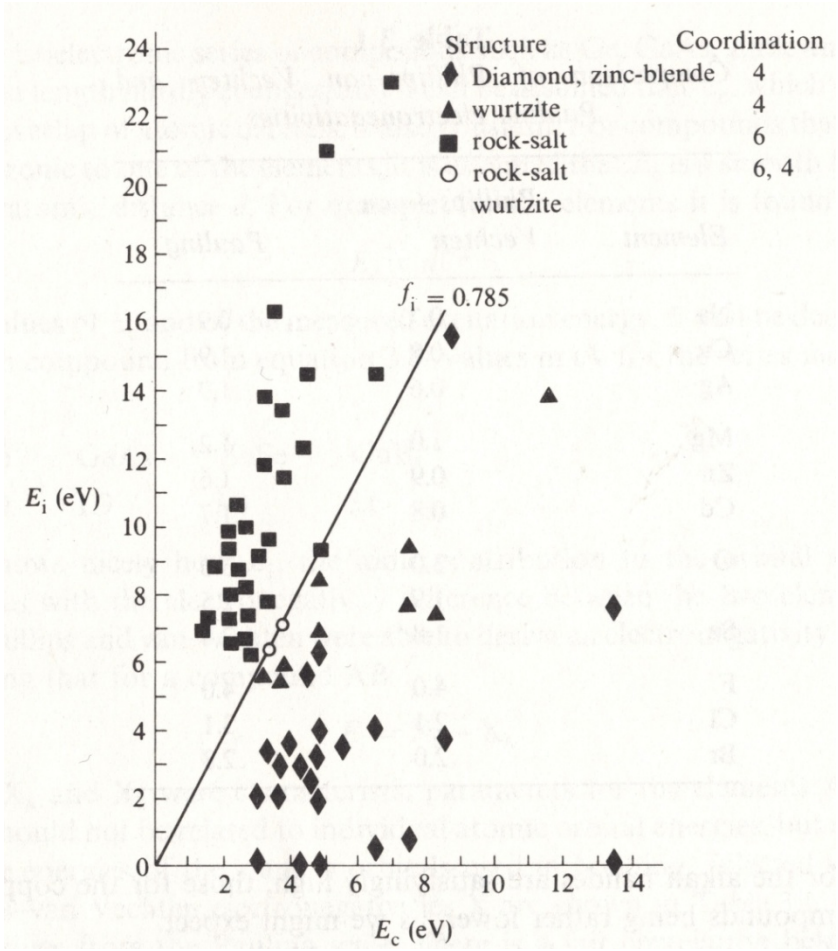
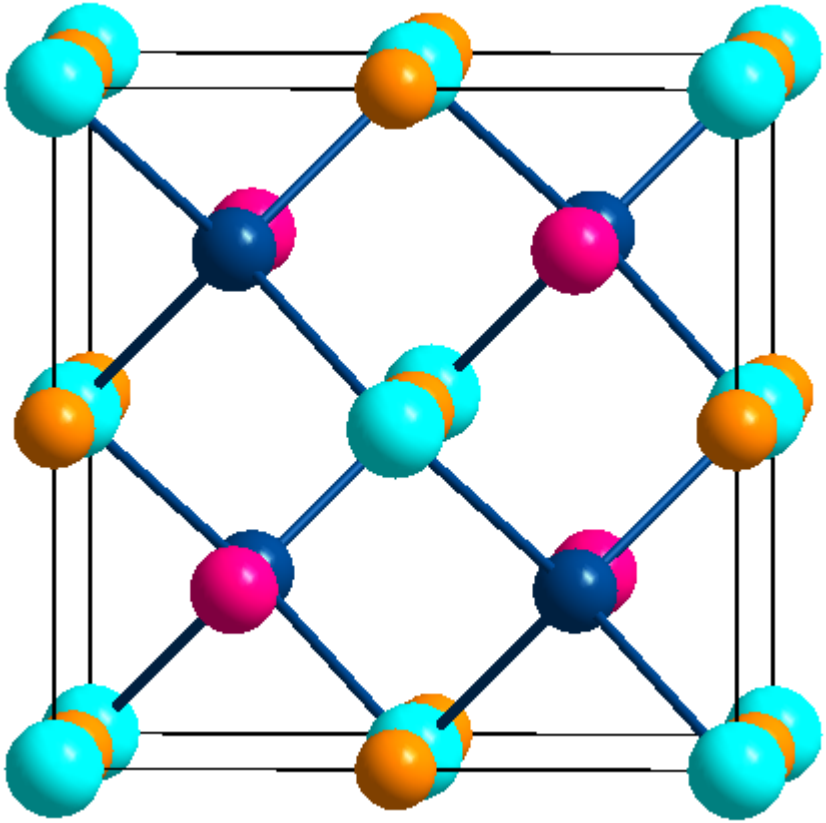
Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

Semiconductors: Structure sorting (Phillips-van Vechten)

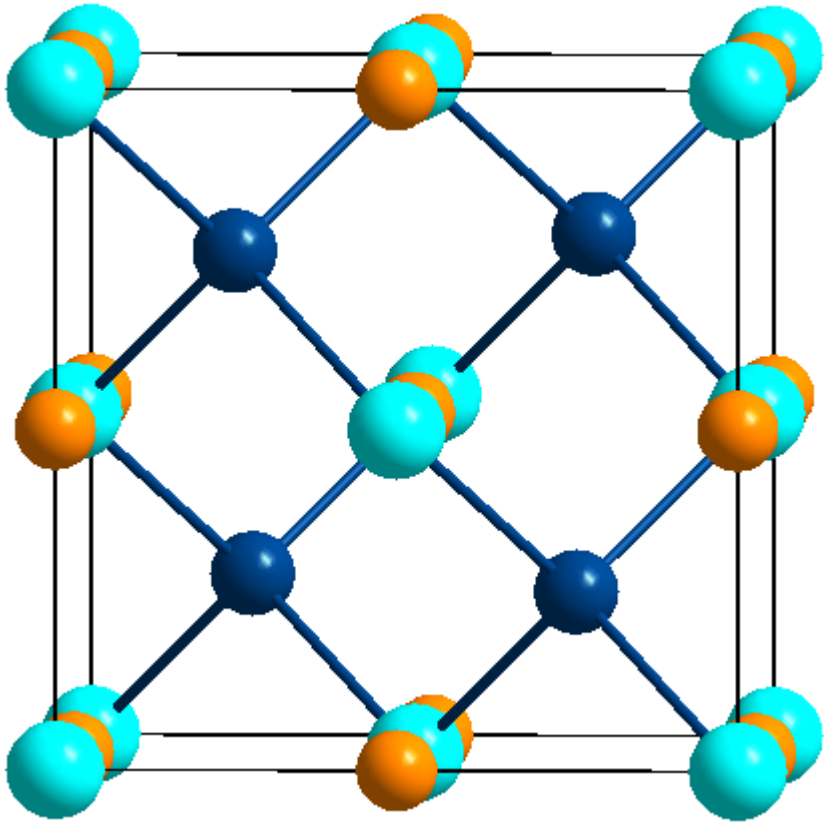


Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



The Heusler crystal structure: XY_2Z
F. Heusler (1903)
4 interpenetrating fcc lattices.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

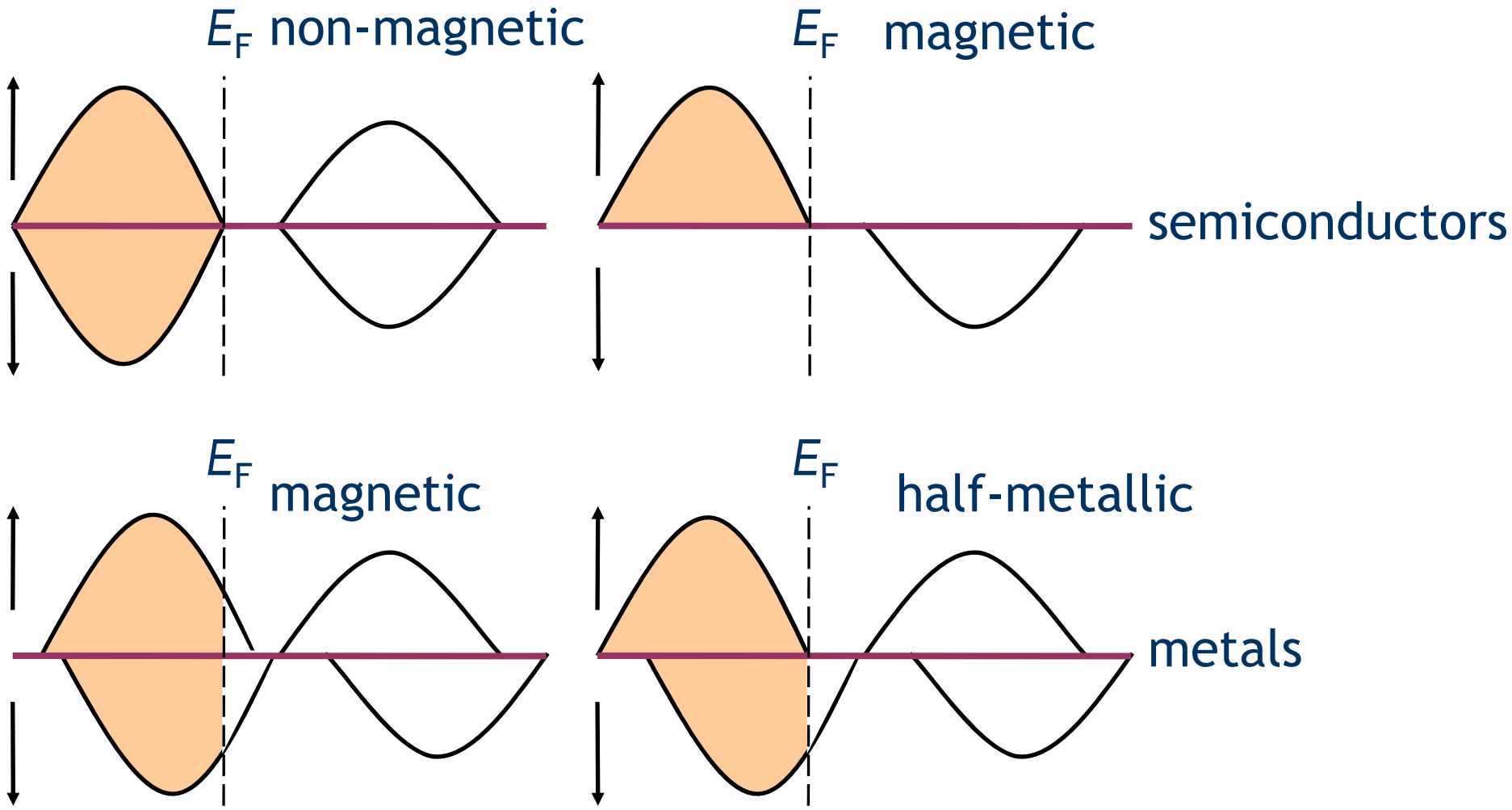


The half-Heusler crystal structure: XYZ. 3 interpenetrating fcc lattices.

AXZ rock-salt with Y in one of the tetrahedral voids.

YZ zinc-blende with X in an octahedral void.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

VOLUME 50, NUMBER 25 PHYSICAL REVIEW LETTERS 20 JUNE 1983

New Class of Materials: Half-Metallic Ferromagnets

R. A. de Groot and F. M. Mueller
Research Institute for Materials, Faculty of Science, Toernooiveld, 6525 ED Nijmegen, The Netherlands

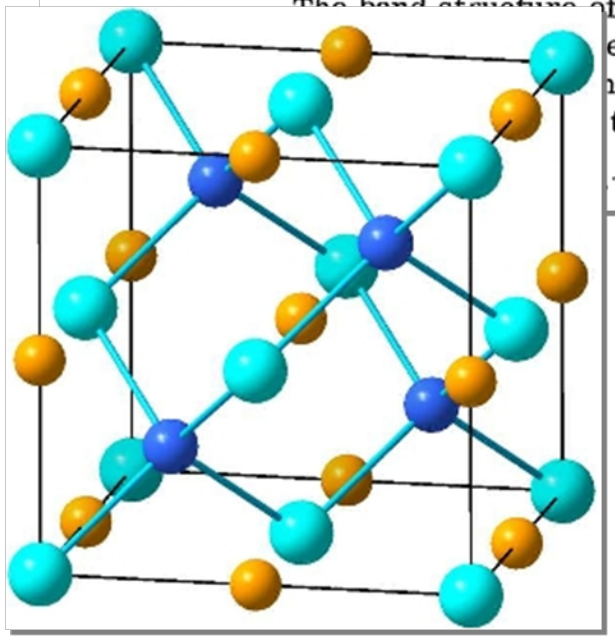
and

P. G. van Engen and K. H. J. Buschow
Philips Research Laboratories, 5600 JA Eindhoven, The Netherlands

(Received 21 March 1983)

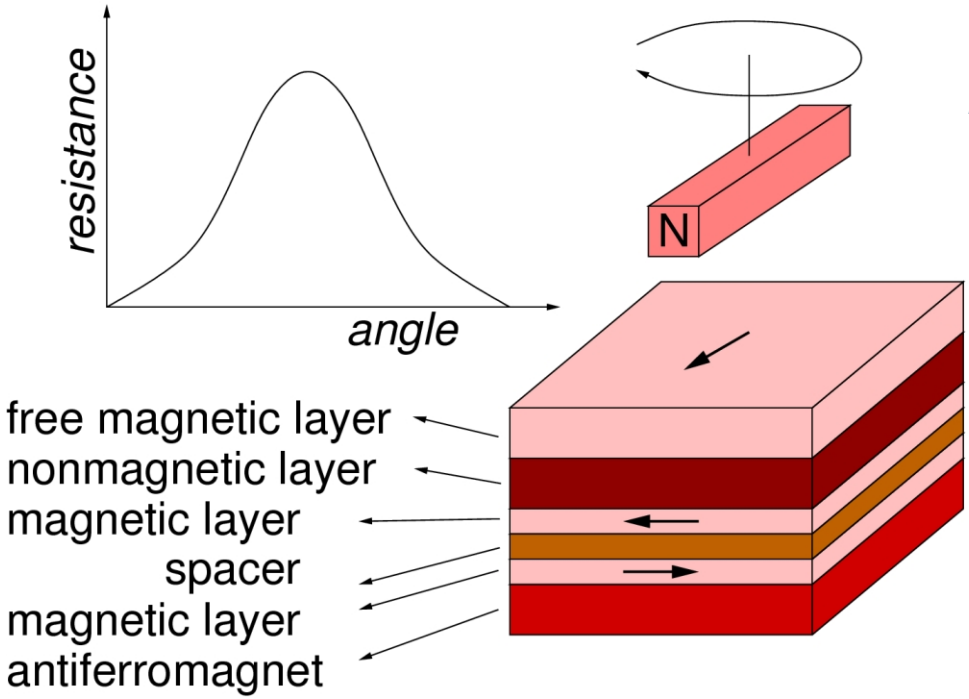
The band structure of Mn-based Heusler alloys of the $C1_b$ crystal structure (MgAgAs ed with the augmented-spherical-wave method. Some of these how unusual electronic properties. The majority-spin electrons the minority-spin electrons are semiconducting.

+x, 71.25.Pi, 75.20.En



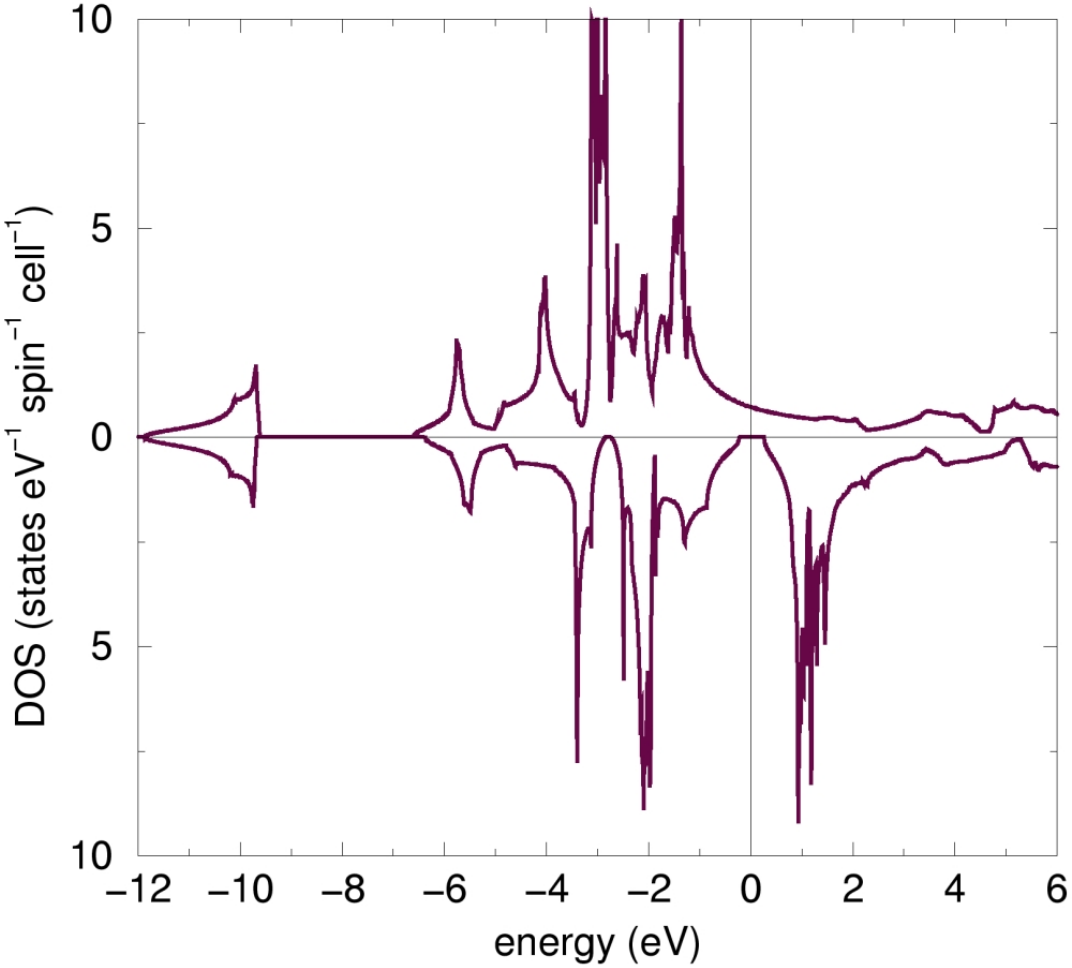
Half Heusler MnNiSb

Magnetoresistive angle sensor:



Modified from Grünberg, *Phys. Today* 54 (2001) 34

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



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

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

APPLIED PHYSICS LETTERS VOLUME 83, NUMBER 3 21 JULY 2003

Molecular-beam epitaxy of the half-Heusler alloy NiMnSb on (In,Ga)As/InP (001)

P. Bach,[a] A. S. Bader, C. Rüster, C. Gould, C. R. Becker, G. Schmidt, and L. W. Molenkamp
Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

W. Weigand, C. Kumpf, and E. Umbach
Physikalisches Institut (EP2), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

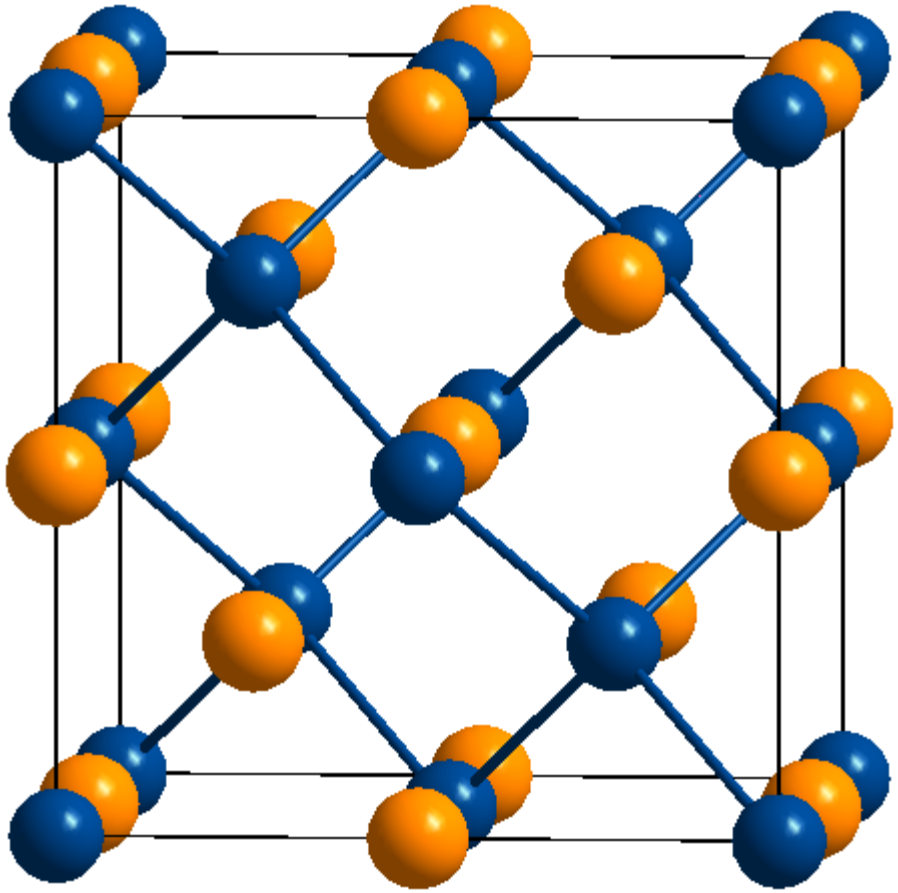
R. Urban, G. Woltersdorf, and B. Heinrich
Simon Fraser University, 8888 University Drive, Burnaby, British Columbia V5A IS6, Canada

(Received 17 March 2003; accepted 4 June 2003)

We report the growth of the half-Heusler alloy NiMnSb on InP (001) by molecular-beam epitaxy using a lattice-matched (In,Ga)As buffer. High-resolution x-ray diffraction confirms a high crystalline quality. Spot-profile analysis low-energy electron diffraction measurements show well-defined surface reconstructions. The samples show the expected high Curie temperature and an uniaxial anisotropy. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1594286]

Half-Heuslers are nearly epitaxial with GaAs: The possibility of spin injection into semiconductors. This is important for any spin-based electronics.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



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), also Öğüt and Rabe (1995), 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.

$18e^- = d^0 + d^{10} + s^2p^6$

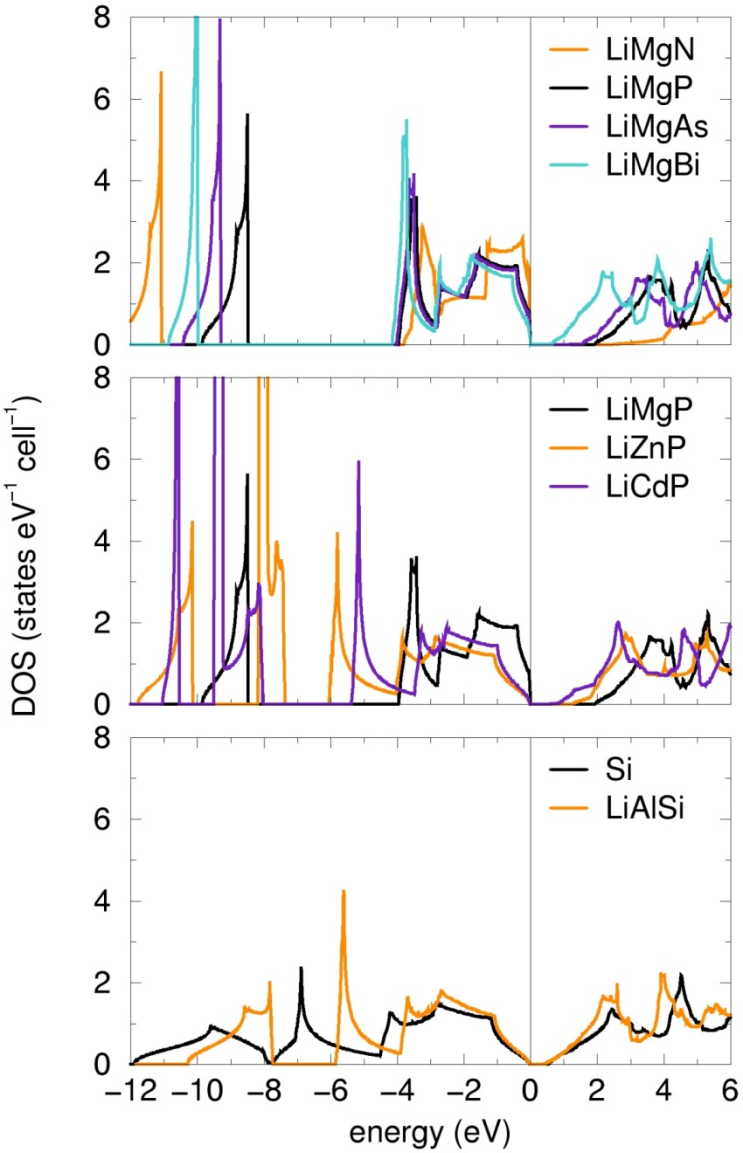
Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

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.

What are the precise nature of the gaps ? How do different constituent elements affect the gaps ? How good is the covalent description of the zinc-blende lattice ?

Gaps in semiconductors as well as in the half-metals.

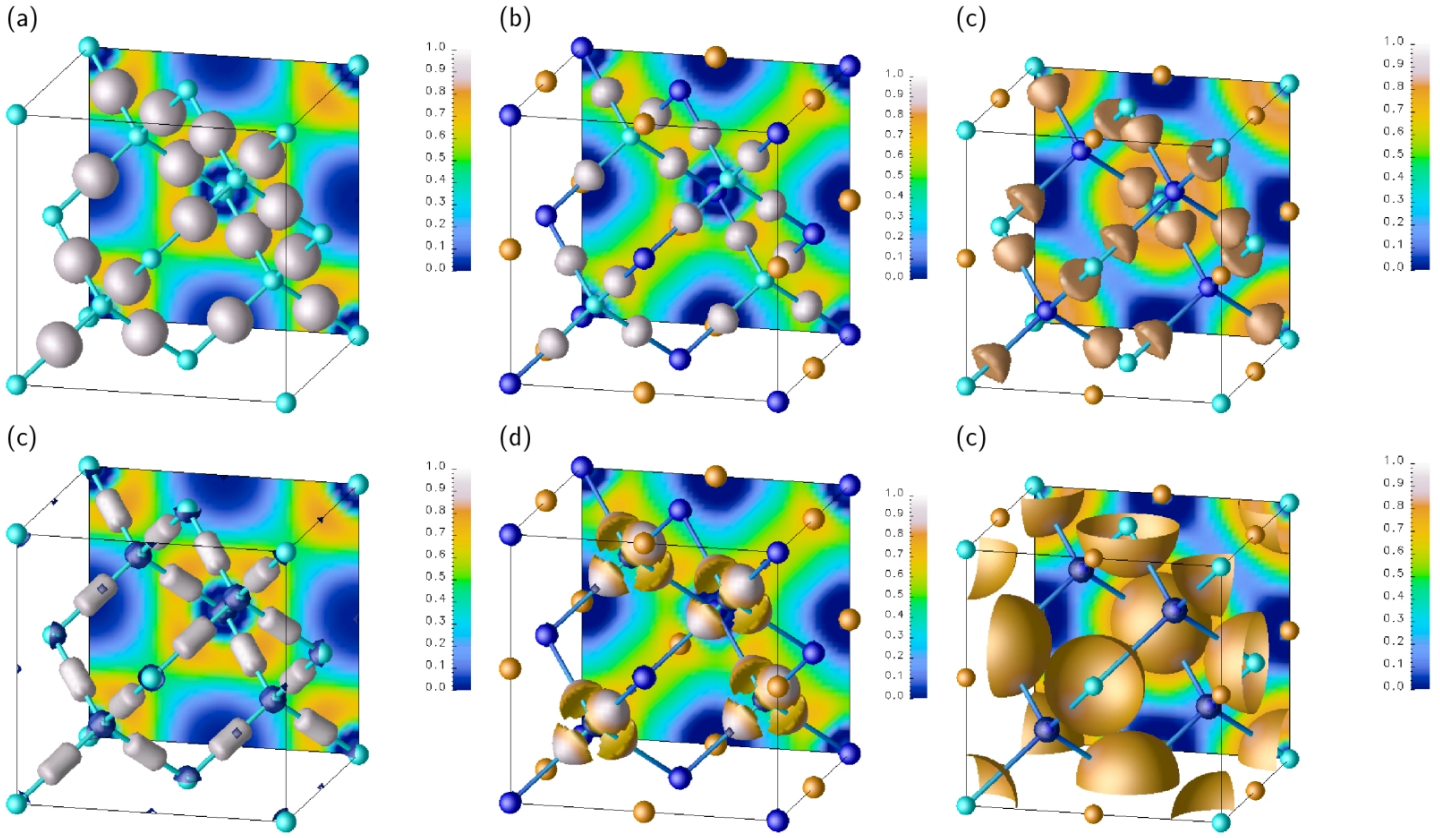
Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



LMTO DOS of 8e half-Heulsers indicates a strong dependence of the band gap on composition of the zinc-blende lattice.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

Si LiAlSi LiMgN

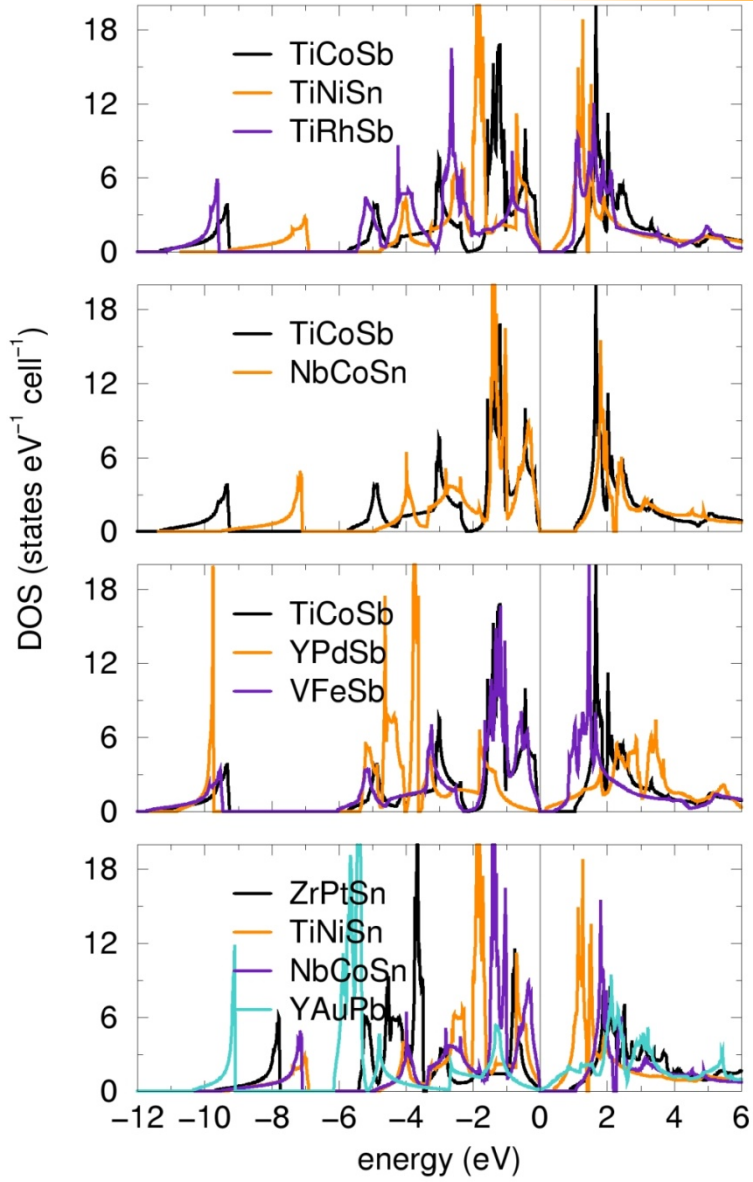


ELF

Charge + ELF

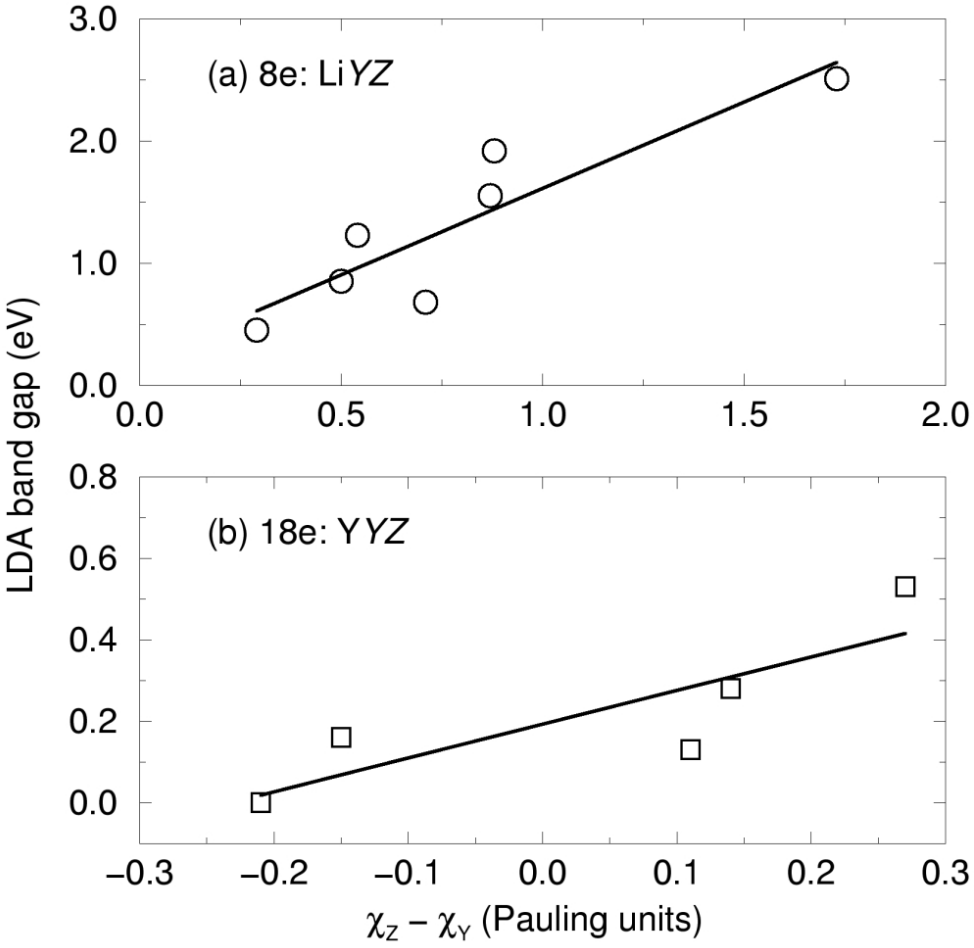
Electron localization functions of the 8e compounds show strongly localized bonding.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



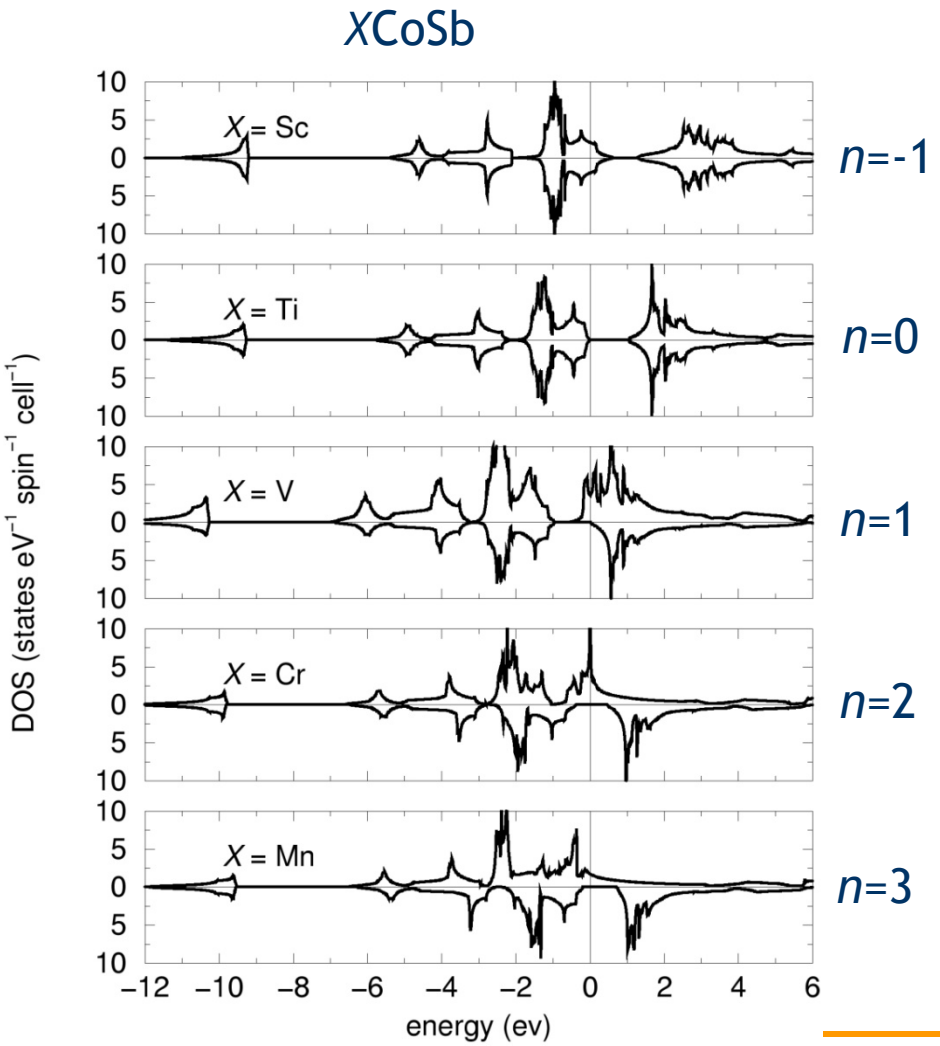
LMTO DOS of 18e half-Heuslers also show rather simple trends in their band gaps.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



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

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers



Magnetic half-Heulser compounds can also be thought of as stuffed zinc-blendes. The band/half-metallic gaps are a little more complex.

Class 3: Semiconductors, stuffed zinc blende, half and full Heuslers

Can one equivalently look for stuffed wurtzites: *hexagonal* semiconducting and half-metallic analogues of the half-Heuslers ? The structure type is known: LiGaGe (SG. $P6_3mc$). Many possibly incorrect determinations in $CaIn_2$ structure.

The structure shown here is CePdSb. Best described as Ce^{3+} stuffing a $(PdSb)^{3-}$ wurtzite lattice, although the $(PdSb)^{3-}$ network is nearly flat/graphitic.