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An Automated Ab Initio Framework for Identifying New Ferroelectrics TESS SMIDT, SEBASTIAN E. REYES-LILLO, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab, ANUBHAV JAIN, Material Science Division, Lawrence Berkeley National Lab, JEFFREY B. NEATON, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab; Kavli Energy NanoSciences Institute at Berkeley — Ferroelectric materials have a wide-range of technological applications including non-volatile RAM and optoelectronics. In this work, we present an automated first-principles search for ferroelectrics. We integrate density functional theory, crystal structure databases, symmetry tools, workflow software, and a custom analysis toolkit to build a library of known and proposed ferroelectrics. We screen thousands of candidates using symmetry relations between nonpolar and polar structure pairs. We use two search strategies 1) polar-nonpolar pairs with the same composition and 2) polar-nonpolar structure type pairs. Results are automatically parsed, stored in a database, and accessible via a web interface showing distortion animations and plots of polarization and total energy as a function of distortion. We benchmark our results against experimental data, present new ferroelectric candidates found through our search, and discuss future work on expanding this search methodology to other material classes such as anti-ferroelectrics and multiferroics.

Tess Smidt
Univ of California - Berkeley

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