数学与系统科学研究院

计算数学所学术报告

报告人：　**Dr. Jie Xu**

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报告题目：

Onsager-theory-based tensor model for nematic phases of bent-core molecules

邀请人：　周爱辉 研究员

报告时间：**2018** 年 **12** 月 **13** 日（周四）

下午 **16:00-17:00**

报告地点：　数学院南楼二层

202 教室

Abstract:

We construct static tensor model for nematic phases of bent-core molecules and star molecules from Onsager theory. The form of free energy is determined by molecular symmetry, which includes the couplings and derivatives of a vector and two second-order tensors, with the coefficients derived as functions of molecular parameters. The model builds a definite mapping from molecular architectures and macroscopic behaviors. We study the nematic phases and elastic constants resulted from different molecular architectures. We incorporate the free energy into hydrodynamics and construct energy dissipative dynamic model. Similar to the static model, the form and coefficients are determined by molecular symmetry and molecular parameters, respectively. We examine the flow modes in shear, where we also focus on the effect of different molecular architectures.

We also discuss theoretical and computational problems arising from the model.

欢迎大家参加！