Abstract Submitted
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Prediction of previously unreported 18-electron ABC materials via first-principles thermodynamics[1] XIUWEN ZHANG, Colorado School of Mines, Golden, CO, ANDRIY ZAKUTAYEV, NREL, Golden, CO, ARPUN NAGARAJA, THOMAS MASON, Northwestern University, Evanston, IL, DAVID GINLEY, National Renewable Energy Laboratory, Golden, CO, ALEX ZUNGER, University of Colorado, Boulder, CO — The eighteen electron s2p6d10 ABC compounds derived from an s2p6 binary plus a column X element such as Ni,Pd,Pt have recently been proposed as new topological insulators and thermoelectric materials. Yet, many potentially stable 18 electron compounds are not reported in standard compilations, raising the question if they are stable or unstable. Here we use "first-principles thermodynamics" [1] to evaluate the thermodynamic stability of the 401 currently undocumented s2p6d10 ABC materials in the groups I-X-VII, II-X-VI, III-X-V, IV-X-IV, II-IX-VII, III-IX VI, IV-IX-V, and V-IX-IV (but excluding the elements Cs, B, Tl, and Po). The calculation follows three steps: (1) Establishing the lowest energy structure of the ternary. (2) Calculating the energies of documented and undocumented potentially competing phases in the A-B-C system. (3) Examining the dynamic stability of the new compound. We report the stable structures, formation enthalpies (corrected for DFT errors) of the new stable compounds, and document the competing phases of the predicted unstable compounds. Recently one of the predicted stable compounds–TaCoSn–has been successfully synthesized. [1] X. Zhang, L. Yu, A. Zakutayev, and A. Zunger, Adv. Funct. Mater. 22, 1425, (2012).

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