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Band Gap Engineering via Local Environment in Complex Oxides[1] TINGTING QI, ILYA GRINBERG, ANDREW RAPPE, University of Pennsylvania — We describe how the electronic structure energy level of the recently-developed highly polar tetragonal perovskite oxides, most prominently $Bi(Zn,Ti)O_3$, can be dramatically changed by a simple rearrangement of the B-cation. Using LDA+Hubbard U, we determine the impact of B-site cation ordering, lattice strain, cation identity, and oxygen octahedral cage tilts on the valence and conduction bands. We find that a combination of ultra-high tetragonality and a careful choice of B-cations can lead to changes of 1-2 eV in the band gap for the same composition, through a change in the B-cation ordering alone. We also find that a layered B-cation ordering exhibits high-mobility 2D hole gas (2DHG) behavior. The lower band gaps of the layered B-cation ordering makes these materials suitable for photovoltaic and photocatalytic applications, due to their good match with the solar spectrum. Our analysis of the crystal structure and the valence and conduction bands shows that these unusual effects can be explained in the framework of crystal field theory and underscores the crucial role that ultra-high tetragonality plays in making the band gap sensitive to the B-cation ordering.

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