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ELECTRONIC STRUCTURE AND STABILITY OF I-II-V FILLED TETRAHEDRAL COMPOUNDS

INVITED PAPER

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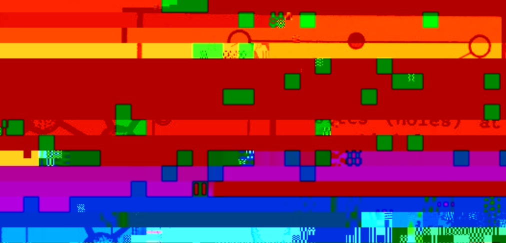
[illegible] possible phases and the electronic structure [illegible] a simple rule developed to understand [illegible]

[illegible] type binary crystals are the most [illegible] packed of all [illegible] tetrahedral coordination for both types of atoms [1]. Their openness [illegible] atomic spheres [illegible] the unit cell is .34, less than half that for the close-packed elements [illegible]



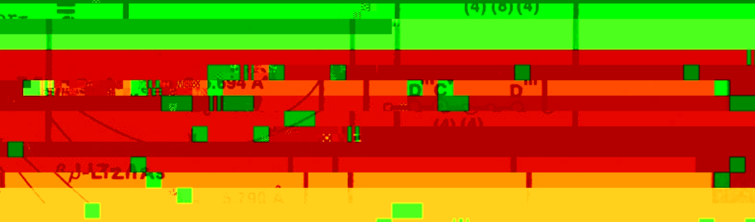
[illegible] sites (holes) at the te[illegible] neighbor tetrahedral distance [illegible]

sites (e.g., the B32 Zintl compounds[5] LiAl, NaTl, or the L2 Heusler al-
loys[6a,b,c] V_CMnAV_A, with V_A=V_C=Co,Ni,Cu,Pd and ... ,In,Sb,Sn). We refer to the structures with partially or completely occupied V_A and V_C sites as "filled tetrahedral structures" (FTS).

NOWOTNY-JUZA COMPOUNDS

The Nowotny-Juza compounds[9], henceforth denoted $A^IB^{II}C^V$ (e.g, LiZnAs), comprise a special cla...

... with B^{II} at the origin τ_1 and C^V at τ_2, ... (A) at the tetra- ... at τ_3 or at τ_4. We de-



... will call the α phase, ... and

Lattice Constant (Å) Atomic Positions

...bstitution of one type of va-
...ound [2] ...

...calculation of the three possible ... phases of a prototypical
..., the ...
...ution of both types of vacant ... We also ...

...recently-developed ... interstitial in- ... denoted $A^{I}B^{II}C^{V}$ (e.g., ... section ... to understand the distortions induced in ... zincblende III-... V-like band structure ... upon inserting He or Li-like atoms. [We refer the reader to Refs. 7-9 for ...

... equilibrium ... equilibrium ...

[illegible] (i) the Zn-As bonds in the α and β [illegible]

[illegible] all exhibit [illegible] local maxima along the bonds), whereas the Li-As bond is almost purely ionic (with no maxima anywhere along the bond direction). This material can [illegible]

[illegible] phase), indicative of a [illegible] structure. The stability of [illegible] α over the [illegible] both of its superior electrostatic stab[illegible]

[illegible]itional stabilization of this [illegible] β phase is hence a [illegible] [illegible]ity and the existence of residual [illegible]

[illegible]ce of extra charge on the Li-As bond relative to the GaAs structure reveal[illegible]s that it originates from the re[illegible] side [illegible] valence charge of Li. Following a transfer of most of its valence electron to the Zn-As bond [illegible] [illegible]d) Li sublattice remains weakly at-[illegible]

[illegible] character of α and β LiZnAs (or. [illegible] the (fictitious) transmu-

, in a two-step process.

Second, trans-

at its interstitial lattice

The great similarity between the band-structure of

ducting phases and that of a III-V deserves further comment.

... low charge density. This figure suggests the lowest conduction bands will show extreme selectivity ... respect to insertion ... atoms ...

... (minima) at ...

... of classifying the ... extended conduction ...

... example ... whereas the lowest conduction band at X for GaP (X ...

closed within

...nd the hypo-

thetical zinc [illegible]ende compound [illegible] (Fig. 5b) [illegible] be a direct band gap semi-

[illegible]

tight-binding viewpoint

[illegible] more weakly [illegible] substitution since
like conduction st[illegible]
their associated charge densities are more [illegible]
[illegible] directly illustrates the [illegible]
[illegible] ar character [illegible]

[illegible]

[1] E. Parthé, Z. Krist 115, 52 (1961), and Crystal Chemistry of [illegible]
ral Structures (Gordon [illegible]

[illegible] 360 (196[illegible]