

数学与系统科学研究院

计算数学所学术报告

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**报告题目: Continuum
Electrostatics for Ionic Solutions
with Nonuniform Ionic Sizes**

邀请人: 周爱辉研究员

报告时间: 2009年9月18日(周五)

下午 4:00—5:00

报告地点: 科技综合楼三层 311

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Abstract: Equilibrium ionic concentrations

predicted by the classical Poisson–Boltzmann theory can often be unrealistically high, since the theory does not describe accurately the excluded–volume effect of ions and solvent molecules. A new, mean–field electrostatic free–energy functional is proposed to include such effects in an ionic solution with multiple ionic species of possibly different ionic sizes. Mathematical analysis is presented on the upper and lower bounds of equilibrium ionic concentrations and the generalized Boltzmann distributions. Unless all the ionic and solvent molecular sizes are assumed to be the same, explicit formulas of such dependence are, however, not available in general. It is nevertheless true that in equilibrium the ionic charge density is a decreasing function of the electrostatic potential. This determines a variational principle with a convex functional for the electrostatic potential. Numerical aspects of this new theory will be discussed.

欢迎大家参加！