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Title: Theory and microscopy -- complementary tools for energy-related applications

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The talk will describe three examples that illustrate the power of combining atomic-scale density-functional calculations of structural properties of complex systems with scanning transmission electron microscopy and electron-energy-loss spectroscopy (EELS). The examples are chosen to highlight energy applications. Colossal ionic conductivity observed in thin layers of ytrria-stabilized zirconia between layers of strontium titanate is explained by theory in terms of a highly disordered oxygen sublattice and confirmed by microscopy and EELS; segregation of Fe antisites in select Li ion diffusion channels in the battery cathode material LiFePO4 is explained by theory in terms of a dynamic energy-lowering process that is unique to systems with one-dimensional diffusion channels and EELS corroborates the theoretical results; the mechanism of the observed white light emission by ultrasmall CdSe is traced by a combination of theory and microscopy to an inherent fluxionality that causes a continuously varying energy gap.
Collaborators: T. J. Pennycook, J. Lee, J. C. Idrobo, M. Varela and S. J. Pennycook. The work is supported by the US Department of Energy Basic Energy Sciences, Materials Science and Engineering Division and by DOE grant DE-FG02-09ER46554.