数学与系统科学研究院

计算数学所定期学术报告

报告人：　**Prof. Hui Zhang**

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报告题目：

新型水凝胶材料的微结构和相变的计算

邀请人：　郑伟英 副研究员

报告时间：**2012** 年 **12** 月 **20** 日（周四）

下午 **16：00~17：00**

（**15：30~16：00** 茶歇）

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 the micro-structure and the phase transition process of Macromolecular Microsphere Composite (MMC) Hydrogel.

Firstly a model to describe the micro-structure of Macromolecular Microsphere Composite (MMC) Hydrogel is proposed in the framework of self-consistent mean field theory (SCFT). The equation system derived by SCFT approximation is solved by a relaxation algorithm. From the numerical simulations of the model, we find that two model parameters play important role in describing the micro-structure of MMC hydrogel, the interactions between two species (polymer chains and MMS spheres) and the volume fraction of MMS spheres. The role of various other model parameters on the structure of the hydrogel is also discussed in this paper. The simulation results are shown to be consistent with the observation from the experiments. Moreover, we also show some new microstructures discovered using the SCFT model.

Then, we use Time-Dependent Ginzburg-Landau(TDGL) mesoscopic model to simulate the phase transition process of macromolecule microsphere composite(MMC) hydrogel. We propose a free energy for such reticular structure, according to the structures of MMC hydrogel and entropy theory. This work generalize the mean field theory confined by Flory-Huggins free energy in polymer blend system. Spectral method is adopted to numerically solve the MMC-TDGL equation. The numerical results are consistent with chemical experiments, showing out the network structure. According to the numerical results at different temperatures, we get that the system shows intermittent phenomenon as upgrading reaction temperature, which is a very good explanation of chemical experiments.

欢迎大家参加！