MICROSTRUCTURES OF CHEMICALLY COMPLEX MATERIALS AND THEIR IMPACTS ON MATERIAL PROPERTIES FROM MULTISCALE SIMULATIONS

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MINISYMPOSIUM

The chemically complex materials, namely, materials with multiple principle chemical components, are drawing increasing attentions in both academia and industries. Examples of emerging chemically complex materials include mixed ion perovskite, high entropy alloys, and van der Waals heterostructures, making them promising advanced materials with applications in advanced electronics, quantum computing, renewable energy, structural materials, or even superconductors. The advantage these materials possess is the wide tunability of material properties, or the potential of attaining multiple functionalities at the same time (e.g. conversion efficiency and life time in perovskite). The microstructure of these chemically complex materials plays a pivotal role in the material properties and performance; nevertheless, owing to the complex combinatorial chemical/permutation space spanned by chemically complex materials, comprehensive insights into their process-structure-property relationship remain a challeng task. In this mini-symposium, we would like to welcome researchers around the world to share and exchange their latest works utilizing computational techniques across both the spatial and temporal length scales to reveal the microstructures of chemically complex materials, and their impacts to the material properties for the structural material, energy storage, catalysis, and renewable energy applications.