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Nanoscale Heterogeneity in Compositionally Complex Ceramic Oxides

ABSTRACT:

Next generation materials of nearly every kind rely on chemical, electronic, and/or magnetic heterogeneity for creating, harnessing, and controlling functionality. High entropy oxides (HEOs), materials exhibiting a single-phase crystal structure containing five or more different cations on single crystallographic lattice sites, 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. We present detailed investigation of the cation site preferences, chemical-short-range order, and magnetic and catalytic properties achieved in specific rare-earth and transition metal-based pyrochlore, fluorite, and spinel HEO families through compositional tuning and variation in synthesis/processing conditions. A combination of local to long-range electron, x-ray and neutron scattering probes are employed to investigate their complex configurational diversity and associated structure-property trends. Experimentally derived models are supported by Density Functional Theory calculations and Metropolis Monte Carlo simulations. This work hints at the exquisite level of detail that may be required in computational and experimental approaches to guide structure-property tuning in emerging HEO materials.

BIO:

Katharine Page is an Assistant Professor of Materials Science and Engineering at the University of Tennessee Knoxville, and a Joint Faculty member with the Neutron Scattering Division at Oak Ridge National Laboratory. She works at the intersection of functional energy materials research and the advancement of x-ray and neutron scattering methods. This includes ventures to understand and control local to long-range ordering in ferroelectric ceramics, energy conversion materials, and nanoscale catalysts, among other topics. She received her PhD in 2008 from the Materials Department at the University of California, Santa Barbara. Kate was a Director's Postdoctoral Fellow and an Instrument Scientist at the Lujan Neutron Scattering Center, Los Alamos National Laboratory through 2014, and then an Instrument Scientist within the Diffraction Group at Oak Ridge National Laboratory until 2019. She has published more than 140 peer-reviewed journal articles and organized dozens of workshops, schools and tutorial sessions on scattering techniques for the scientific community. She is a recipient of the Department of Energy (DOE) Early Career Award and the NSF Career Award. She received an Exceptional Service Award from the Neutron Scattering Society of America in 2018 and she is a 2019 recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE). Kate lives in Oak Ridge, Tennessee, with her husband, Dr. Michael Crowell, and their children, Wriston (age 11) and Abbie (age 5).