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High-Throughput Screening of Perovskite Alloys for Piezoelectric Performance and Formability RICKARD ARMIENTO, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden, BORIS KOZINSKY, Research and Technology Center, Robert Bosch LLC, GEOFFROY HAUTIER, Institut de la Matière condensée et des Nanosciences (IMCN), European Theoretical Spectroscopy Facility, Université Catholique de Louvain, Belgium, MARCO FORNARI, Department of Physics, Central Michigan University, GERBRAND CEDER, Department of Materials Science and Engineering, Massachusetts Institute of Technology — We use high-throughput computational density functional theory to screen a large chemical space of perovskite alloys for systems with the right properties to accommodate a morphotropic phase boundary (MPB) in their composition-temperature phase diagram, a crucial feature for high piezoelectric performance. We start from alloy end-points previously identified in a high-throughput computational search. An interpolation scheme is used to estimate the relative energies between different perovskite distortions for alloy compositions with a minimum of computational effort. Suggested alloys are further screened for thermodynamic stability. The screening identifies alloy systems already known to host a MPB, and suggests a few new ones that may be promising candidates for future experiments. Our method of investigation may be extended to other perovskite systems, e.g., (oxy-)nitrides, and provides a useful methodology for any application of high-throughput screening of isovalent alloy systems. Preprint available at <http://arxiv.org/abs/1309.1727>

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