

## SMS Spring 2024 Seminar Series

Friday April 4 | 3pm | Biodesign Auditorium

### Design and Predictive Synthesis of Multi-Anion Chalcogenides Using Retrosynthetic Chemistry

Mixed-anion chalcogenides are an important class of semiconductors that can be fine-tuned for specific applications. While chalcogens form solid solutions in simple binary crystal systems, ordering can occur in more complex structures with more than one crystallographically distinct anion site. In this talk, I will explain how we can exploit these features to synthesize ordered multi-anion chalcogenides using a reverse-engineering approach. Crystallographic analysis is used to identify single-anion host structures where ordering will occur, and additionally, the specific Wyckoff position each chalcogen will prefer to occupy. The analysis provides a guide for generating new crystalline solids in a predictable manner and is inspired by the retrosynthetic methods used in organic chemistry. We have applied the technique to a variety of crystal systems with varying structural and compositional features and I will discuss the rules and guidelines for predicting local ordering in crystalline solids. Mixing anions can also facilitate rearrangements of polyhedral building blocks from the single-anion hosts and drive formation of new structures. The reverse-engineering approach is expected to accelerate the discovery of new compounds and provide a platform for studying how local atomic ordering affects the properties of crystalline solids.

### James Hodges, PhD (hosted by Jason Khoury)

*Professor, Penn State*

James M. Hodges received his Ph.D. degree in Chemistry at the Pennsylvania State University in 2016 under the tutelage of Raymond E. Schaak, where his research focused on the synthesis, characterization, and electrochemistry of inorganic nanocrystals. After completing his Ph.D. he spent three years as a postdoctoral fellow at Northwestern University working with Mercuri Kanatzidis developing new chalcogenides for thermoelectric applications. He then spent three years as Senior Scientist in the New Materials Group at Honeywell UOP, where he designed microporous material for catalysis and adsorption technologies that led to 9 patents. In 2022, he joined the Chemistry Department at Penn State, where his group is working on several areas of solid state chemistry including mixed-metal oxides for heterogeneous catalysis and exploratory synthesis multi-anion materials. Jim is currently the chair of the Solid State Chemistry subdivision of Inorganic Chemistry at ACS.

