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Structuring Intuition: Strategies to Predict Novel Functions

R. Armiento,(1) B. Kozinsky, (2) G. Hautier, (3) G. Ceder, (3) and M. Fornari

Prof. Marco Fornari
Department of Physics
Central Michigan University

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(1) Linkoping University, Sweden
(3) Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge MA, USA
(2) Research and Technology Center, Robert Bosch LLC, Cambridge MA, USA
(4) Department of Physics, Central Michigan University, Mt. Pleasant, MI, USA.

Abstract: First principles methodologies have grown in accuracy and applicability to the point where systematic searches of novel compositions with optimized properties are within reach. Such searches require well-defined screening criteria for the desired functional properties, high-throughput data generation tools, data structuring and organization, schemes for estimating alloy properties, and strategies to validate the predictions. To design novel lead-free piezoelectrics, for instance, we have distilled specific search criteria for large tetragonal strains and formation of morphotropic phase boundaries (MPB); these include “phase coexistence”, “ion activities” and “structural instabilities” of phase diagram end-points. The quantities have been computed for a large chemical space and quantitative information was organized in a database. We also developed interpolation schemes to predict properties of novel piezoelectric alloys and tested stability. Our search included 3969 perovskitic compounds and pointed to 49 phase diagram end-points and three specific MPB alloy families.