

II. POSITIVE VERSUS NEGATIVE EFFECTIVE

spin-orbit splitting. The main disadvantages of orbitals for $\xi_{so} < 0$ is the small absolute value of their atomic spin-orbit splitting relative to 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 orbitals is the possible intra-atomic mixing in the VBM of p -like states coming from low-lying unoccupied orbitals of the 5 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 d_{xy} , or by placing it next to more electronegative atoms and thereby enforcing the anion role, such as in the case of LuPtBi. This design principle suggests that materials involving elements such as Pt ($\xi_{so}^d = 1.5 \text{ eV}^2$), Ir ($\xi_{so}^d = 1.3 \text{ eV}^2$), Os ($\xi_{so}^d = 1.06 \text{ eV}^2$), or Re ($\xi_{so}^d = 0.85 \text{ eV}^2$) should be considered when searching for new topological insulators. Overall, the Au element occupies

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