演題: Navigating stability and metastability in the synthesis of novel functional materials

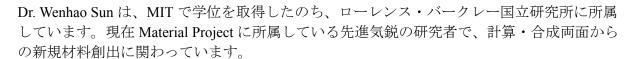
講師: Dr. Wenhao Sun

Lawrence Berkeley National Laboratory, the U.S.A.

日時: 2019年6月28日(金) 13:30~14:30

場 所: 工学部材料·化学棟大会議室 (MC526)

主催:新学術領域研究「複合アニオン化合物の創製と新機能」



Abstract: Despite rapid progress in the computational design of novel functional materials, the materials discovery pipeline remains bottlenecked by the difficulty of reliably synthesizing predicted compounds in the lab. Developing a theoretical foundation for predictive materials synthesis requires a more quantitative understanding of *metastable* phases, which often appear as kinetic byproducts during materials formation. By mapping the thermodynamic landscape of crystalline metastability, and calculating relative nucleation rates between competing polymorphs, we can construct synthesis maps to navigate through the thermodynamic and kinetic energy landscape towards desired material phases. I will showcase several applications of this *ab initio* framework to predict non-equilibrium crystallization pathways of carbonate minerals and functional manganese oxides in hydrothermal synthesis, and conclude with thermodynamic strategies for the discovery and synthesis of metastable thin-film nitride semiconductors. Mastering metastability will deepen our fundamental understanding of nucleation and crystal growth, and can expand the search space for functional technological materials beyond equilibrium phases and compositions.

本講演は、大学院総合化学院『化学研究先端講義(修士課程選択科目)/ 総合化学特別研究第二(博士後期課程選択科目)』の一部として認定されています。

連絡先:工学研究院応用化学部門 三浦章(内線:7116)

フロンティア化学教育研究センター