Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Design and discovery of heterostructural alloys AARON HOLDER, SEBASTIAN SIOL, PAUL NDIONE, HAOWEI PENG, ANDRIY ZAKUTAYEV, STEPHAN LANY, NREL, BETHANY MATTHEWS, JANET TATE, Oregon State Univ., BRIAN GORMAN, Colorado School of Mines, ROY GORDON, Harvard, LAURA SCHELHAS, MIKE TONEY, SLAC — The tailoring of materials properties by alloying is routinely utilized to design materials for targeted technological applications. Despite the great successes of alloying in isostructural systems, heterostructural alloying remains a fundamentally unexplored area. In heterostructural alloys, the crossover between different crystal structures enables a new parameter for control over structure and properties by variation of the composition. Here, we present a complementary theoretical and experimental investigation of novel semiconducting metal chalcogenide alloys to develop design principles and approaches for utilizing heterostructural alloying as a materials design strategy. We use *ab initio* methods to predict the structural and electronic properties of novel alloys with commensurate and incommensurate lattice symmetries. Non-equilibrium deposition methods are employed to overcome thermodynamic solubility limits and produce metastable thin-film samples across the entire alloy composition range. The prediction, theory-guided combinatorial synthesis, and characterization of heterostructural alloys demonstrate the design and discovery of functional metastable materials. Our approach establishes a new route for the control of structure-property and composition-structure relationships by accessing non-equilibrium phase space to develop new materials with uniquely tailored properties.

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Date submitted: 06 Nov 2015 Electronic form version 1.4