



PLENARY LECTURE

Exploring layered solids over broad length scales

Scott T. Misture

Layered solids and their 2-D derivatives represent an important class of materials that have electrochemical, catalytic, ferroic and related properties. Characterizing such materials is often a challenge, but advances in powder diffraction methods and analysis have led to improved understanding of stacking and layer disorder. If one considers also the critically important roles of defects and dopants and their convolution with stacking and layer disorder that defines material properties, it becomes clear that we must describe both the local and long-range structural features simultaneously. Extending powder diffraction studies to total scattering and pair distribution functions (PDFs) yields data that captures the local and long range structures required to assess simultaneously the defects/dopants and layer-to-layer correlations. It is often the case that complementary characterization tools can be used in concert with PDF studies, but only the PDF spans desired length scales. Although poor and/or anisotropic crystallinity makes fitting robust and reliable models to the PDF challenging, the community has made strong strides forward in strategies that provide access to defect/dopant distributions and layer disorder simultaneously, in both real and reciprocal space, with estimates of statistical reliability. A brief overview of our advances in using these tools for ambient and in-situ study of materials and devices will be presented.

Keywords: **stacking disorder, nanosheets, PDF analysis, Bayesian statistics**