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Half-Heusler semiconductors as piezoelectrics ANINDYA ROY, UC Santa Barbara, JOSEPH W. BENNETT, KARIN M. RABE, DAVID VANDERBILT, Rutgers University — We use a first-principles rational-design approach to demonstrate the potential of semiconducting half-Heusler compounds as a previously-unrecognized class of piezoelectric materials. We scan a large number of compounds, testing for insulating character and calculating structural, dielectric, and piezoelectric properties. Of the 792 compounds considered, 234 are found to be nonmetallic, of which 189 are further found to be elastically stable. We compare the computed structural parameters to available experimental values for the half-Heusler compounds considered that have been experimentally studied, as reported in the Inorganic Crystal Structure Database. Calculated piezoelectric coefficients (d_{14}) and electromechanical coupling factors (k_{14}) are often high enough to compare favorably with those of piezoelectrics currently in use. We analyze how factors such as electronegativity and ionic radius influence the piezoelectricity of the compound. Moreover, we show that even if toxic or expensive elements are excluded, we are still left with many combinations having reasonably high piezoelectric response. Our results provide guidance for the experimental realization and characterization of high-performance materials of this class that may find practical applications.

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