

Tailoring defect-strain coupling of complex oxides for energy conversion and storage

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Solid-state electrochemical devices – electrolysis cells, fuel cells, and batteries – require materials that can transport ions rapidly, catalyze interfacial reactions, and withstand the chemical stresses inherent in operation. These properties derive in part from the types, arrangements, and dynamics of point defects – atomic scale anomalies including vacancies, interstitials, dopants, and electronic species. This talk will focus on our recent work uncovering the relationships between strain, defect equilibria/kinetics, and functional properties in ion-conducting perovskite oxides. Case studies to be highlighted include: 1) lowering deleterious chemical expansivity in ceramics that “breathe,” 2) raising surface catalytic activity through chemo-mechanical actuation, and 3) boosting ionic conductivity through strain engineering. This work involves both bulk ceramic and thin film synthesis, through sol-gel and pulsed laser deposition methods, respectively. We then apply various *in situ* diffraction, spectroscopic, electrochemical, optical, thermogravimetric, and dilatometric characterization methods up to ~1000 °C in precisely controlled chemical potential environments to assess links between defect chemistry, crystal/micro-structure, and resulting functional behavior. By understanding and tailoring chemo-mechanical coupling, we are able to develop new electrodes and electrolytes that are more efficient and durable.