Abstract Submitted
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**Experimental Realization of Theoretically Predicted New Stable Inorganic ABX Materials**[1] ANDRIY ZAKUTAYEV, National Renewable Energy Laboratory, XIUWEN ZHANG, Colorado School of Mines, LIPING YU, University of Colorado, STEPHAN LANY, DAVID GINLEY, National Renewable Energy Laboratory, ALEX ZUNGER, University of Colorado — Inorganic materials with ABX stoichiometry are an important class of compounds that is under research for numerous applications. Systematic search across databases and literature indicates that many ABX materials are unreported [1], for example 29 out of 45 materials in the V-IX-IV 18-electron family. Theoretical calculations reveal that 8 of these V-IX-IV materials are thermodynamically stable, including 4 new materials with half-Heusler structure. Thin film combinatorial synthesis experiments using sputtering, x-ray fluorescence and x-ray diffraction confirm that one of these materials TaCoSn is stable in the predicted half-Hesuler structure. [2] Despite being made of three metallic elements, TaCoSn is a semiconductor, but the band gap of this material is difficult to measure due to a high concentration of interstitial cobalt defects. [1] Adv. Func. Mat. 22, 1425 (2012) [2] J. Am. Chem. Soc. 135, 10048 (2013)

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Andriy Zakutayev
National Renewable Energy Laboratory

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