

origin of the hitherto mysterious difficulty to obtain simultaneously electronic band inversion and thermodynamic stability. We will refer to the electronic structure associated with the geometrical motif shown in Figure 1 (which we will show, enables topological insulation) as the “topological gene.” We then identify the topological gene in oxide perovskites as being a lone-pair electron-rich B atom (e.g., Te, I, Bi rather than Ti, Nb, Y, respectively) at the octahedral site in the cubic ABO_3 . Oxides tend to have larger predicted inversion energies (Δ

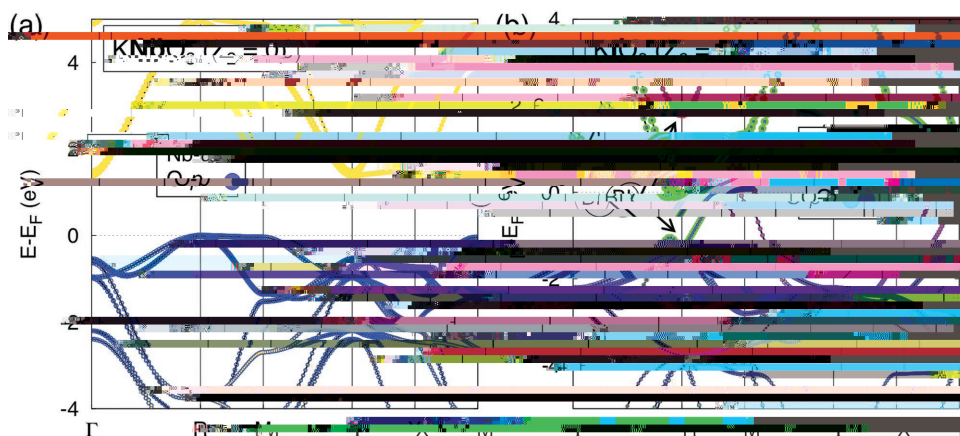


Figure 3. Band structure plots for KNO₃ (Z₂ = 0) and KNO₂ (Z₂ = 4). The Fermi level (E_f) is indicated by a horizontal line, and the topological invariant Z₂ is shown in the top right corner of each plot.

being the lowest-energy structures of specific ABO₃ compounds, relative to the lowest-energy phase. The A position in ABO₃ with the S1 (prototype compound: CaTiO₃) structure is the cube vertices (Ca sites in CaTiO₃) and the B position is part of the BO₆ octahedra (Ti sites in TiO₆ of CaTiO₃), similarly for S2–S15 types. We considered the swapping of A and B elements on the ABO₃ atomic site to create BAO₃, and found that this lowers the energy for 33 structures in our calculations, which are marked by italicized text in Figure 4, meaning that the lowest energy structure is BAO₃. The lattice parameters (as well as band gaps) of the relaxed crystal structures

in Figure 4 are provided in Table S1 (Supporting Information). In addition to stability, Figure 4 also denotes if according to the calculated topological invariant Z₂ the compound is a TI or a normal insulator. We find from such total energy minimizations that the BO₆ octahedral unit with the said electron rich B atom tends to distort toward a stabler, noncubic crystal structure^{31,32} and that this distortion removes the topological insulation. Therefore, the stability gene and TI gene tend to contradict each other for the ABO₃ compounds at ambient conditions: ABO₃ oxides that are stable are not TIs and structures that are TIs are not stable.

II _A	VI _B		VII _B		VIII _B	
	Te	Se	Ti	Sn	Ga/In	Al/Sb
Ba	BaTeO ₃	BaSeO ₃	BaTiO ₃	BaSnO ₃	BaGaO ₃	BaAlO ₃
	<i>S1 (26): NI</i>	<i>S1 (26): NI</i>	<i>S1 (26): NI</i>	<i>S1 (26): NI</i>	<i>S1 (26): NI</i>	<i>S1 (26): NI</i>
	S2 (76): NI	S3 (37): NI	S4 (37): NI	S5 (37): NI	S6 (37): NI	S7 (37): NI
	S8 (37): NI	S9 (37): NI	S10 (37): NI	S11 (37): NI	S12 (37): NI	S13 (37): NI
	S14 (37): NI	S15 (37): NI	S16 (37): NI	S17 (37): NI	S18 (37): NI	S19 (37): NI
Sr	SrTeO ₃	SrSeO ₃	SrTiO ₃	SrSnO ₃	SrGaO ₃	SrAlO ₃
	<i>S1 (232): NI</i>	<i>S1 (232): NI</i>	<i>S1 (232): NI</i>	<i>S1 (232): NI</i>	<i>S1 (232): NI</i>	<i>S1 (232): NI</i>
	S2 (43): NI	S3 (43): NI	S4 (43): NI	S5 (43): NI	S6 (43): NI	S7 (43): NI
	S8 (43): NI	S9 (43): NI	S10 (43): NI	S11 (43): NI	S12 (43): NI	S13 (43): NI
	S14 (43): NI	S15 (43): NI	S16 (43): NI	S17 (43): NI	S18 (43): NI	S19 (43): NI
Ca	CaTeO ₃	CaSeO ₃	CaTiO ₃	CaSnO ₃	CaGaO ₃	CaAlO ₃
	<i>S1 (70): NI</i>	<i>S1 (70): NI</i>	<i>S1 (70): NI</i>	<i>S1 (70): NI</i>	<i>S1 (70): NI</i>	<i>S1 (70): NI</i>
	S2 (52): NI	S3 (52): NI	S4 (52): NI	S5 (52): NI	S6 (52): NI	S7 (52): NI
	S8 (52): NI	S9 (52): NI	S10 (52): NI	S11 (52): NI	S12 (52): NI	S13 (52): NI
	S14 (52): NI	S15 (52): NI	S16 (52): NI	S17 (52): NI	S18 (52): NI	S19 (52): NI

Figure 4. Crystal structures of ABO₃ compounds. The table lists the ABO₃ compounds, their topological invariant Z₂, and their stability status (NI for normal insulator, TI for topological insulator). The structures are color-coded: blue for normal insulators and red for topological insulators. The topological invariant Z₂ is shown in the top right corner of each cell.

demonstrate that the cubic perovskite (S1, see red squares in Figure 7a,b) tends to be stabilized by external pressure. At pressure of 15 GPa (35 GPa), the S1 phase that contains the topological gene becomes the lowest-enthalpy structure for BaTeO_3 (RbIO_3). We further check the effect of external pressure on the band inversions in cubic BaTeO_3 and RbIO_3 , finding that the band inversion is not removed by external pressure (see Figure 7c,d), but on the contrary, increased by the pressure from 2.3 eV at 0 GPa to 3.4 eV at 35 GPa for BaTeO_3 , and from 3.0 eV at 0 GPa to 3.8 eV at 35 GPa for RbIO_3 .

unstable than band-inverted oxides is because destabilizing band inversion drives structural distortions that often remove the topo-

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