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An Automated Ab Initio Approach for Identifying Small Band Gap Ferroelectric TESS SMIDT, SEBASTIAN REYES-LILLO, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab, JEFFREY NEATON, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab; Kavli Energy NanoSciences Institute at Berkeley — Small band gap ferroelectrics are scarce and yet hold promise for optoelectronics applications. In this work, we leverage the electronic and symmetry requirements that give rise to ferroelectricity to search for new small band gap ferroelectrics using the Materials Project and Inorganic Crystal Structure Database. We create an automated workflow that combines database queries, symmetry tools and high-throughput DFT to identify candidate classes of ferroelectrics. Using density functional theory and beyond, we reveal accurate band gap trends for new and previously synthesized compounds. The effect of chemical doping on the polarization and energy barrier is discussed for select cases.

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