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Thermodynamic Stability of Topological Insulators DEMET USANMAZ, PINKU NATH, JOSE J. PLATA, Department of Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina 27708, USA, GUS L.W. HART, Department of Physics and Astronomy, Brigham Young University, Provo, UT 84602, MARCO B. NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, Denton, Texas 76203, USA, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics, and Chemistry, Duke University, Durham, North Carolina 27708, USA, CENTER FOR MATERIALS GENOMICS TEAM, G. L. W. HART COLLABORATION, M. B. NARDELLI COLLABORATION — Well known three-dimensional TIs such as Bi_2Te_3, Bi_2Se_3, Bi_2Te_2Se, Sb_2Te_2Se, have been the subject of research due to potential application for spintronic devices. TIs have large bulk band gap and metallic surface states at the special time-reversal-invariant momentum (TRIM) points of the Brillouin zone. These fascinating properties constitute the current carry along the surface and not conduct current through the bulk. Creating heterostructures of TIs has recently been demonstrated to be advantageous for controlling electronic properties. In addition to the importance of the electronic properties of materials, thermodynamic stability is the key for manufacturability of materials. Guided by cluster expansion, we have investigated the thermodynamic stability of TI interfaces.

Demet Usanmaz
Department of Mechanical Engineering and Materials Science,
Duke University, Durham, North Carolina 27708, USA

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