Northeastern University
College of Engineering

October 3, 2025 | Egan Center (EC) 306 | 1:30PM

Distinguished Seminar Speaker

Fast-Track Materials Discovery Beyond Equilibrium for Energy and Sustainability

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Abstract: The development of stable multicomponent materials remains a central challenge in inorganic chemistry and chemical engineering. In systems containing multiple elements, positive mixing enthalpy, size and valence mismatch, and structural incompatibility tend to drive phase separation, especially under equilibrium conditions. Traditional doping strategies for tuning electronic structure and defect chemistry have had some success but are fundamentally constrained by narrow solid-solution windows. To address these limitations, we developed a non-equilibrium flame synthesis technique capable of producing multicomponent solid solutions across alloys, ceramics, and metal-organic frameworks. This method enables rapid evaporation, nucleation, and growth within milliseconds, establishing a well-defined thermodynamic and kinetic pathway for kinetically trapping metastable phases. When combined with entropy-driven stabilization, this approach yields two types of material outcomes, depending on the configurational entropy of the system: high-entropy systems with five or more elements tend to form stable single-phase solid solutions, while systems with two to four components undergo controlled *in situ* exsolution in response to mild enthalpic stimuli. This unified strategy is broadly applicable to thermocatalysis, electrocatalysis, and critical mineral recovery, and offers a robust framework for materials design beyond the limits of equilibrium-based methods.

Biography: Dr. Chaochao Dun joined Lawrence Berkeley National Laboratory in June 2019 and currently serves as a project staff scientist at the Molecular Foundry. He earned his Ph.D. from the Center for Nanotechnology and Molecular Materials in the Physics Department at Wake Forest University in 2017. At Berkeley Lab, Chaochao is leading three main research thrusts: (I) synthesizing multicomponent materials via non-equilibrium flame-aerosol method for energy conversion and storage; (II) designing sorbents and redox-active clusters for recovering critical minerals; and (III) mechanism-oriented studies that link defect chemistry and kinetics/thermodynamics to performance, supported by multi-scale characterization.

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