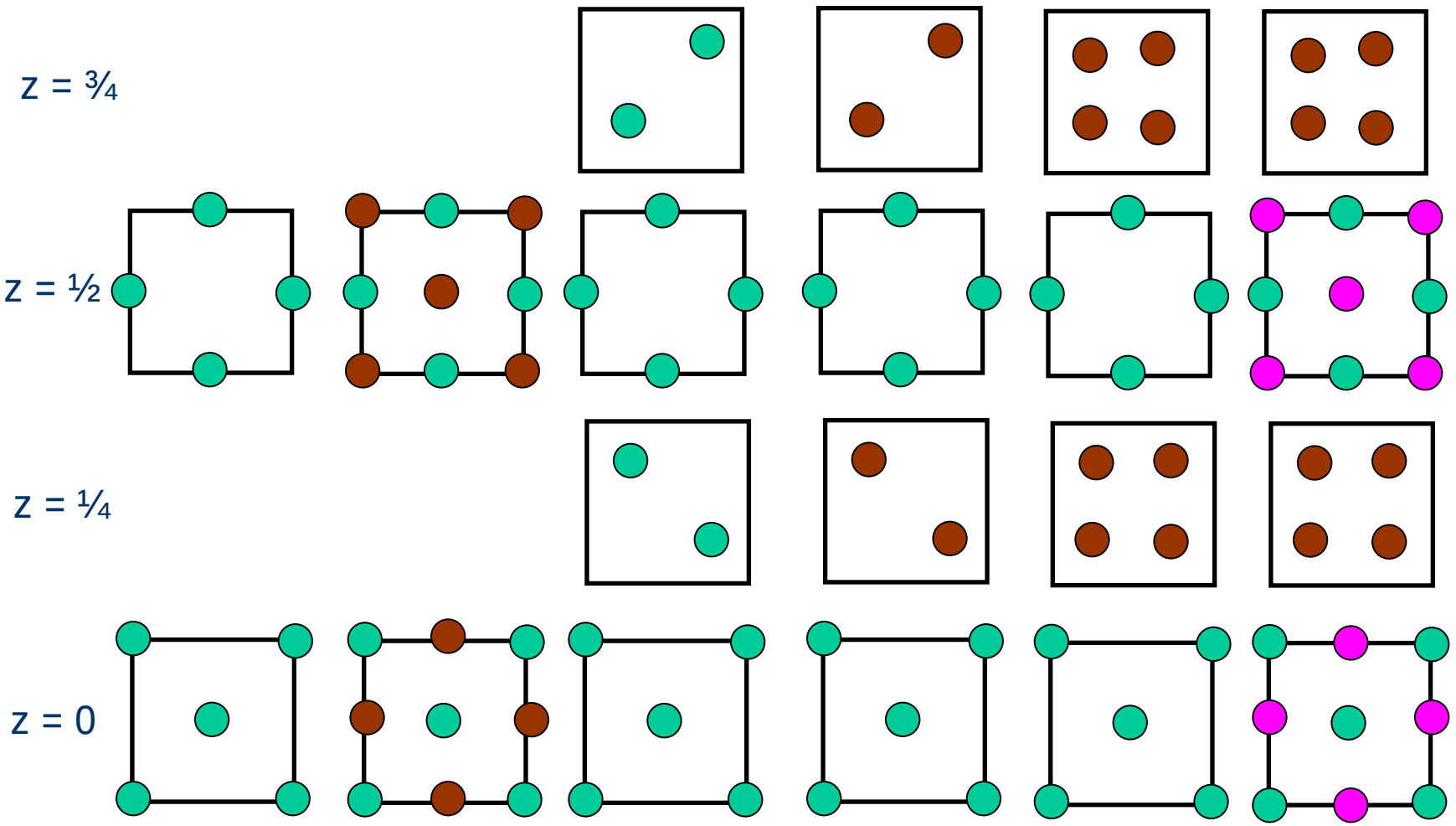
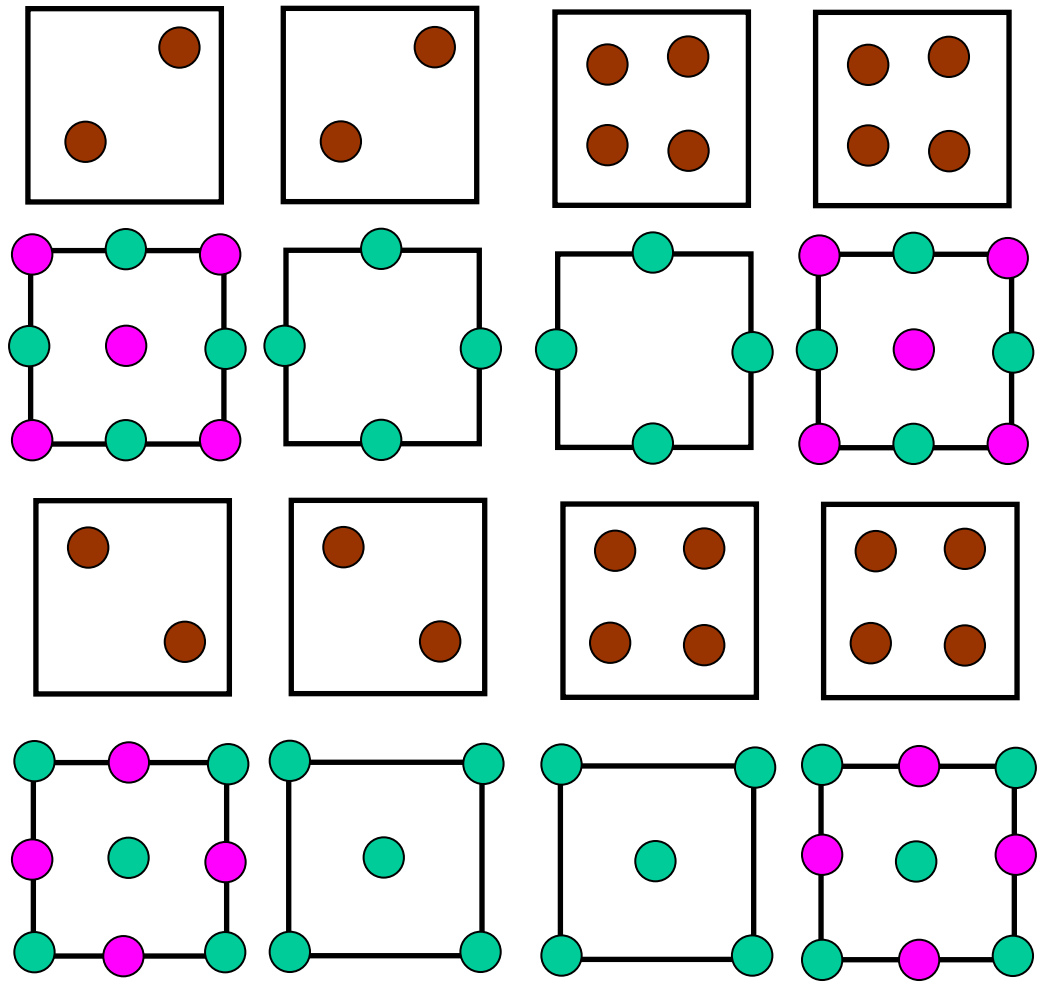
Class 10: Half-Heuslers, Heuslers, half-metallic ferromagnetism



Class 10: Half-Heuslers, Heuslers, half-metallic ferromagnetism



half-Heusler *F-43m* | zinc blende *F-43m* | fluorite *Fm-3m* | Heusler *Fm-3m*

Heusler compounds comprise four interpenetrating *fcc* lattices.

The first Heuslers compounds, including $MnCu_2Al$ [P. Heusler, *Verh. Deutsch Phys. Ges.* **5** (1903) 219] were of great interest when discovered, because they were ferromagnetic in the absence of "ferrous" elements.

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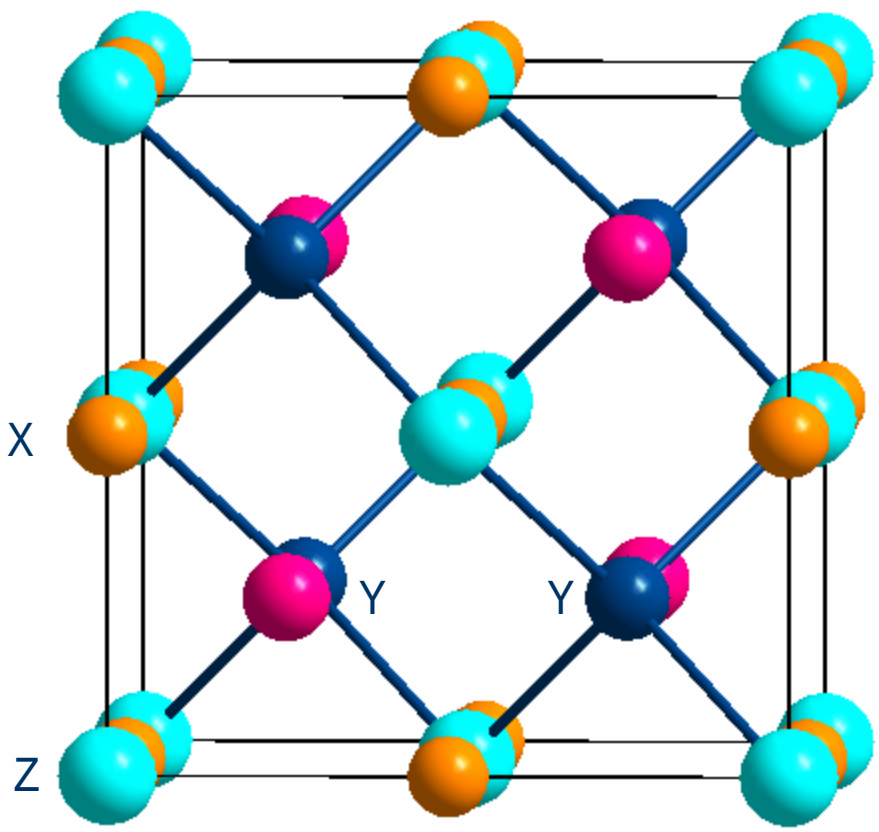
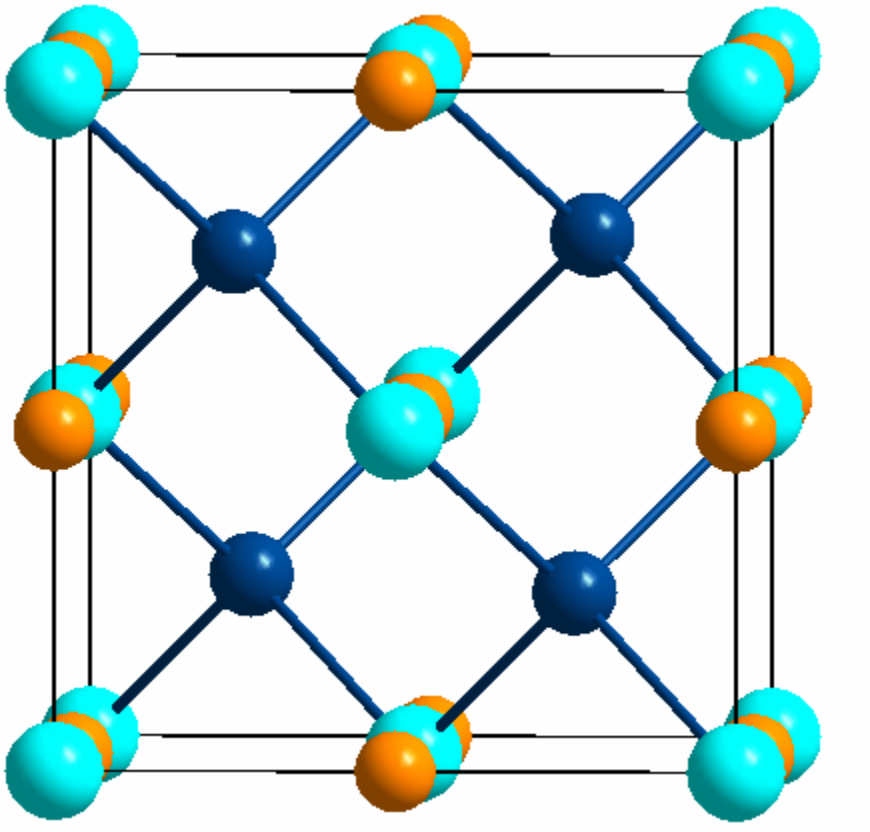
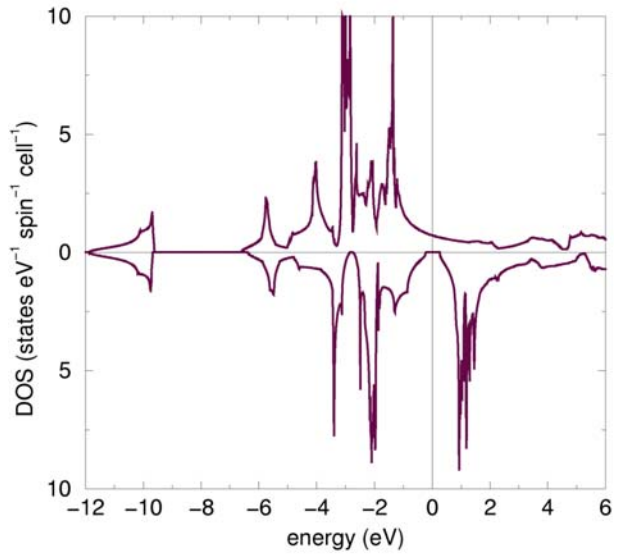


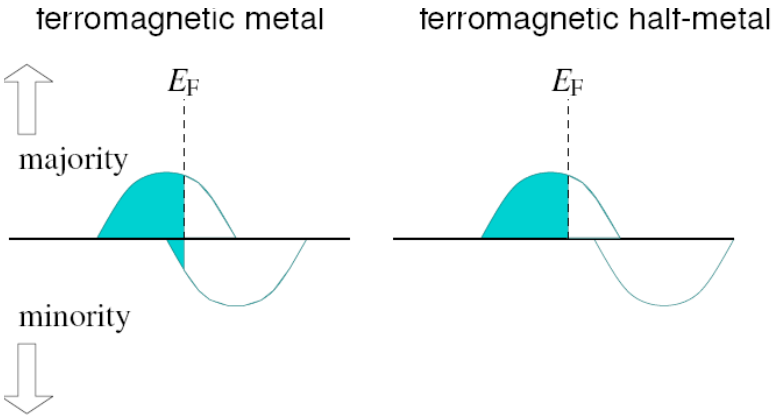
XY_2Z Heusler



XYZ half-Heusler

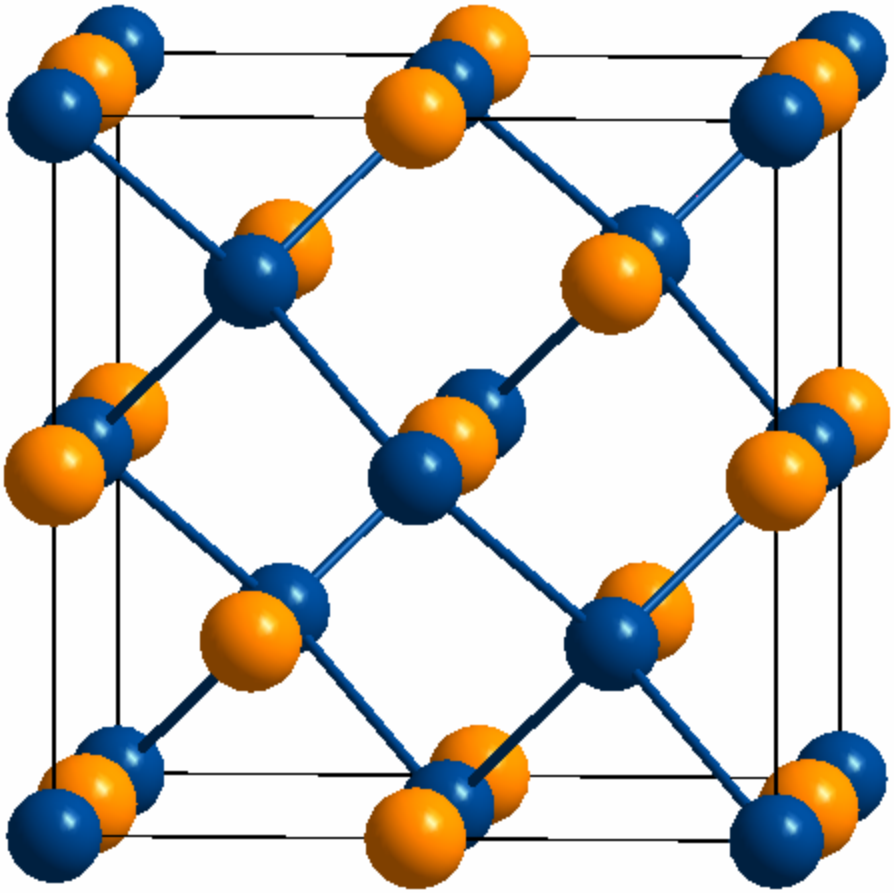
Half-Heuslers (also labeled $C1_b$, and MgAgAs)





MnNiSb (deGroot 1983) has states at the Fermi energy only in one spin direction, and is gapped in the other. The calculated magnetic moment is precisely 4 μ_B

New class of materials: Half-metallic ferromagnets, *Phys. Rev. Lett.* **50** (1983) 2024.



The Zintl-Klemm concept and valence compounds: The example of LiAl (Li^+Al^-). Al^- is isoelectronic with C and forms a diamond lattice. The Li^+ ions stuff the Al^- lattice. Note the 8 electron rule operates.

The contribution of Whangbo *et al.* (2000) Galanakis *et al.* (2002):

Instead of 8 electrons, 18 valence electrons suggests a gap. For example, TiNiSn and TiCoSb are 18 electron semiconductors.

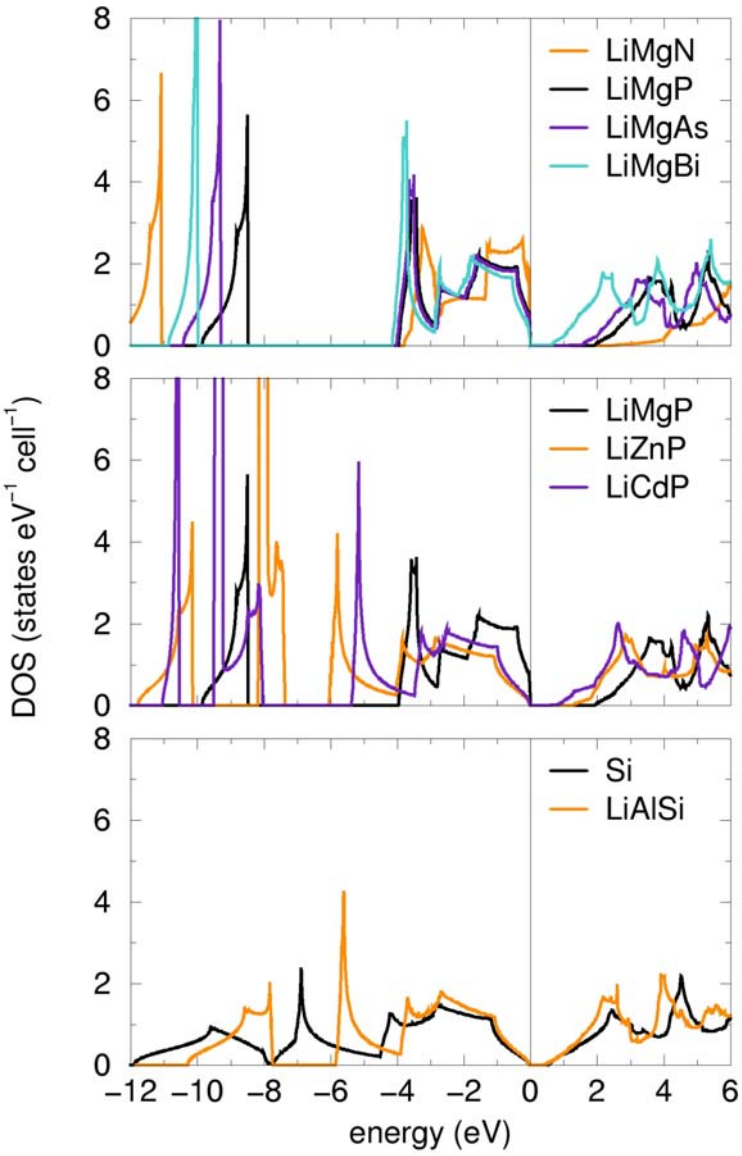
TiCoSb = Ti^{4+} + $(CoSb)^{4-}$; $(CoSb)^{4-}$ = GaSb forming a zinc-blende lattice. Ti is in the octahedral hole.

$18e^-$ = d^0 + d^{10} + s^2p^6 Magnetic compounds (Whangbo):

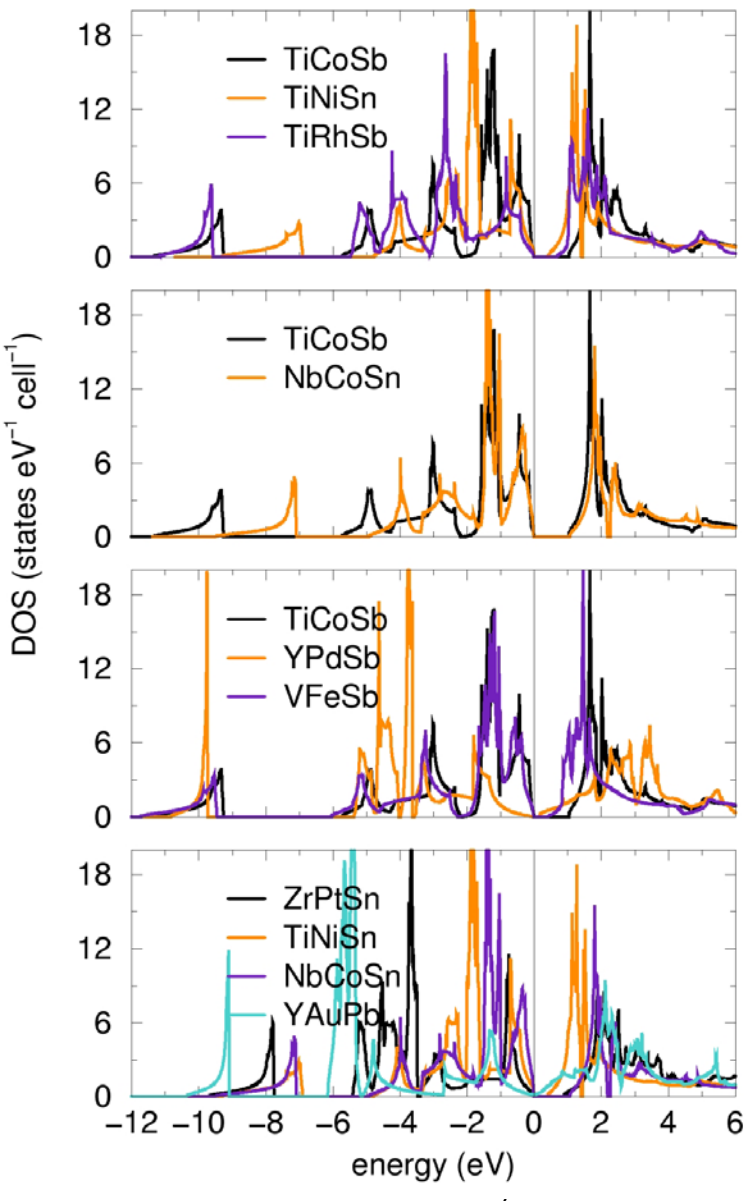
If the number of electrons is 17 or 19, a paramagnet or a Stoner ferromagnet results depending on the DOS at the Fermi energy. If it is 22 (MnNiSb), a local-moment ferromagnet is formed.

Class 10: Half-Heuslers, Heuslers, half-metallic ferromagnetism

8 electron



18 electron



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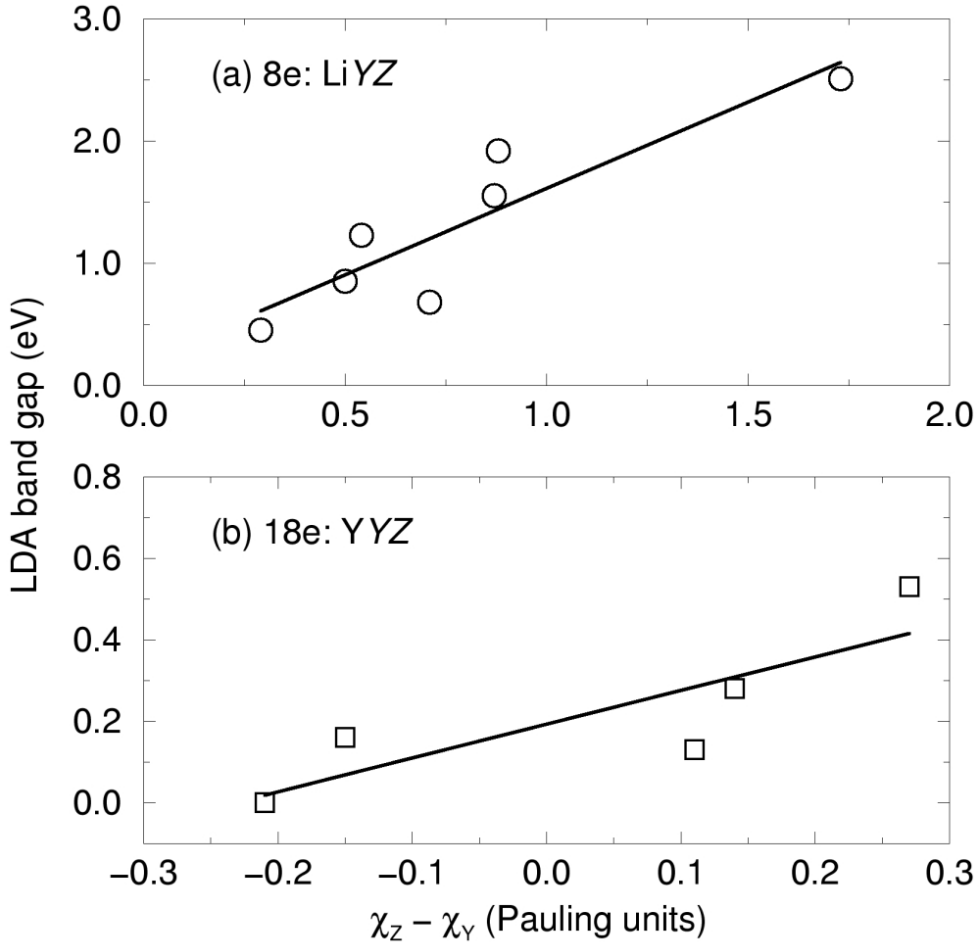
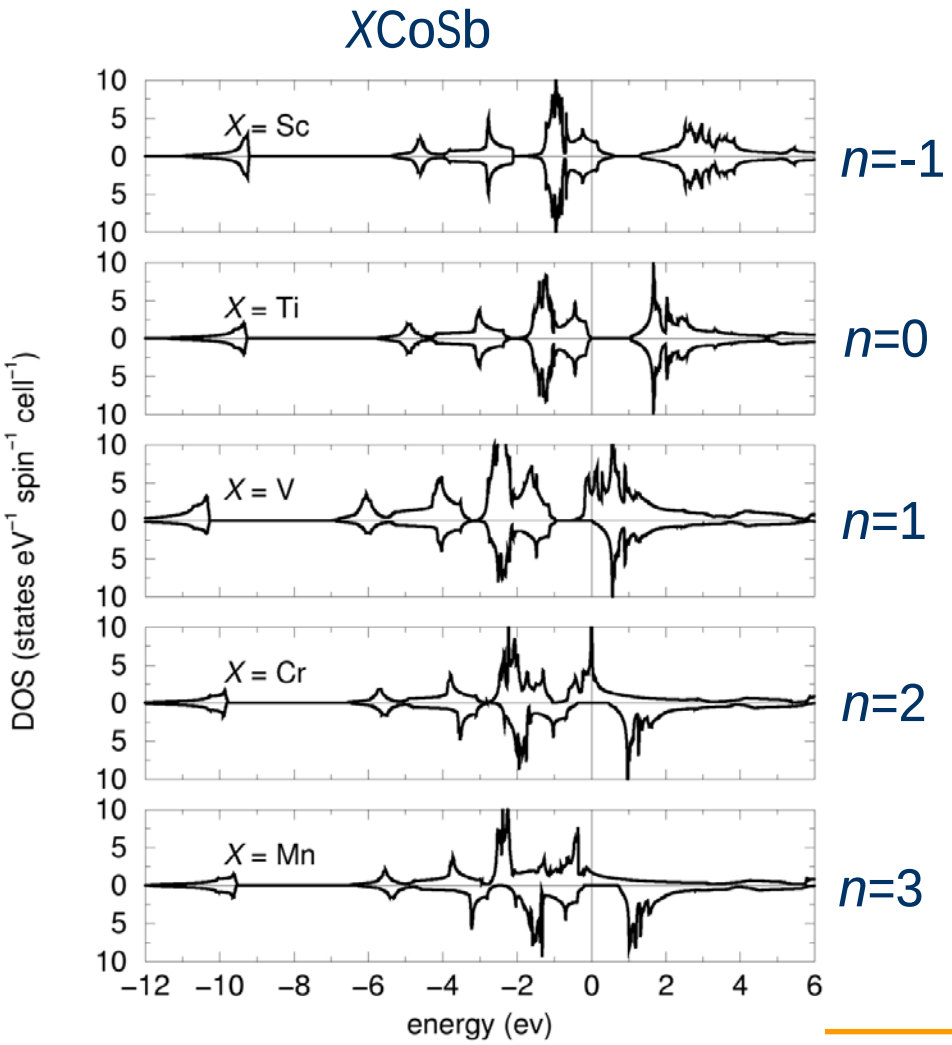
ri x6129 seshadri@mrl



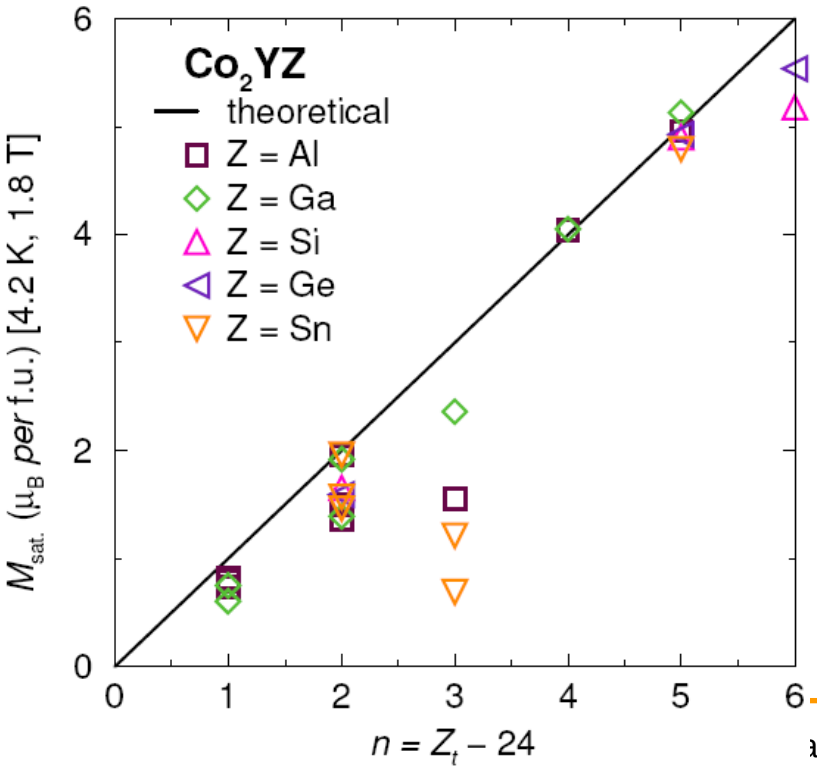
The band gaps of some 8*e* and 18*e* half-Heuslers depend on the electronegativity of the ions in the zinc-blende framework.



Magnetic compounds: 18*e* is a non-magnetic semiconductor. The rest are magnetic half-metals.

Heuslers: The 24 electron rule: [Galanakis, Dederichs, Papanikolau, *Phys. Rev. B* **66** (2002) 174429], Slater-Pauling behavior and the origin of the half-metallicity of the full-Heulser alloys

$M_t = Z_t - 24$



Data from Buschow *et al. J. Magn. Magn. Mater.* **38** (1983) 1.