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Informatics-aided computational design of functional layered oxides PRASANNA V BALACHANDRAN, Los Alamos National Laboratory, Los Alamos, NM, JOSHUA YOUNG, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, TURAB LOOKMAN, Los Alamos National Laboratory, Los Alamos, NM, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University, Evanston, IL — We discuss a data-driven *ab initio* protocol with predictive capability to design and accelerate the discovery of noncentrosymmetric (NCS) inorganic oxides. Our approach synergistically integrates applied group theory, materials informatics and density functional theory (DFT) to uncover geometry-chemistry-symmetry guidelines for computational design of new NCS materials, specifically oxygen octahedra containing basic building units. Using this approach, we identify new and previously unknown compositions with potential for realizing NCS structures in the bulk n=1 Ruddlesden-Popper (RP) oxides. We then validate our predictions using DFT calculations. Our approach enables rational design and engineering of both crystal structures and functionalities.

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