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Lifting Phase Diagrams Out of Flatland

When synthesizing a new material, one often starts by consulting the thermodynamic phase diagram. There are four main varieties of phase diagrams today: 1) Temperature–Pressure; 2) Temperature–Composition; 3) Ellingham (T, μ_{O2}); and 4) Pourbaix diagrams (pH, Redox potential). However, these 2D phase diagrams do not account for many other forms of thermodynamic work that may be operative during nucleation and growth—such as surface, elastic, electromagnetic and electrochemical work. Here, I will describe a geometric process to 'lift' 2D phase diagrams into higher dimensions, exposing these additional forms of thermodynamic work on the axes. By properly accounting for these hidden thermodynamic variables, we can reconcile many surprising experimental observations of non-equilibrium intermediates during multistep crystallization—for example as often observed during 'panoramic synthesis.' Visualizing phase stability along these additional thermodynamic axes further enables us to design rational processing routes to novel metastable materials under far-from-(bulk)-equilibrium conditions. I will conclude with a broader vision for the construction and deployment of high-dimensional phase diagrams, which may serve as a powerful new conceptual framework for the design and synthesis of advanced functional materials.

Wenhao Sun joined the University of Michigan as an Assistant Professor of Materials Science and Engineering in January 2020. He performed his undergraduate studies at Northwestern University, double majoring in Materials Science and Engineering and Applied Mathematics, and obtained his PhD in Materials Science and Engineering from MIT. The Sun Research Group uses high-throughput density functional theory, applied thermodynamics, and materials informatics to deepen our fundamental understanding of synthesis–structure–property relationships, while exploring new chemical spaces for functional technological materials. In 2020, Wenhao was named a Materials Horizons Emerging Investigator, and received the Department of Energy Early Career Award to support his research on, 'Temperature-Time-Transformation (TTT) Diagrams for Predictive Solid-State Ceramic Synthesis'.

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Tech Institute Rm. LR4, 4:00-5:00 p.m.

Zoom meeting link:
https://northwestern.zoom.us/j/99345784357
Meeting ID: 993 4578 4357