



香港中文大學化學系  
Department of Chemistry  
THE CHINESE UNIVERSITY OF HONG KONG

# The Chinese University of Hong Kong

## Department of Chemistry - Research Seminar Series

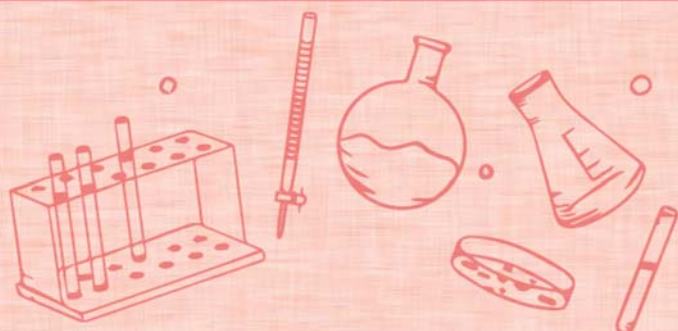


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### Structures and Dynamics of Topological Defects in Driven and Active Nematic Liquid Crystals

17 February 2023 (Friday)  
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## Structures and Dynamics of Topological Defects in Driven and Active Nematic Liquid Crystals

Abstract:

Topological defects are important for regulating the structural, optical, and rheological properties of liquid crystals. Current research interests in liquid crystal defects are motivated by their potential applications as a template to direct self-assembly and their autonomous motion capabilities in active liquid crystals. However, our understanding of their structures in driven and active systems is limited by their microscopic size and transient behavior. Therefore, simulations can provide a convenient platform to elucidate their emergence, structures, and dynamics. In this talk, I will discuss our recent efforts in employing different simulation methods combined with experiments to characterize disclination behaviors in nematic liquid crystal in static state, under driven flows, or driven by active stresses. First, we use molecular dynamics to examine nanoscopic structures and thermodynamics of disclinations and find that the molecular system can be well understood by continuum theories. We next combine continuum simulation and experiment to study the super-elastic properties of disclinations and their emergent structures in tumbling, lyotropic liquid crystals under a pressure-driven flow. Lastly, we predict a new symmetry breaking mechanism for self-propelling disclinations in active chiral nematics. As such, our multiscale simulations have provided a deeper understanding of topological defects in out-of-equilibrium nematic liquid crystals, which could facilitate their applications in sensing, photonics, material transport, and rheology.