

Joint APS/CNM WK#3: Interpreting Hierarchical Data at Nanocenters and X-ray User Facilities

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Understanding the evolution of materials *in situ* and under *operando* conditions is fundamental to the rational design and precise control of material properties and requires concerted experimental and theoretical efforts. The key information about the material evolution is contained in the lattice and electronic structures across hierarchies of relevant length and time scales, and is captured using different electron and x-ray spectroscopy, diffraction and imaging instrumentations at national nano and x-ray user facilities. However, the depth of information contained therein can be hard to fully exploit due to the complex nature of the data using typical approaches to analysis. The goal of this workshop is to initiate a discussion focused on increasing the efficiency and amount of information extracted from hierarchical datasets. To make sense of these experimental observations needs a coherent framework to merge large datasets with rigorous theoretical calculations and modeling to validate the questions at hand.

Recent advancement at DOE nanocenters and x-ray user facilities including the improvement of electron and x-ray source qualities, the use of large two-dimensional detectors, and the development of high throughput data acquisition protocols fueled an explosion of user data approaching TB for a single experiment. Meanwhile, modeling complicated material systems is computationally expensive due to the large number of atoms involved and the small energy difference between different configurations. These new challenges in domain science parallel the rapid progress in high-power computing and artificial intelligence, which provides new opportunities to accelerate the understanding and discovery of materials. The bottleneck is bridging the knowledge gap between the domain experts and computing scientists, and between domain experts with different experimental/theoretical areas of expertise.

This workshop will bring together experts in electron/x-ray diffraction, spectroscopy and imaging, atomic simulations, and computing scientists to focus on the following cross-cutting frontiers, including (1) high-throughput feature extraction from large experimental dataset, and the role of HPC in streamlining the data analysis; (2) coherent interpretation of multiple x-ray and electron measurements as higher dimensional data, with the help of machine learning; (3) formation and validation of hypothesis towards supervised experiments at user facilities.