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High-Throughput Density Functional Theory Categorization of Ferroelectric Ternary Perovskite Oxides for Use as High-Performance Piezoelectrics RICKARD ARMIENTO, Massachusetts Institute of Technology, BORIS KOZINSKY, Bosch Research and Technology Center, MARCO FORNARI, Central Michigan University, GERBRAND CEDER, Massachusetts Institute of Technology — We present a nearly exhaustive density functional theory (DFT) survey over the chemical space of perovskite compounds on ABO3 form, with the aim of identifying alloy end points for new piezoelectric materials. Our screening criteria on the DFT results selects 85 relevant compounds, among which all well known alloy end points for high performance piezoelectrics are present. We analyze the compounds with respect to macroscopic polarization, born effective charges, and energy differences between different structure distortions. We discuss the energy features that cause the high piezoelectric performance of the well known piezoelectric lead zirconate titanate (PZT), and to what extent these features are rare among the found compounds. The results are used to discuss relevant isovalent alloys of the selected compounds.

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