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Digital Layered-Manganites: Madelung Energy Effects on Atomic Structure and Properties B. NELSON-CHEESEMAN, MSD, Argonne Natl Lab, J. RONDINELLI, MSE, Drexell Univ, H. ZHOU, APS, Argonne Natl Lab, M. NIKIFOROV, CNM, Argonne Natl Lab, E. BARNES, MSE, Penn State Univ, A. SHAH, MRL, Univ of IL Urbana-Champaign, S. BADER, MSD/CNM, Argonne Natl Lab, V. GOPALAN, MSE, Penn State Univ, A. BHATTACHARYA, MSD/CNM, Argonne Natl Lab — The atomic monolayer control of molecular beam epitaxy allows one to explore non-equilibrium dopant-cation configurations in correlated oxide thin films, enabling new electronic phases and magnetic properties to emerge. We report the effects of digital A-site cation doping on electronic phase stability and competition in perovskite-derived manganites. In such digitally synthesized films, Madelung energy constraints are expected to play a primary role in minimizing local Coulomb forces. We correlate changes in the electrical and magnetic properties of the ordered manganites and the resulting crystal structures (Mn-O bond lengths and O-Mn-O bond angles) to the compositionally equivalent control films, i.e. those with randomly distributed A-site dopant-cations. DFT calculations predict that these different layering patterns produce different local and extended crystallographic distortions, including a potential multiferroicity induced by a hitherto unknown mechanism. Synchrotron surface X-ray diffraction measurements in combination with COherant Bragg Rod Analysis at the Advanced Photon Source is used to investigate the resulting atomic structure of the different layering variants, while Second Harmonic Generation and Piezoforce Microscopy investigate the ferroelectric properties.

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