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Defect-Induced Segregation and Lattice Stability of BSCF Perovskites[1] MAIJA KUKLJA, ONISE SHARIA, Materials Science and Engineering Department, University of Maryland, College Park, MD, USA, YURI MASTRIKOV, Institute for Solid State Physics, University of Latvia, Kengaraga str. 8, Riga LV-1063, Latvia, EUGENE KOTOMIN, Max Planck Institute for Solid State Research, Heisenbergstr., 1, D-70569, Stuttgart, Germany — Among novel advanced materials for clean energy, $\mathbf{Ba}_x\mathbf{Sr}_{1-x}\mathbf{Co}_{1-y}\mathbf{Fe}_y\mathbf{O}_{3-\delta}$(**BSCF**) are considered as promising materials for cathodes in solid oxide fuel cells (SOFC) and oxygen permeation membranes. BSCF exhibits a good oxygen exchange performance, mixed ionic and electronic conductivity, high oxygen vacancy concentration, and low diffusion activation barrier, which largely define the oxygen reduction chemistry. However, understanding the interplay between the structural disorder and crystalline stability in BSCF is extraordinarily complex and essentially unexplored. We present first principles calculations of an ideal BSCF crystal and the crystal containing point defects, Frenkel and Schottky disorders, cation and antisite exchanges, and a set of relevant solid-solid solutions. We discuss possible mechanisms of defect-induced (in)stability, solid-state decomposition reactions, and phase transitions of the BSCF lattice as a function of oxygen vacancy concentration for cubic and hexagonal BSCF in the context of available experiments. This research explains the observed SOFC performance reduction and provides insights on enhancing energy conversion.

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