How to discover new solids containing alkali metals: predictive screening, facile synthesis and in situ studies

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Chemistry Seminar on predictive screening of materials

Monday April 13 at 4 pm in 126 Schrenk

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Abstract: Materials discovery can be accelerated by the development of synthesis methods and in-situ characterization techniques allowing for the rapid "screening" of multicomponent systems, while theoretical predictions of new compounds' structure and thermodynamic stability can yield the desired roadmap for the targeted synthesis. However, the sluggish kinetics of solid-state reactions entails the necessity of high temperatures and long annealing times, often leading to the stabilization of the thermodynamically stable products.

We are interested in unconventional synthesis methods toward solid-state materials, using reactive, salt-like precursors. Our synthesis is guided by real-time reaction monitoring and theoretical predictions. I will show how new ternary compounds containing alkali metals (Li, Na, K) can be discovered using this approach. I will further discuss their structural features established by comprehensive diffraction methods, and physical properties.

About the speaker: Dr. Julia V. Zaikina is a solid state chemist interested in non-conventional synthesis routes to complex solids and understanding of their atomic and electronic structure with the goal of creating new functional materials that address current scientific challenges in sustainable energy. She has B.S. and M.S. degrees in Chemistry, and Ph.D. degree in solid-state and inorganic chemistry. After two postdoctoral stints at Florida State University and UC Davis, she has joined the faculty at Iowa State as an Assistant Professor in 2017, and in 2023 was promoted to Associate Professor. She is a recipient of NSF CAREER award, 2021 Margaret C. Etter Early Career Award from American Crystallographic Association (ACA), 2022 LAS Award for Early Achievement in Research and most recently Trapp Innovation Award.