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**Atomic Order Modeling of Nanodomains in Solid-Oxide Fuel Cell Materials**[1] PAUL DALACH, DON ELLIS, Northwestern University, AXEL VAN DE WALLE, California Institute of Technology — Yttria-stabilized zirconia (YSZ), $(La_x,Sr_{1-x})(Fe_y,Cr_{1-y})O_{3-z}$ (LSFCr), and $(La_x,Sr_{1-x})(Ru_y,Cr_{1-y})O_{3-z}$ (LSRCr) were modeled using first principles Density Functional theory (DFT) and DFT-derived thermodynamic statistical cluster expansion methods. Cluster expansions were trained using theoretical structural energies to develop semi-analytical energy expressions for each material's configuration space.[2] A lattice Monte Carlo algorithm was used to thermally equilibrate structures of fixed concentration. Thermally equilibrated atomic ordering data were analyzed to reveal nanodomains below current experimental diffraction resolution limits and correlate local atomic features to material properties, such as aging and ionic diffusion in YSZ and B-site metal precipitation in the lanthanum perovskites.

[1]US DOE-BES
[2]A. van de Walle, Nature Materials 7, 455 - 458 (2008)

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