Meiji Institute for Advanced Study of Mathematical Sciences Center for Mathematical Modeling and Applications

Meiji University Center for Mathematical Modeling and Applications

第51回 現象数理学コロキアム



Tetrahedral Liquids: From a Tale of Two Liquids to a Tale of Topology

※ 講演は英語で行います。

Abstract:

Water is a classic example of tetrahedral liquids, where the nature of the molecular interactions favour local, short-ranged tetrahedral order. Water exhibits a host of anomalous thermodynamic properties, many of which are also displayed by tetrahedral liquids. The existence of a phase transition between a low-density liquid (LDL) and a high-density liquid (HDL) for water was originally hypothesised more than three decades ago to account for its thermodynamically anomalies and has now been well-established more generally for tetrahedral liquids by a significant body of computational studies. However, the experimental verification of this liquid-liquid phase transition (LLPT) has proved elusive, in particular, for water. An enduring puzzle is how a pure substance can have two distinct liquid phases. In this presentation, I will describe how we developed a colloidal model of water, exploiting hierarchical self-assembly, to throw light on this puzzle. Our work reveals a topological distinction between the two liquids for water, and more generally for tetrahedral liquids, showing that the LDL is unentangled and the HDL – containing an ensemble of topologically complex motifs, including links and knots – is entangled. I will also illustrate how entanglement can emerge as a general mechanism for densification, with a hierarchy of topological transitions in a model tetrahedral liquid, which is known to densify via two successive LLPTs. Our results thus unravel a topological perspective of the tale of two liquids, which should have far-reaching implications for understanding LLPTs in tetrahedral liquids.

講演者:Dwaipayan Chakrabarti University of Birmingham (UK) WPI-SKCM2, 広島大学(客員准教授) 2025年8月19日(火) 16:00~17:30 会場:明治大学中野キャンパス 高層棟6階研究セミナー室3 ※ 参加費無料、事前登録制。



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