegie Mellon University. During the Ph.D. period, his research was centered on studying the reaction mechanisms of a human-made biomimetic catalyst for green applications. His quality research has been highly recognized with a four-year continuous award of the prestigious Mellon presidential fellowship. He also served as the chair of the environmental group of the ACS (American Chemical Society) Pittsburgh local chapter. During his term, he lead his team to win the ChemLuminary award for outstanding sustainability activities. After graduation, he carried on his passion toward green chemistry by joining the Center for Green Chemistry and Green Engineering at Yale as a postdoc research associate. His current active role is leading the research consortium forged by four universities to design safer chemicals with reduced likelihood to incur toxicity.

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