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The search for multifunctional polar materials JOSEPH BENNETT, KARIN RABE, Department of Physics and Astronomy, Rutgers University — One strategy in the search for new polar semiconducting (and possibily magnetic) materials is to check systems already synthesized and reported as polar in the literature to determine the intrinsic magnitude and switchability of the polarization, the band gap and magnetic properties. In many examples where a polar space group was found, neither polarization or band gap measurements were made because the sample as grown was too conductive. Using a combination of ICSD searching and symmetry analysis, we first identify potentially interesting polar materials and screen out those that are reported to definitely be metallic. We then use first-principles density functional theory (DFT) calculations to investigate the ground state structures of these experimentally synthesized materials for which limited data is available. These calculations will help us to develop criteria for screening candidate systems for polar, magnetic and semiconductive behavior, and broaden the search for new examples of these important functional materials.

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