数学与系统科学研究院

计算数学所学术报告

报告人：　　**Xubo Lin**

（ ***Beijing Advanced Innovation Center for Biomedical Engineering, Beihang University (BUAA), Beijing, China*** ）

报告题目：

Membrane Domain Dynamics and Its Biological Effects: Insights from Molecular Dynamics Simulations

邀请人：　卢本卓 研究员

报告时间：**2019** 年 **3** 月 **28** 日（周四）

上午 **10:00-11:00**

报告地点：　　数学院南楼七层

714 教室

Abstract:

Plasma membrane is critical to the functions of cells due to its role in selectively exchanging matter and signals between inside and outside the cell. Many efforts have been made to reveal the correlation between its functions and dynamics. It is generally agreed that its main components including lipids and proteins can segregate into nanoscale dynamic membrane domains of different compositions and properties. We have performed a series of molecular dynamics simulations to elucidate both the in-leaflet and inter-leaflet membrane domain dynamics. We found the in-leaflet membrane domain stability could be quantified by lipid chain order differences rather than thicknesses between different domains. Meanwhile, the in-leaflet membrane domain stability might further affect the partitioning dynamics of transmembrane peptides and the clustering dynamics of membrane-bound proteins. The inter-leaflet membrane domain dynamics (domain registration/anti-registration), which might be critical to signal transduction, is dominated by the inter-leaflet coupling. In addition to lipid chain interdigitation, we recently found cholesterol flip-flop rate as well as lipid cis double bond position could also modulate the coupling. Weak inter-leaflet coupling will induce obvious dynamic domain registration and anti-registration, which may correspond to an alternating intrinsic membrane potential. Combing all the points above, we believe insights provided by molecular dynamics simulations will be useful for understanding roles of membrane domains.

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