

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:

Multi-step umbrella sampling and its application in trans-membrane permeation of ions

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报告地点: **数学院科技综合楼**

三层 311 报告厅

Abstract:

Multi-target umbrella sampling is an important technique in free energy calculation of phase transitions. In this sampling technique, it is crucial to find a few proper reaction coordinates in obtaining a continuous transition trajectory and an accurate free energy profile. However, when the system is complex, it is usually very hard to find the reaction coordinates. In this talk, we discuss a multi-step strategy to perform multi-target umbrella samplings. A weighted least square analysis method (Welsam) is designed to obtain the free energy profile along the transition path. The (local) reaction coordinates can be obtained from the trajectory jumps. This strategy has been successfully applied in the study of trans-membrane permeation process of ions. Proper reaction coordinates are designed and continuous transition trajectories are obtained in a relatively easier way. Our work makes clear the trans-membrane permeation mechanism of ions for the first time, in which a water chain is formed across the membrane to bridge the permeation of ions. With the presence of the water chain, the free energy barrier is significantly reduced for thick membranes.

欢迎大家参加！