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：

Introduction to finite-temperature density functional theory calculations

邀请人：　刘歆副研究员

报告时间：**2017** 年 **11** 月 **9** 日（周四）

上午 **9:30-10:30**

报告地点：数学院科技综合

301 报告厅

报告摘要：

In this work, a novel ring polymer representation for multi-level quantum system is proposed for thermal

average calculations. The proposed representation keeps the discreteness of the electronic states: besides position and momentum, each bead in the ring polymer is also characterized by a surface index indicating the electronic energy surface. A path integral molecular dynamics with surface hopping (PIMD-SH) method ("DS" method) is also developed to sample the equilibrium distribution of ring polymer configurational space. Besides, The infinite-swap limit of this representation has been investigated, which provides an alternative formulation for thermal average calculations and overcomes the limitations of the "DS" method. We also introduce a multi-scale integrator to efficiently sample the infinite-swap limit. This is joint work with Jianfeng Lu.

欢迎大家参加！