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PLENARY LECTURE

Tuning Chemical Short Range Order in the Solid State

Katharine Page

It is widely recognized in catalysis, energy storage and conversion, and a wide array of other functional materials areas that unique properties and characteristics are governed by intricate structural-chemical relationships. Locally ordered cation and anion motifs offer a gamut of possibilities but remain a challenge because experimental tools to observe them are limited. We present recent efforts to apply and extend X-ray and neutron total scattering and related probes to explore *chemical short range order* and associated structure-property responses in solid state materials. First, we will present our work uncovering universal B-site cation ordering in mixed metal inverse spinel oxides, materials of interest as high voltage cathodes in Li-ion batteries. It is found that the degree and length-scale of cation order depend on the charge and ionic radii difference between constituents, unifying the view of many observed physical properties in the structural archetype. Ongoing efforts to increase the reversibility of charge-discharge chemistries will be described. Second, we will present structure-property characteristics of pyrochlore $Ln_2M_2O_7$ materials, a new family in the emerging class of high entropy oxides (HEOs). HEOs exhibit a single-phase crystal structure containing five or more different metal cations of the same amount on single crystallographic lattice sites. The resulting configurational disorder promises unique property characteristics, such as increased structural stability (by impairing the migration of defects) and multi-functional "cocktail" effects (through high numbers of possible element combinations and their interactions). We combine numerous local structure probes and a complex modeling framework to explore the characteristics that specific participating cations and synthesis conditions impart to the family, demonstrating a rich tunability of associated properties. These examples highlight a broader theme of our research aimed at extracting crystal structure models from experimental data with the detail needed to guide and validate solid state theories, and design new and improved functional materials. Current challenges and future opportunities in this arena will be discussed.

Keywords: **Total scattering; neutron scattering; chemical short range order; spinel oxides; pyrochlore oxides**