

数学与系统科学研究院

计算数学所学术报告

报告人: **Dr. Beibei Huang**

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报告题目:

**Computational Challenges in
Modeling of Self-assembly of
Charged Polymers**

邀请人: 卢本卓 研究员

报告时间: 2015 年 9 月 28 日 (周一)

上午 10:00-11: 00

报告地点: 数学院南楼七层

702 会议室

Abstract:

Self-assembly is a spontaneous and reversible organization of molecular units into ordered structures. The self-assembly process plays an important role in materials science and life science. My talk focus on the computer simulation of self-assembly by linear charged polymers in ionic solution. In one case Poisson-Boltzmann (PB) theory is considered in the numerical simulation of self-assembly phenomenon, and in another case it is incorporated with the Single Chain Mean Field (SCMF) theory to simulate several charged nanosystem numerically.

欢迎大家参加！