Probing the Local Atomic Structure of High-Entropy Oxides

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High entropy oxides (HEOs) have attracted great interest in diverse fields because of their inherent opportunities to tailor and combine materials functionalities. The control of local order/disorder in the class is by extension a grand challenge towards realizing their vast potential. Pair distribution functions (PDF) obtained from total scattering (high energy synchrotron X-ray and Neutron scattering) can reveal both the local and intermediate range structure of crystalline and disordered materials. As we all know that conventional reciprocal space diffraction only probes the average long-range structure of the Bragg planes, and information from EXAFS and XANES is limited to no more than third coordination shell, PDF can reveal both local distortions and measure the structural coherence up to several tens of Ångstrøm. With optimized sample environments PDFs can also be collected under in situ mechanical and electrical fields. A combination of multiple approaches using STEM-EDS, PDFgui (graphical interface built on the PDFfit2 engine), TOPAS v6 (combined reciprocal and real space neutron PDF data) and RMCProfile (Reverse Monte Carlo software) were performed throughout this work. The experimental total scattering PDF activity will be closely supported by density functional theory (DFT) calculations and further Metropolis Monte Carlo simulations (MCS) simulations. This work hints at the exquisite level of detail that may be needed in computational and experimental data analysis to guide structure-property tuning in the emerging HEO materials.

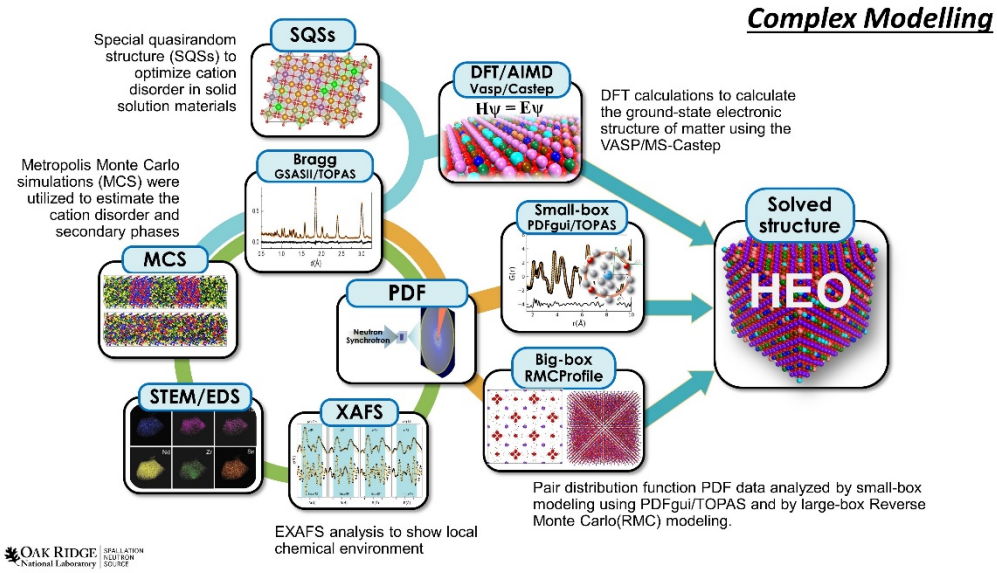

Figure 1