

UCSD NANOENGINEERING/CHEMICAL ENGINEERING
SEMINAR SERIES

Wednesday, May 1, 2024

Seminar Presentation: 11:00am - 12:00pm

SME Room 248*“Success Stories in Computationally-Driven
Materials Discovery”***Dr. Corey Oses, PhD***Assistant Professor
Department of Materials Science and Engineering
Johns Hopkins University*

Abstract: Computational approaches are increasingly employed to guide and understand experiments, offering a systematic and accelerated path to materials discovery. Automated ab-initio frameworks like aflow++ have rapidly expanded the volume of materials data, enabling the use of data-science methods for the prediction of new materials. These approaches have been used to study superconductors and thermoelectrics, and have proved fruitful with the discovery of new permanent Heusler magnets, superalloys, high-entropy ceramics, and phase change memory compositions. This talk explores these success stories, highlighting physics-based modeling of thermodynamic and vibration properties, descriptor development, screening approaches, and active-learning schemes driving these discoveries.

Biosketch: Corey Oses, an assistant professor of materials science and engineering at Johns Hopkins University, leads the Entropy for Energy laboratory focusing on the discovery of materials for clean and renewable energy. Specifically, Oses looks to leverage the stabilizing effects of disorder to innovate nuclear-waste immobilization, waste-heat conversion, and electric storage technologies. He completed his bachelor’s degree in applied and engineering physics from Cornell University in 2013 and his PhD in materials science from Duke University in 2018. More information can be found at entropy4energy.ai.