Stephen Holoviak

Computational methods, such as density functional theory (DFT), molecular dynamics (MD) simulations, and applied data science techniques such as Bayesian optimization enable the discovery and design of material systems and their properties at a faster rate and lower cost than experiment alone. The Sinnott group focuses on a diverse group of material systems using these techniques to model the next generation of materials with our experimental collaborators. One example is the study of Pt-based oxygen reduction reaction (ORR) catalysts using a Bayesian optimization technique to rapidly parameterize computationally affordable models to simulate nanoparticles in an explicit water environment and under an externally applied voltage. Transition metal dichalcogenide (TMDs) heterostructures such as (Mo/W)$S_2$ are investigated using DFT for their ferromagnetic and anti-ferromagnetic properties. As a part of the Materials Research Science and Engineering Center (MRSEC) at Penn State, we also explore complex oxides populated by many elements at random using DFT calculations. We primarily focus on rocksalt high-entropy oxides (HEOs) for fundamental understanding as well as rare-earth fluorite-based HEOs for fast oxygen conductivity. As contributors to the Energy Frontier Research Center on Fast and Correlated Ion Transport in Polymer-based Electrolytes, we work with an interdisciplinary team modeling complex polymer-ceramic interfaces for applications in electrochemical energy storage devices.