数学与系统科学研究院

计算数学所学术报告

报告人： 徐振礼 研究员

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报告题目：

Self-Consistent Continuum Theory for Coulomb Many-Body Systems in Inhomogeneous Environments

邀请人： 谢和虎 副研究员

报告时间： 2014 年 8 月 22 日（周五）

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：

In this talk, I will present recent work on modeling and simulations of nanoscale electrostatic systems in inhomogeneous dielectric media with strong many-body correlation effects. We consider Monte Carlo simulations and continuum models by self-consistent field theory for electrolytes including dielectric-boundary, ion-correlation, and excluded-volume effects. For particle simulations, we developed efficient algorithm for treating dielectric interfaces. For continuum theory, we derived self-energy-modified Poisson-Boltzmann equations for equilibrium systems and Poisson-Nernst-Planck equations for charge transport. We studied the asymptotic properties of the models, discussed efficient algorithms for these PDE models. By both continuum and particle simulations, we attempt to understand many-body properties of systems with dielectric interfaces, arising from soft matter and biological applications.

欢迎大家参加！