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：

Phase-Field Free Energy and Boundary Force for Molecular Solvation

邀请人：　陈志明 院士

报告时间：2019 年 6 月 3 日（周一）

上午 10:00-11:00

报告地点：　数学院南楼七层

702 教室

Abstract:

We discuss a phase-field variational model for the solvation of charged molecules with implicit solvent. The solvation free-energy functional of all phase fields consists of the surface energy, solute excluded volume and solute-solvent van der Waals dispersion energy, and electrostatic free energy. The last part is defined through the electrostatic potential governed by the Poisson-Boltzmann equation in which the dielectric coefficient is defined through a phase field. We prove Gamma-convergence of the phase field free-energy functional to its sharp-interface limit. We also define the dielectric boundary force for any phase field as the negative first variation of the free-energy functional, and prove the convergence of such force to the corresponding sharp-interface limit.

欢迎大家参加！