CNM WK #7: Artificial Intelligence for Autonomous Synthesis and Processing

Time: Full-day
Date: Wednesday, April 22
Workshop location: Building 440, Room A105/106
Organizers: Jie Xu (CNM), Pierre Darancet (CNM), Subramanian Sankaranarayanan (CNM), Hua Zhou (APS), Xiao-Min Lin (CNM), and Logan Ward (ANL)

Description: The need for optimized synthesis and processing conditions is ubiquitous in technology, impacting fields as diverse as electronics, medicine, metallurgy, solar energy conversion, and multifunctional coatings. However, obtaining a target material with desired properties is time intensive because of the high dimensional and complex synthetic and processing parameters space. The sampling of the large synthetic and processing landscape is generally done through human intuition, based on the knowledge of physical chemistry principles, and trial-and-error approaches, leading to clustered, sparse, and incomplete datasets.

In the past decade, automated robotic technologies have been shown to markedly increase productivity in both medicine and materials science research fields by offloading repetitive works from human scientists and performing experiments in faster speed, greater precision, and better accuracy. With the aid of high performance computing in recent years, artificial intelligence (AI) has been successfully applied to hard materials and small molecule discovery and engineering. Physically informed machine learning approaches including clustering, regression, and Bayesian methods, as well as artificial neural networks, have been applied towards these elements, and have made use of (and added to) publicly accessible databases. This new experimental paradigm has enormous potential benefits, as the robotic hardware and AI software technologies required to realize this goal are just reaching maturity. The proposed workshop will address the main progress and challenges in the research of AI-guided materials synthesis and processing, and cover the entire life cycle of these studies, from computational design, physically guided AI, experimental automation, to control methods, synthetic databases, and robotic integration.