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Electronic structure of Tl2Hg3Te4 and related systems - possible topological insulators ANDREW BACZEWSKI, S.D. MAHANTI, Michigan State University, MERCOURI KANATZIDIS, Northwestern University — Topological insulators (TI) have attracted considerable interest in condensed matter physics in recent years. The origin of TI behavior in 3D systems is band inversion at time reversal invariant points throughout the Brillouin zone, induced by a strong spin-orbit interaction (SOI). Motivated by this physics, we have looked at the electronic structure of $Tl_2Hg_3Te_4$ and related systems focusing on the physics of band gap formation, parentage of near-gap states, and the influence of SOI. Calculations within the GGA give a band gap of 0.48 (0.33) eV in the absence (presence) of SOI, in reasonable agreement with a recent band structure calculation[1]. However, there is no SOI-induced band inversion at the Γ point because the lowest conduction band (LCB), which is mainly Hg s, lies below a Tl p band, suggesting that Tl2Hg3Te4 is probably not a TI. Replacing Hg by other divalent atoms may make the Tl p band the LCB, resulting in a system that may be a TI. To this end, we will discuss the electronic structures of several possible candidates. [1] S. Johnsen, et. al., Chem. Mater., 2011, 23 (19), pp 4375 to 4383

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