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Band-structure predictions for A2BX4 discovery compounds[1] STEPHAN LANY, V. STEVANOVIC, National Renewable Energy Lab., Golden, CO, A. ZUNGER, University of Colorado at Boulder, CO — The inverse design of materials requires to predict the existence and the properties of previously unknown materials. We have performed a computational search for thermodynamically stable materials within the family of A2BX4 compounds (A, B = main group and 3d cations; X = O, S, Se, Te) resulting in the theoretical discovery of about 100 previously unreported compounds. The challenge for the prediction of band-structures and optical spectra is to obtain accurate results for a wide range of materials within a single computational scheme, so that unknown materials can be predicted with confidence. Whereas the main group chalcogenides are rather accurately predicted by many-body GW calculations, large deviations from experiment are observed for many 3d oxides. In particular, we find that the 3d orbitals consistently occur at too high energies, independent on whether they are occupied (e.g., Cu2O) or unoccupied (e.g., TiO2). While the exact nature of these issues are under investigation, we pursue here a pragmatic approach, using attractive on-site potentials with a single parameter for each 3d element, which leads to good agreement with experiment for binary and ternary 3d oxides. We use this approach to predict the band-structures of the discovery compounds.

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