

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Interpolation schemes for high-throughput prediction of new piezoelectric alloys RICKARD ARMIENTO, Massachusetts Institute of Technology, BORIS KOZINSKY, Research and Technology Center, Robert Bosch LLC, MARCO FORNARI, Central Michigan University, GERBRAND CEDER, Massachusetts Institute of Technology — Systematic discovery of materials with optimized properties based on first principles methodologies requires well-defined descriptors, in addition to the automation infrastructure for calculations and data analysis. We have designed a set of computationally affordable descriptors for enhanced piezoelectric performances and analyzed the chemical space for oxides with the perovskite structure. Our results include phase stability for the most promising compositions and ad hoc interpolation schemes that have been exploited to identify 49 alloys with favorable properties.

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Date submitted: 11 Nov 2011

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