



Institute colloquium

Topology, molecular simulation, and machine learning as routes to exploring structure, dynamics, and phase behavior in atomic and molecular crystals

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The different solid structures or polymorphs of atomic and molecular crystals often possess different physical and chemical properties. Structural differences between organic molecular crystal polymorphs can affect, for example, bioavailability of active pharmaceutical formulations, the lethality of contact insecticides, and diffusive behavior in host-guest systems. In metallic crystals, structural differences may determine how different phases may be used in electronic device applications. Crystallization conditions can influence polymorph selection, making an experimentally driven hunt for polymorphs difficult. These efforts are further complicated when polymorphs initially obtained under a particular experimental protocol “disappear” in favor of another polymorph in subsequent repetitions of the experiment. Theory and computation can potentially play a vital role in mapping the landscape of crystal polymorphism. Traditional force-field based methods for predicting crystal structures and investigating solid-solid phase transformation behavior face their own challenges, and therefore, new approaches are needed. In this talk, I will show, by leveraging concepts from mathematics, specifically geometry, topology, and machine learning, a force-field free method for predicting molecular crystal structures is possible. The new approach yields predictions of structures at least an order of magnitude faster than traditional energybased methods. Once a polymorph landscape is obtained, techniques of molecular simulation and machine learning can be used to predict the kinetics of structural phase transitions between different polymorphs. In this way, I hope to present a convincing case that new paradigms are emerging in our ability to predict molecular crystal structures and determine kinetics of polymorphic phase transformations.

Monday, November 6, 2023 11:30am - 12:30pm

Raiffeisen Lecture Hall



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