

数学与系统科学研究院

计算数学所学术报告

报告人: **Prof. Dexuan Xie**

(*University of Wisconsin-Milwaukee, USA*)

报告题目:

**New Dielectric Continuum Models
for Biomolecular Electrostatics and
Their Mathematical Studies**

邀请人: 周爱辉研究员

报告时间: **2010 年 12 月 20 日(周一)**

上午 10: 00~11: 00

报告地点: 科技综合楼三层 **311**

计算数学所报告厅

Abstract:

Electrostatic interactions play an important role in molecular biology, biochemistry, bioengineering, and many other fields. They have been modeled in several different kinds of dielectric continuum models for large scale biomolecular simulations, which include the well known Poisson-Boltzmann equation and the nonlocal dielectric model. In this talk, I will report a new dielectric continuum model that we developed recently using the density functional theory of hard-sphere mixture fluid. I then will describe a numerical protocol for solving this new model. Finally, I will present some mathematical results on the analysis of a typical nonlocal dielectric model. This project is supported in part by NSF grant #DMS-0921004.

欢迎大家参加!