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：

Mean-Field Description of Ionic Size Effects: A Numerical Approach

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报告时间：**2011** 年 **6** 月 **17** 日（周五）

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报告地点：　　科技综合楼三层 **311**

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Abstract:

Ionic size effects are significant in many biological systems. Mean-field descriptions of such effects can be efficient but also challenging. When ionic sizes are different, explicit formulas in such descriptions are not available for the dependence of the ionic concentrations on the electrostatic potential, i.e., there is no explicit, Boltzmann type distributions. This work begins with variational formulations of the continuum electrostatics of an ionic solution with such non-uniform ionic sizes as well as multiple ionic valences. An augmented Lagrange multiplier method is then developed and implemented to numerically solve the underlying constrained optimization problem. Extensive numerical tests demonstrate that the mean-field model and numerical method capture qualitatively some significant ionic size effects, particularly those for multivalent ionic solutions, such as the stratification of multivalent counterions near a charged surface. The ionic valence-to-volume ratio is found to be the key physical parameter in the stratification of concentrations. All these are not well described by the classical Poisson--Boltzmann theory, or the generalized Poisson--Boltzmann theory that treats uniform ionic sizes. Finally, various issues such as the close packing, limitation of the continuum model, and generalization to molecular solvation are discussed. This is joint work with Shenggao Zhou and Zhongming Wang.

欢迎大家参加！