DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

Department of Materials Science and Engineering

Proposal of Thesis

3 pm August 31st, 2023
in Hill Seminar Room, Lebow Engineering Center room # 240

Understanding the effects of chemical complexity on structural and mechanical properties of refractory high entropy alloys

Name: Chris Tandoc
Advisor: Prof. Yong-Jie Hu

Abstract

Refractory high entropy alloys (RHEAs) are a captivating class of materials that have garnered significant attention in recent years due to their exceptional combination of mechanical, thermal, and chemical properties. These alloys, composed of multiple refractory transition metal elements as principal elements, exhibit remarkable resistance to extreme environments, making them promising candidates for applications in aerospace, energy, and other high-performance industries. The multi-principal element composition represents a departure from traditional dilute alloy design, and consequently, presents the potential to unlock novel combinations of properties but also limits the effectiveness of classical alloy design principles. Two specific challenges are 1) the expansive compositional space that can be spanned by a multi-principal element composition and 2) local fluctuations in chemistry that arise due to random mixing of atoms in a solid-solution lattice. To address these design challenges, the use of computational techniques including *ab-initio* calculations and machine learning is proposed to develop high throughput tools that can efficiently screen the RHEA composition space for promising candidate materials. The application of probability theory and atomistic simulations is also proposed to model the distribution of defect properties across local chemical fluctuations in RHEAs and explore the implications for plastic deformation mechanisms.