False metals, real insulators, and degenerate gapped metals

[redacted]

[redacted]

"acceptor state" inside the principal band gap if its formation costs a "reconstruction (rec) energy" $|E_{rec}|$ that is smaller than the energy gained by transferring q electrons from the conduction band to these lower energy acceptor states $|q\Delta E|$, where ΔE is the band energy difference for electrons in the conduction/valence band and localized states. In general, spontaneously formed acceptor states may be [illegible] (e.g., cation vacancies) as in $BaNbO_3$, $Ca_6Al_7O_{16}$, and $Ag_3Al_{22}O_{34}$ and lead to (i) the observed off-stoichiometry even at low temperatures,[23,28–31] (ii) reduced metallicity and, at the extreme, even to (iii) the emptying of the conduction band and thus a metal to insulator transition. But such acceptor states may also be [illegible],

While recently developed open access databases[20,43–45] of elec-

standard tight binding,[47] k·p,[48,49]

It turns out that each of these symmetry-breaking modalities can result in energy lowering, leading to local symmetry breaking. The electronic structure can react to the existence of such distributions,

XC density-functional (i.e., SCAN) without an on-site interelectronic repulsion, i.e., $= 0$ eV. $CuBi_2O_4$ is also a wide band gap magnetic insulator, which recently attracted significant attention for catalysis,[97] thus suggesting that eight-band fermions near the Fermi level found in hypothetically nonmagnetic $CuBi_2O_4$ are not likely to be realized.

B. Local spin motifs: Allowing for a polymorphous spin network can convert a false metal to a real paramagnetic insulator

Paramagnetic (PM) compounds have non-zero local but zero total magnetic moments. Until recently, the properties of such systems have been explored as properties of globally average nonmagnetic structures [Fig. 7(a)],[14,92,98–101] leading invariably to metallic prediction in contrast with the known insulating properties of many if not most PM ABO_3 phases. Because of this, there has been a long-term belief that many properties of PM systems cannot be described within DFT methodology, and higher-order methods [e.g., dynamical mean-field theory (DMFT)

$SrBiO_3$ as a topological compound, but this structure is not the stable phase.

: Fig. 9(d) illustrates how the formation

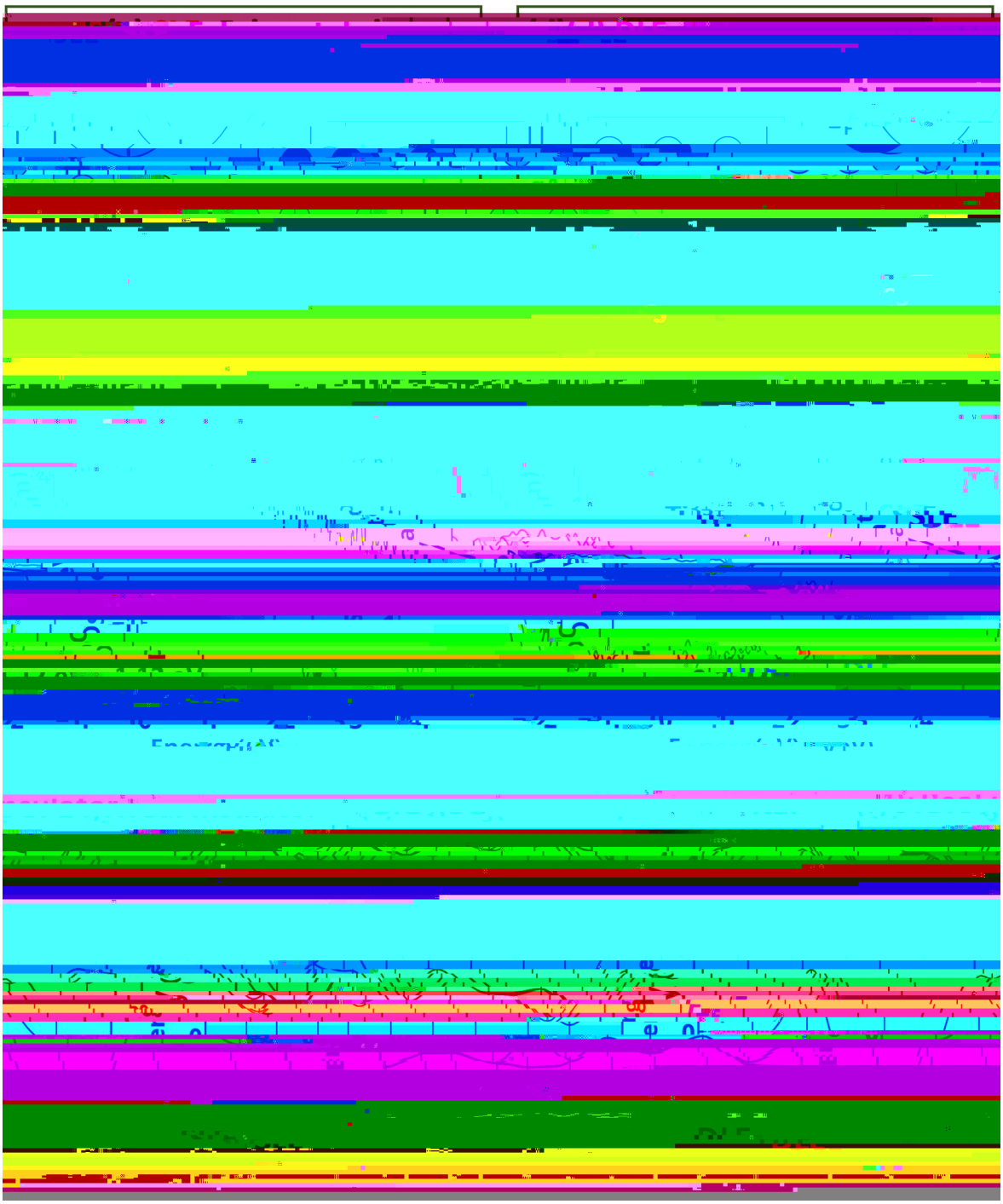

FIG. 9. A (LSE), ( ) ( ) ( ) ( ) (D E) ( ) ( ) ( )
S LSE 16 .
T 2 (S 12) L ( ) P3E+ S G
LSE S 3 (S 221) F ( ) S .( )
G 16 T 2 (S 12) E
T D E. . 114. ( ) P3E+ S G
D E S 3 (S 14) T
( ) 0.26 S

conflict with available experimental data showing that the compound is an AFM insulator with a wide band gap at low temperature.[129]

conductors [Fig. 11(c)], the formation of donor vacancy results in the moving electrons from the donor level to the hole states in the valence band, which can restore the part of the energy needed to form the vacancy. Similarly, for n-type degenerate gapped metal [Fig. 11(d)], the formation of acceptor vacancy can result in decay of conducting electrons to the acceptor level restoring part of the energy needed to create the vacancy. Such electron–hole recombination can result in spontaneous vacancy formation, which can induce significant deviation from stoichiometry at low-temperatures.[23,31,139,140] To examine the possibility of the instability of stoichiometric Ba_4As_3 and $Ag_3Al_{22}O_{34}$, we study the formation of As vacancy (donor) in the Ba_4As_3 and Ag vacancy (acceptor) in $Ag_3Al_{22}O_{34}$. Taking into account all experimentally known stoichiometric phases in Ba–As and Ag–Al–O phases, the range of chemical potentials for stability of Ba_4As_3 and Ag_3Al_{22}

results suggest that both compounds are unstable with respect to

(see below TiO_2:Li) behaving as a defect level, except that the defect here is ▯▯▯ *c*. This situation is common when the localizing sublattice atom can exist in more than one FOS, such as Ti^{3+} and Ti^{4+}. In the dilute defect limit, this latter situation is often discussed as polaron—a quasiparticle originating from the interactions of electrons/holes with a lattice ion, often causing local distortions.[148,149]

formation of h-trapped states in Figs. 6(e), 8(b), and 9(f). Here, $YNiO_3$ and $SrBiO_3$ are the compounds having disproportionation in the low-

correlated systems: Dynamical mean-field theory," J. Phys.: Condens. Matter 9, 7359 (1997).
[105]T. Yoshida, A. Ino, T. Mizokawa, A. Fujimori, Y. Taguchi, T. Katsufuji, and Y.

[149]T. Holstein, “Studies of polaron motion: Part I. The molecular-crystal model,” Ann. Phys. 8, 325 (1959).
[150]A. R. Elmaslmane, M. B. Watkins, and K. P. McKenna, “First-principles modeling of polaron formation in TiO_2 polymorphs,” J. Chem. Theory Comput. 14, 3740 (2018).
[151]A. C. M. Padilha, H. Raebiger, A. R. Rocha, and G. M. Dalpian, “Charge storage in oxygen deficient phases of TiO_2: Defect Physics without defects,” Sci. Rep. 6, 28871 (2016).
[152]J. P. Allen and G. W. Watson, “Occupation matrix control of d- and f-electron localisations using DFT + U,” Phys. Chem. Chem. Phys. 16, 21016 (2014).
[153]G. F. Koster and J. C. Slater, “Simplified impurity calculation,” Phys. Rev. 96, 1208 (1954).
[154]