II. POSITIVE VERSUS NEGATIVE EFFECTIVE

spin-orbit splitting. The main disadvantages of d orbitals for $\lambda_{so} < 0$ is the small absolute value of their atomic spin-orbit splitting relative to p orbitals with the same principal quantum number.[35] Because of the light anion, this might not appear as an obvious concern. Yet, another pitfall of $5d$ orbitals is the possible intra-atomic mixing in the VBM of p-like states coming from low-lying unoccupied orbitals of the $5d$ elements.[36] Such onsite mixing can be prevented though by the adequate choice of local symmetry, which forbids mixing of p states and d states such as h, O or by placing it next to more electronegative atoms and thereby enforcing the cation role, such as in the case of α-LuPtBi. This design principle suggests that materials involving elements such as Pt (λ_{so}^{5d} 1.5 eV[21]), Ir (λ_{so}^{5d} 1.3 eV[21]), Os (λ_{so}^{5d} 1.06 eV[21]), or Re (λ_{so}^{5d} 0.85 eV[21]) should be considered when searching for new topological insulators. Overall, the Au element occupies

perturbation) as it is the case for crystal-“eld splitting or strain.