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COMBINING X-RAY AND NEUTRON DIFFRACTION AND MODELLING FOR BETTER UNDERSTANDING ADVANCED MATERIALS

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Many advanced materials, such as thermoelectrics, phosphors for light emitting diodes, electrodes and solid electrolytes for batteries, etc. are difficult objects for stand-alone crystal structural analysis based on diffraction techniques due to intrinsic high disorder of one of the sublattices. Traditional diffraction data analysis based on atom-centric models with explicitly declared atomic positions is often unstable or unable to fully capture all the details due to correlations between variables. Additional difficulties arise from the limitations of X-ray diffraction in locating light elements and distinguishing elements with close atomic numbers (e.g. Mn/Ni/Ci). Combining X-rays with neutrons and traditional diffraction data analysis with other approaches, such as Maximum Entropy Method, and atomistic modelling and theoretical symmetry analysis allows to paint a more complete picture. I will illustrate the point using our recent studies of several such structurally complex systems, such as NASICON and P2-types and phosphor polyanion frameworks. All of them have been studies for decades and yet complementing experiment with theory and modelling revealed new features which help understand and improve properties.

Topic

Advanced Materials

Primary author(s) : AVDEEV, Max (Australian Nuclear Science and Technology Organisation, Australian Centre for Neutron Scattering)

Presenter(s) : AVDEEV, Max (Australian Nuclear Science and Technology Organisation, Australian Centre for Neutron Scattering)

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