



Introduction to Heusler compounds: From the case of Fe_2VAl

Chin Shan Lue (呂欽山)

2017-03-28-NTU

Outline

1) Introduction to Heusler compounds

Full-Heusler compounds

Half-Heusler compounds

2) Case study of Fe_2VAl

3) Promising characteristics of Heusler compounds

Thermoelectric properties

Spintronic applications

Topological materials

4) Summary

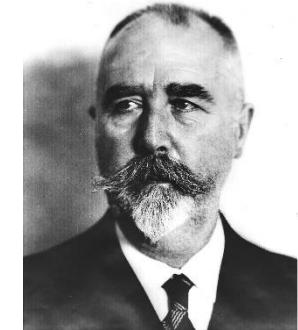
Heusler compounds

Full-Heusler compounds: X_2YZ

Half-Heusler compounds: XYZ

First full-Heusler Cu₂MnAl in 1903

First half-Heusler NiMnSb in 1951



Fritz Heusler
(Germany)

More than 1000 real Heusler compounds

1 H 1.008	2 Li 6.94	3 Be 9.0122	4 Na 22.990	5 Mg 24.305	6 K 39.098	7 Ca 40.078	8 Sc 44.956	9 Ti 47.867	10 V 50.942	11 Cr 51.996	12 Mn 54.938	13 Fe 55.845	14 Co 58.933	15 Ni 58.693	16 Cu 63.546	17 Zn 65.38	18 B 10.81	19 C 12.011	20 N 14.007	21 O 15.999	22 F 18.998	23 Ne 20.180													
3 Li 6.94	4 Be 9.0122	5 Mg 24.305	6 K 39.098	7 Ca 40.078	8 Sc 44.956	9 Ti 47.867	10 V 50.942	11 Cr 51.996	12 Mn 54.938	13 Fe 55.845	14 Co 58.933	15 Ni 58.693	16 Cu 63.546	17 Zn 65.38	18 B 10.81	19 C 12.011	20 N 14.007	21 O 15.999	22 F 18.998	23 Ne 20.180															
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.630	33 As 74.922	34 Se 78.97	35 Br 79.904	36 Kr 83.798	37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.95	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.29
55 Cs 132.91	56 Ba 137.33	57-71 * 137.33	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)	87 Fr (223)	88 Ra (226)	89-103 # (265)	104 Rf (268)	105 Db (271)	106 Sg (270)	107 Bh (277)	108 Hs (276)	109 Mt (281)	110 Ds (280)	111 Rg (285)	112 Cn (286)	113 Nh (286)	114 Fl (289)	115 Mc (289)	116 Lv (293)	117 Ts (294)	118 Og (294)

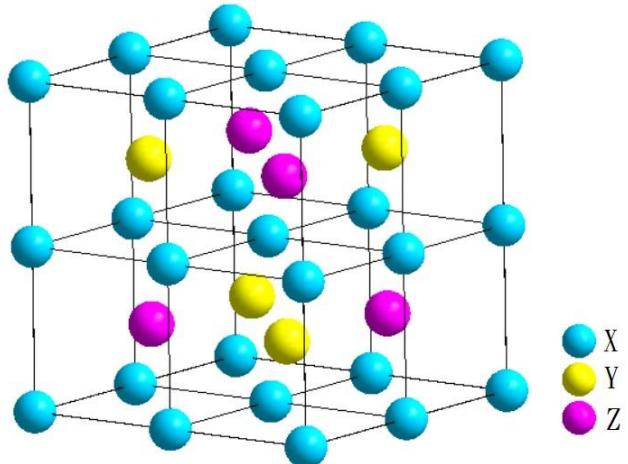
* Lanthanide series

57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05	71 Lu 174.97
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Actinide series

89 Ac (227)	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)
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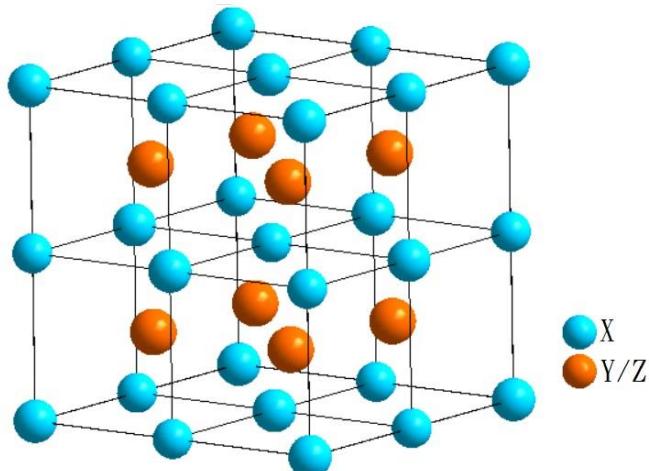
Common crystal structures of Heusler compounds



First determination of crystal structure
for Cu_2MnAl by **Otto Heusler** in 1934

$\text{L}_2\text{1}$ structure

Cu_2MnAl -type
16 atoms per unit cell
 Fe_2VAl , Ru_2NbGa , Ni_2MnGa (HT), ...

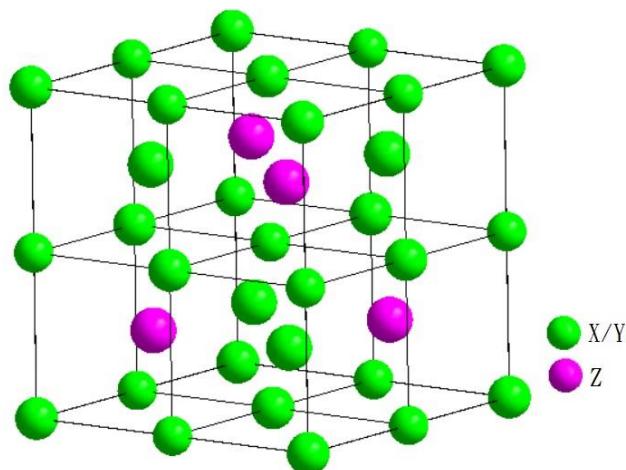


Anti-site disorder

B2 structure

CsCl -type
2 atoms per unit cell
 Co_2MnAl , Ru_2NbAl , Ru_2VAl , ...

X = Y



Binary compounds X_3Z

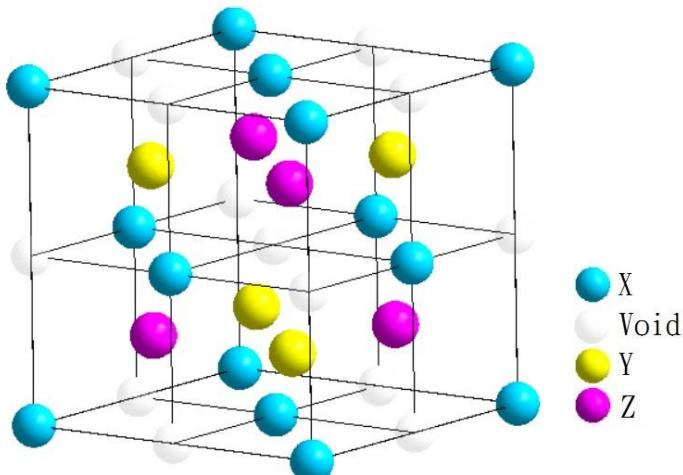
DO₃ structure

BiF₃-type

16 atoms per unit cell

Fe₃Al; Fe₃Ga; Fe₃Si, ...

X + void



Half-Heusler XYZ

C1_b structure

MgAgAs-type

12 atoms per unit cell

NiMnSb, NiZrSn, CoTiSb, ...

Various properties of Heusler compounds

Ferromagnetism: Co_2MnZ , $\text{Pd}_2\text{Mn}(\text{In},\text{Sn})$, ...

Superconductivity: Pd_2YSn ($T_C = 4.9 \text{ K}$), Ni_2NbSn , Pd_2ErSn , ...

Shape memory behavior: Ni_2MnGa (Martensitic transformation $T_M = 220 \text{ K}$), ...

Semiconducting: Fe_2VAl , Ru_2TaAl , IrNbSb , NiHfSn , CoTiSb , ...

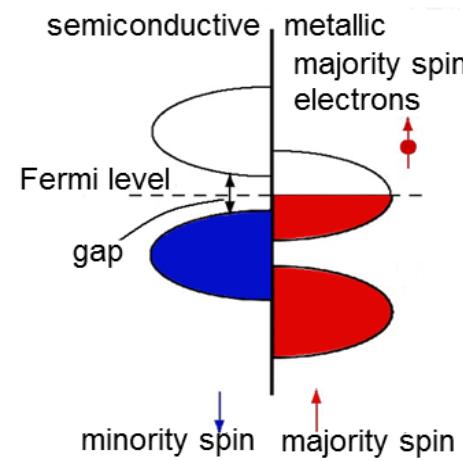
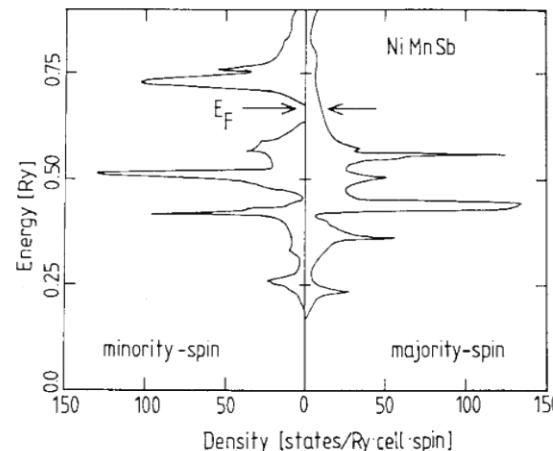
VOLUME 50, NUMBER 25

PHYSICAL REVIEW LETTERS

20 JUNE 1983

New Class of Materials: Half-Metallic Ferromagnets

R. A. de Groot and F. M. Mueller



Unusual physical behavior in Fe_2VAI

Paramagnetic behavior in Fe_2VAI by Webster & Ziebeck in 1983

VOLUME 79, NUMBER 10

PHYSICAL REVIEW LETTERS

8 SEPTEMBER 1997

Semiconductorlike Behavior of Electrical Resistivity in Heusler-type Fe_2VAI Compound

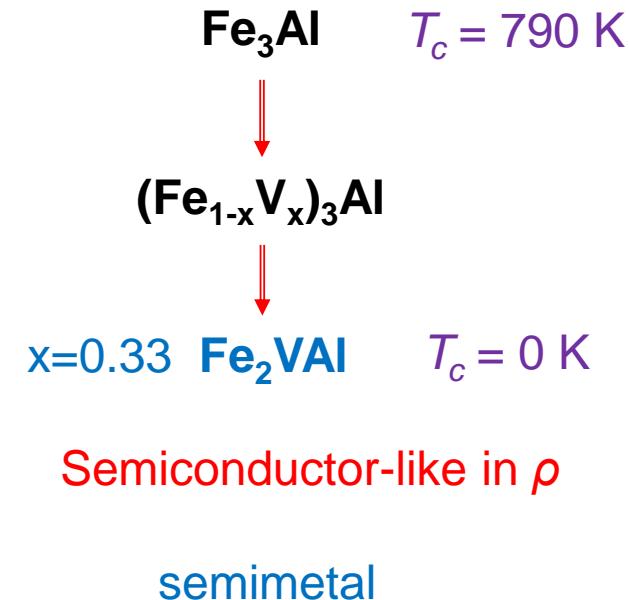
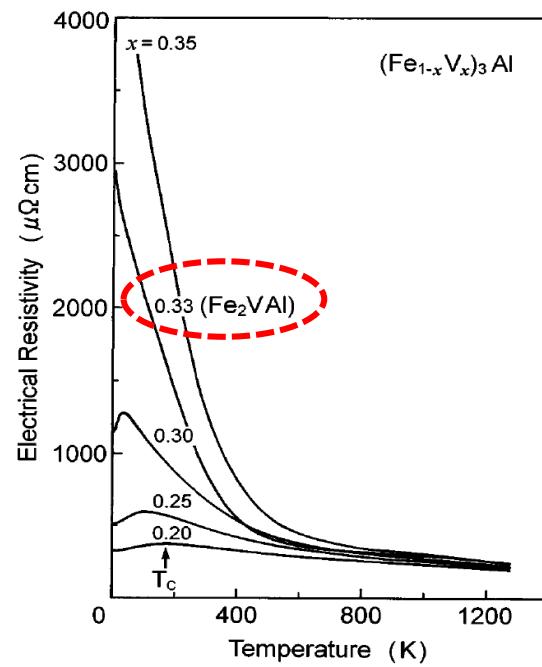
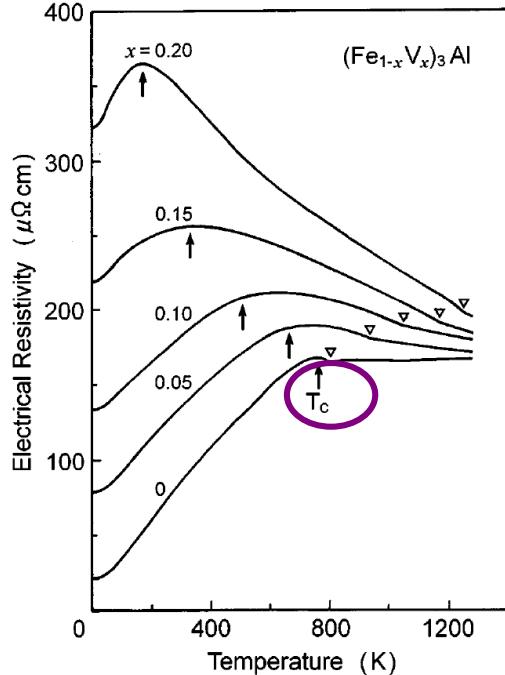
Y. Nishino, M. Kato, and S. Asano

Department of Materials Science and Engineering, Nagoya Institute of Technology, Showa-ku, Nagoya 466, Japan

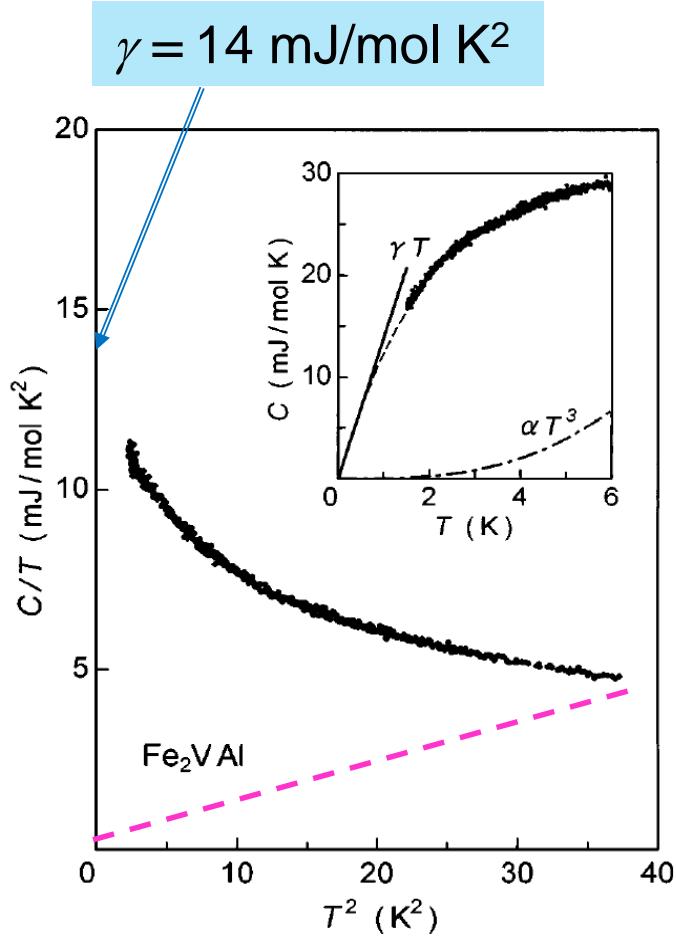
K. Soda, M. Hayasaki, and U. Mizutani

Department of Crystalline Materials Science, Nagoya University, Chikusa-ku, Nagoya 464-01, Japan

(Received 7 March 1997)



Possible 3d heavy fermion for Fe_2VAI



Expected behavior for ordinary semimetals (low Fermi-level DOS)

$\gamma = 1.07 \text{ mJ/mol K}^2$

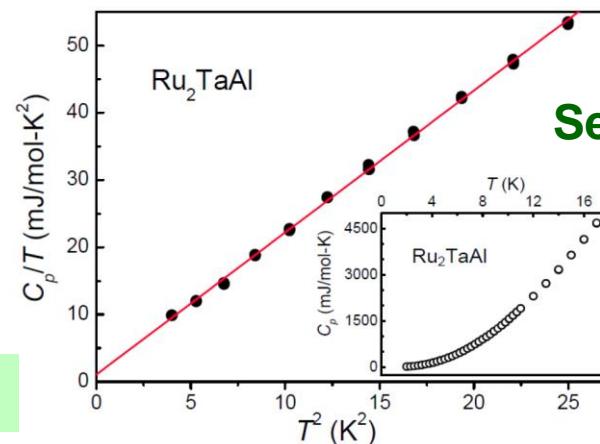
Low- T $C = C_e + C_{ph} = \gamma T + \beta T^3$

$C/T = \gamma + \beta T^2$

Sommerfeld coefficient based on free electron model

$$\gamma_{th} = \frac{\pi^2 k_B^2}{3} N(E_F) \propto m_e$$

$$\frac{\gamma_{exp}}{\gamma_{th}} = \frac{m^*}{m_e} \approx 50 - 100 \quad \text{for } \text{Fe}_2\text{VAI}$$



Semimetallic Ru_2TaAl

$$\frac{\gamma_{exp}}{\gamma_{th}} \approx 3$$

from C. M. Wei et al.

Simple concept for heavy fermions

f-electron heavy fermions

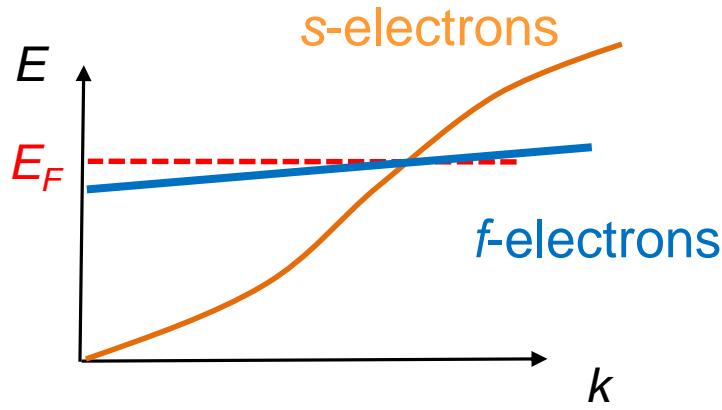
CeAl₃ $\gamma = 1620 \text{ mJ/mol K}^2$

CeCu₆ $\gamma = 1300 \text{ mJ/mol K}^2$

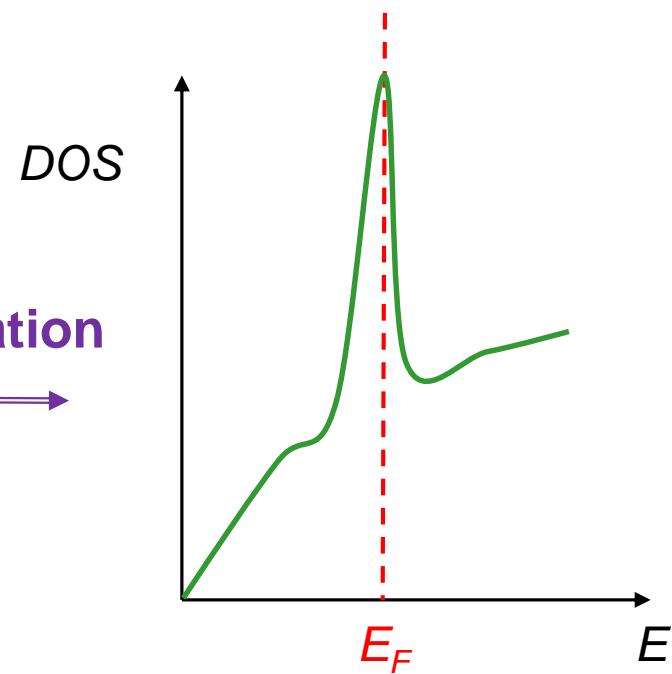
UBe₁₃ $\gamma = 1100 \text{ mJ/mol K}^2$

U₂Zn₁₇ $\gamma = 500 \text{ mJ/mol K}^2$

.....



hybridization



It is less likely to observe heavy fermion behavior in *d*-electron systems since the corresponding wave-functions of *d*-orbitals are more dispersive.

d-electron heavy fermion???

Spinel LiV₂O₄ $\gamma = 420 \text{ mJ/mol K}^2$

PRL 78, 3729 (1997); PRL 85, 1052 (2000)

PRL 89, 267201 (2002); PRL 99, 167402 (2007)

Nat. Comm. 3, 981 (2012); PRL 113, 236402 (2014);

.....

Band structure calculations for Fe_2VAI

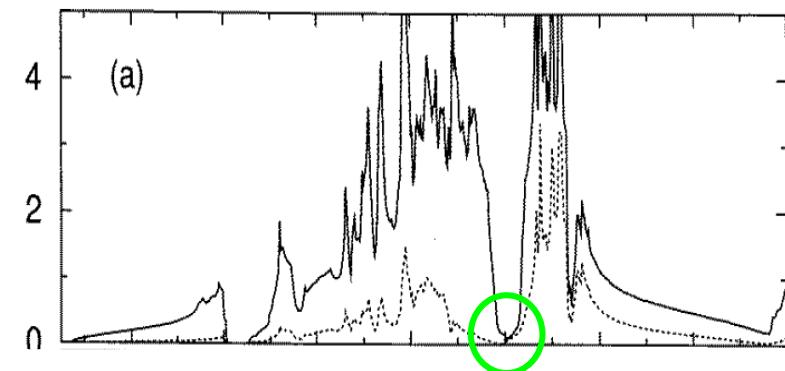
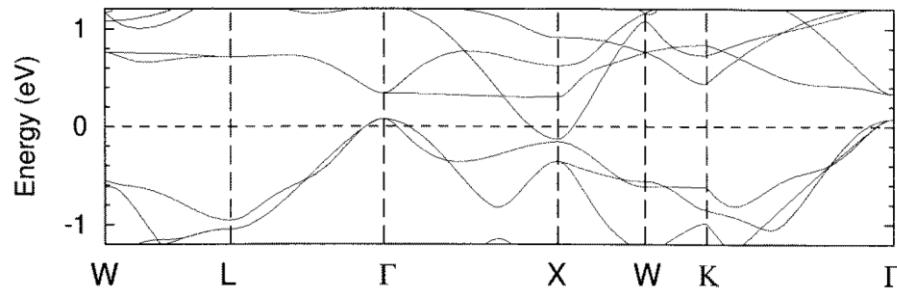
J. Phys.: Condens. Matter **10** (1998) L119–L126. Printed in the UK

LETTER TO THE EDITOR

Electronic structure of possible 3d ‘heavy-fermion’ compound Fe_2VAI

郭光宇

G Y Guo[†], G A Botton[‡] and Y Nishino^{||}



$$N(E_F) = 0.08 \text{ states/eV atom}$$

Electronic structure, local moments, and transport in Fe_2VAI ,

D. J. Singh & I. I. Mazin, Phys. Rev. B 57, 14352 (1998)

Excitonic correlations in the intermetallic Fe_2VAI ,

R. Weht & W. E. Pickett, Phys. Rev. B 58, 6855 (1998)

Hybridization-induced band gaps in transition-metal aluminides,

M. Weinert & R. E. Watson, Phys. Rev. B 58, 9732 (1998)

Electronic structure and magnetism of $\text{Fe}_{3-x}\text{V}_x\text{X}$ ($\text{X}=\text{Si, Ga, and Al}$) alloys by the KKR-CPA method, A. Bansil, et al., Phys. Rev. B 60, 13396 (1999)

NMR evidence for semimetallic behavior in Fe_2VAl

PHYSICAL REVIEW B

VOLUME 58, NUMBER 15

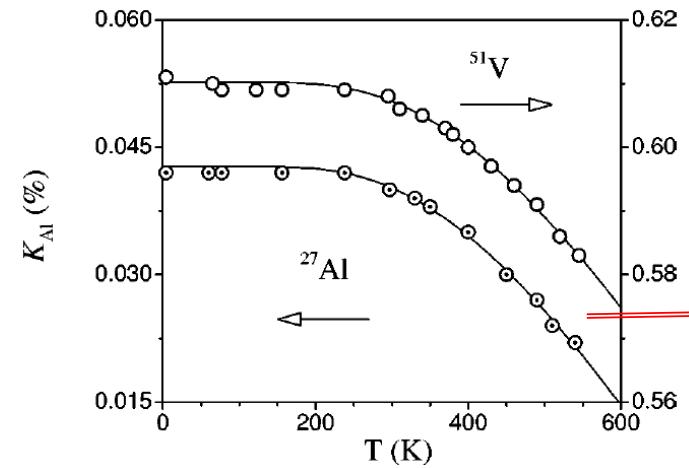
15 OCTOBER 1998-I

Semimetallic behavior in Fe_2VAl : NMR evidence

Chin-Shan Lue* and Joseph H. Ross, Jr.[†]

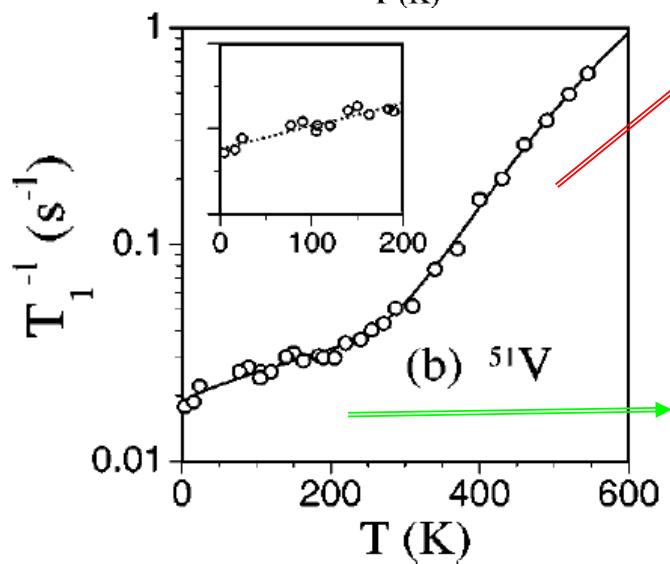
Department of Physics, Texas A&M University, College Station, Texas 77843-4242

(Received 3 June 1998)



Thermally excited carriers
across electronic bands near E_F

Activation energy $E_A \sim 0.27 \text{ eV}$



Korringa relation $1/T_1 T \sim C[N(E_F)]^2$

Low V-3d $N(E_F) = 0.11 \text{ states/eV atom}$

Question of possible 3d heavy fermion for Fe₂VAL

THIRD SERIES, VOLUME 60, NUMBER 20

15 NOVEMBER 1999-II

RAPID COMMUNICATIONS

Rapid Communications are intended for the accelerated publication of important new results and are therefore given priority treatment both in the editorial office and in production. A Rapid Communication in Physical Review B may be no longer than four printed pages and must be accompanied by an abstract. Page proofs are sent to authors.

Field-dependent specific heat in Fe₂VAL and the question of possible 3d heavy fermion behavior

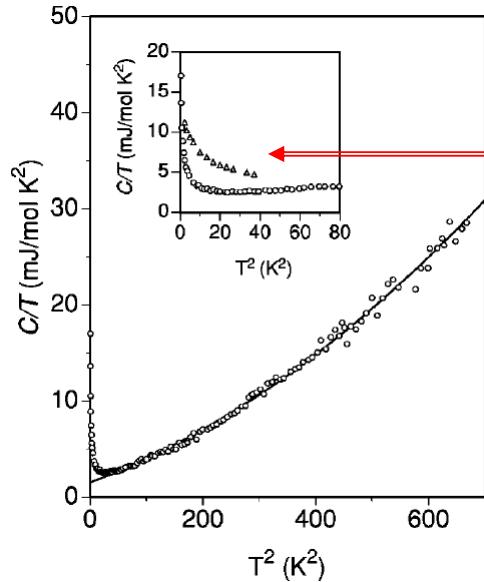
C. S. Lue* and Joseph H. Ross, Jr.[†]

Department of Physics, Texas A&M University, College Station, Texas 77843-4242

C. F. Chang and H. D. Yang

Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan

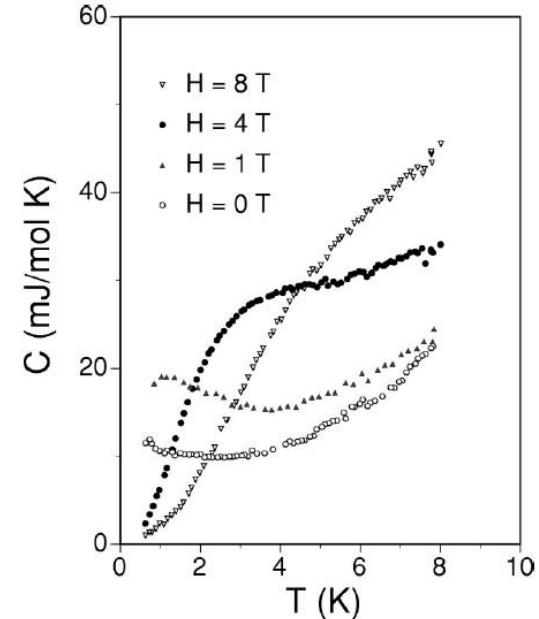
(Received 19 August 1999)



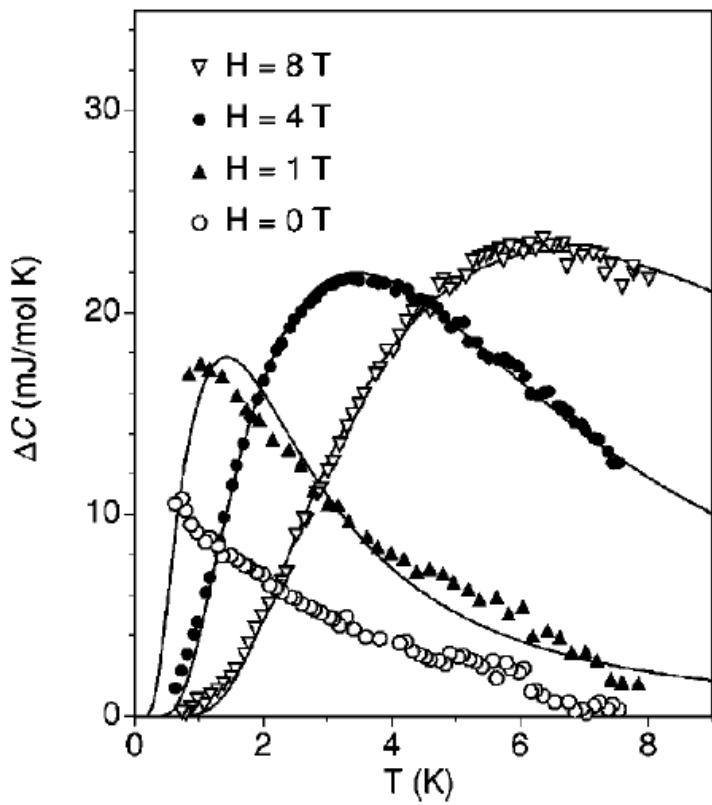
Field-dependent

Field-dependent

Small $\gamma = 1.5 \text{ mJ/mol K}^2$



False heavy fermion behavior in Fe_2VAl



For non-interacting magnetic clusters with spin $J > 1/2$, the magnetic specific heat can be generated by the so-called multi-level Schottky function as

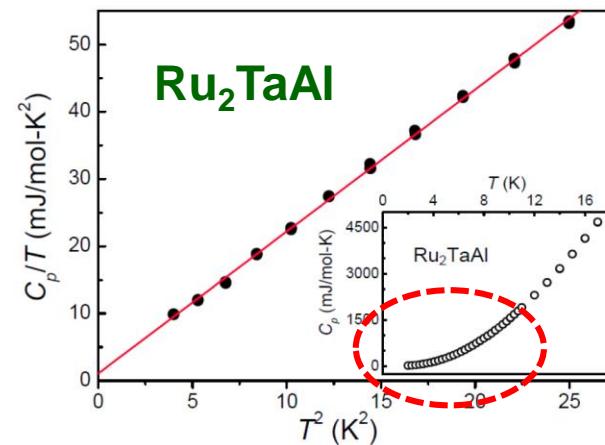
$$C_m = Nk_B \left[\frac{x^2 e^x}{(e^x - 1)^2} - (2J+1)^2 \frac{x^2 e^{(2J+1)x}}{(e^{(2J+1)x} - 1)^2} \right]$$

$$x = \frac{g\mu_B H}{k_B T}$$

$$J = \frac{3}{2} \rightarrow \mu = g\mu_B \sqrt{J(J+1)} = 3.7\mu_B$$

$f = 0.36\%$ population per formula unit

**The low- T upturn in C is not intrinsic;
It is reasonably associated with
magnetic clusters due to anti-site
disorder in real samples.**



Effects of magnetic clusters in Fe₂VAL, Fe₂VGa and Fe₂TiSn

“Weak ferromagnetism induced by atomic disorder in Fe₂TiSn”,

A. Ślebarski, M. B. Maple, et al., Phys. Rev. B 62, 3296 (2000)

“Kondo-type behavior in Fe_{2-x}M_xTiSn(M=Co,Ni)”,

A. Ślebarski, M. B. Maple, et al., Phys. Rev. B 63, 214416 (2001)

“Fe–3s core-level splitting and local magnetism in Fe₂VAL”,

Phys. Rev. B 63, 054419 (2001)

“Superparamagnetism and magnetic defects in Fe₂VAL and Fe₂VGa”,

J. Phys.: Condens. Matter 13, 1585 (2001)

“Structure and magnetic order in Fe_{2+x}V_{1-x}Al”,

J. Phys.: Condens. Matter 13, 5487 (2001)

“NMR and Mössbauer study of spin dynamics and electronic structure of Fe_{2+x}V_{1-x}Al and Fe₂VGa”,

Phys. Rev. B 67, 224425 (2003)

“Transport and magnetic properties of the Heusler-type Fe_{2-x}V_{1+x}Al system
(-0.01≤x≤0.08)”,

Phys. Rev. B 71, 094425 (2005)

“Evidence for cluster glass behavior in Fe₂VAL Heusler alloys”,

Phys. Rev. B 78, 064401 (2008)

Band structure calculations for Fe₂VAI

J. Phys.: Condens. Matter **10** (1998) L119–L126. Printed in the UK

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R. Weht & W. E. Pickett, Phys. Rev. B 58, 6855 (1998)

Hybridization-induced band gaps in transition-metal aluminides,

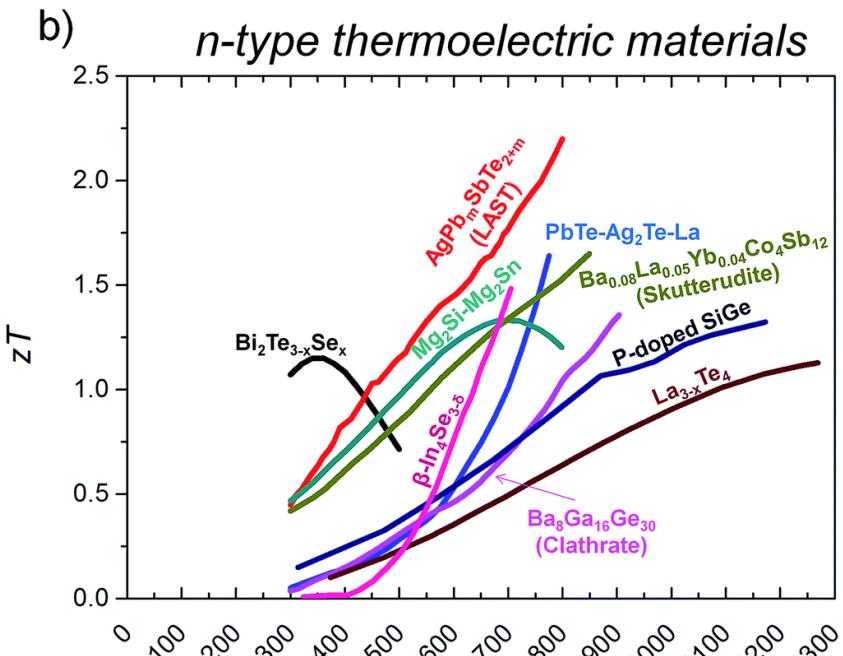
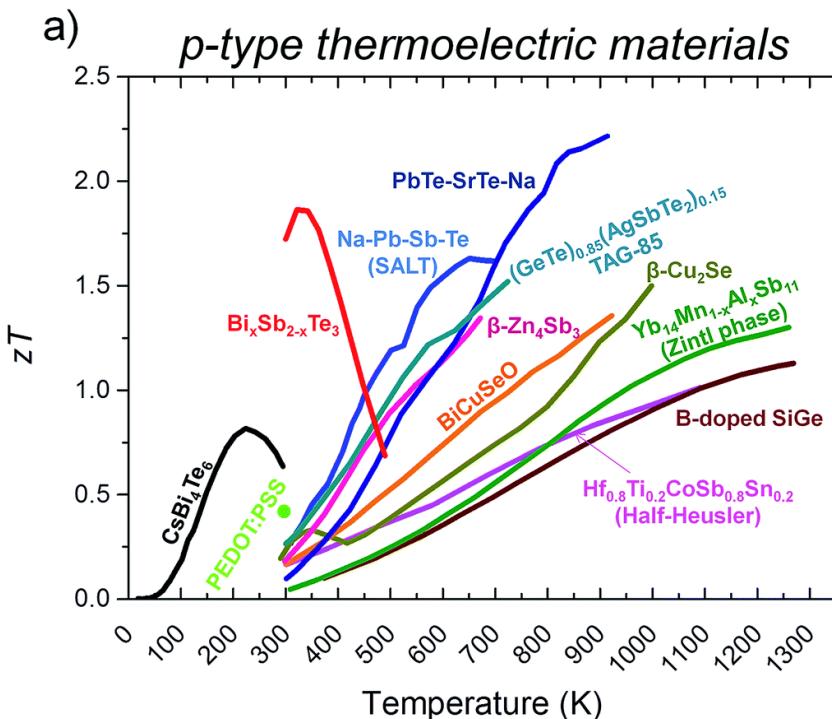
M. Weinert & R. E. Watson, Phys. Rev. B 58, 9732 (1998)

Electronic structure and magnetism of Fe_{3-x}V_xX (X=Si, Ga, and Al) alloys by the KKR-CPA method, A. Bansil, et al., Phys. Rev. B 60, 13396 (1999)

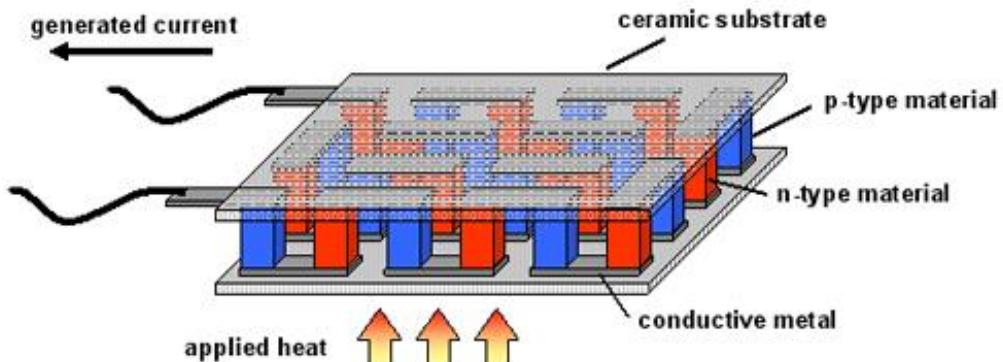
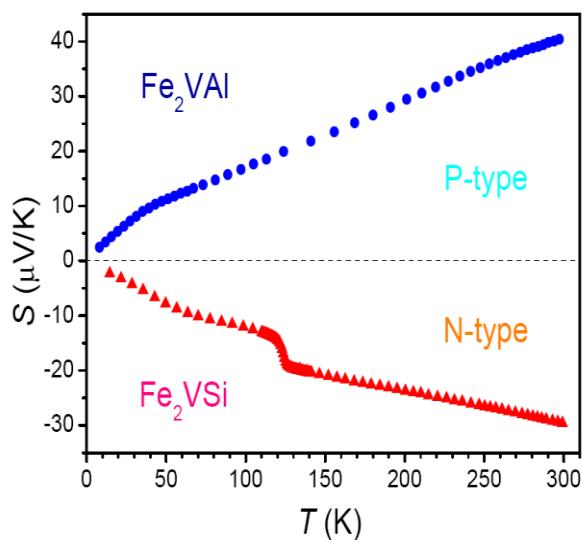
More first-principles calculations on Fe₂VAI

- “Electronic structure and x-ray magnetic circular dichroism in Heusler-type Fe_{2-x}V_{1+x}Al: First-principles calculations”,
Phys. Rev. B 77, 134444 (2008)
- “Density functional study of elastic and vibrational properties of the Heusler-type alloys Fe₂VAI and Fe₂VGa”,
Phys. Rev. B 80, 125108 (2009)
- “Electronic and **thermoelectric properties** of Fe₂VAI: The role of defects and disorder”,
Phys. Rev. B 83, 205204 (2011)
- “Effect of onsite Coulomb repulsion on **thermoelectric properties** of full-Heusler compounds with pseudogaps”,
Phys. Rev. B 84, 125104 (2011)
- “Low-Dimensional transport and **large thermoelectric power factors** in bulk semiconductors by band engineering of highly directional electronic states”,
Phys. Rev. Lett. 114, 136601 (2015)
- “Quantum many-body intermetallics: Phase stability of Fe₃Al and small-gap formation in Fe₂VAI”,
Phys. Rev. B 95, 045114 (2017)
-

Thermoelectric materials



RSC Advances 5, 52 (2015)



Thermoelectric generator module

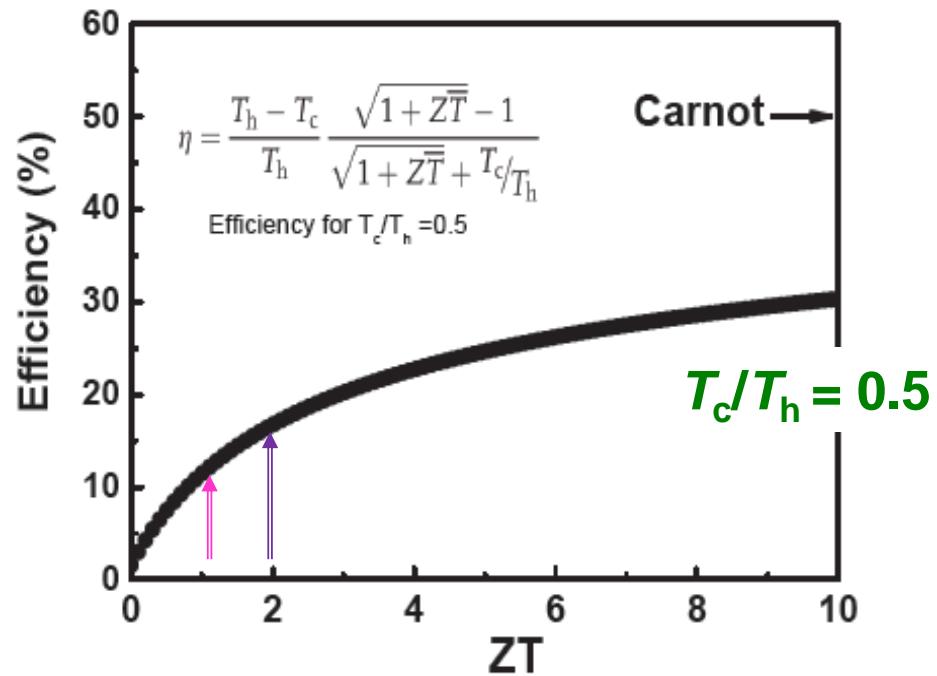
Thermoelectric efficiency

η : Generated electrical energy/Absorbed heat energy

$$\eta_{\max} = \left(\frac{T_h - T_c}{T_h} \right) \frac{\sqrt{1 + Z\bar{T}} - 1}{\sqrt{1 + Z\bar{T}} + \frac{T_c}{T_h}}, \quad \text{with} \quad Z = \frac{S^2}{\rho\kappa}, \quad \bar{T} = \frac{T_c + T_h}{2}.$$

ZT: Figure of merit
熱電優質

$$ZT = 1 \rightarrow 10.8\% \\ ZT = 2 \rightarrow 16.4\%$$



Thermoelectric performance

$$ZT = S^2 T / \rho (\kappa_e + \kappa_l)$$

S : Seebeck coefficient

ρ : electrical resistivity

κ_e : electronic thermal conductivity

κ_l : lattice thermal conductivity

Naive expectation:

$$S = 200 \mu\text{V/K}$$

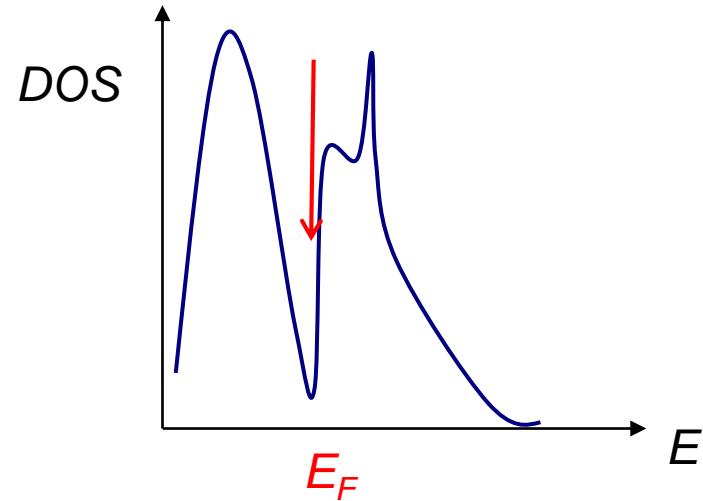
$$\rho = 1000 \mu\Omega\text{-cm}$$

$$\kappa = 2 \text{ W/m-K}$$

$$ZT=1 \text{ at } 500 \text{ K}$$

Physical approach based on Mott equation,

$$S_e \propto \frac{1}{e} \left(\frac{1}{N(E)} \frac{\partial N(E)}{\partial E} \right)_{E=E_F}$$



Chemical approach by partially substituting heavy elements and/or vacancies to enhance the phonons scattering and thus reduce the contribution of κ_l .

A simple rule with number of valence electrons

Full-Heusler compounds with L_21 -type structure

Total number of valence electrons per formula unit VEC = $Z_t = 24$

In principles → Semiconductors

In reality → Semimetals

Fe_2VAI , Fe_2VGa , Fe_2TiSn , Ru_2NbGa , Ru_2TaAl , Ru_2TiSi ,

Half-Heusler compounds with C_b1 -type structure

Total number of valence electrons per formula unit VEC = $Z_t = 18$

In principles → Semiconductors

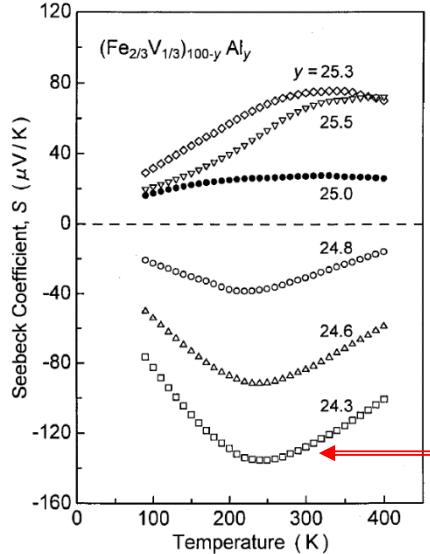
In reality → Semimetals

NiTiSn , NiZrSn , NiHfSn , CoTiSb , FeVSb

Thermoelectric studies of Fe_2VAl and related compounds

Effect of off-stoichiometry on the transport properties of the Heusler-type Fe_2VAl compound

Nishino et al., Phys. Rev. B 63, 233303 (2001)



Large S

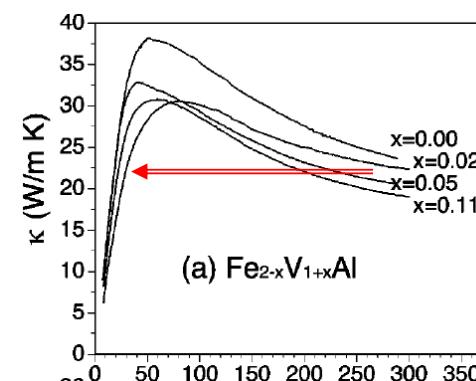
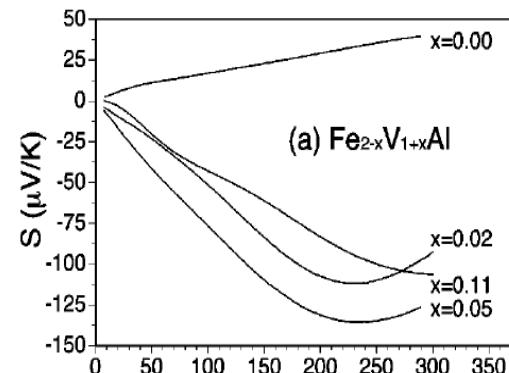
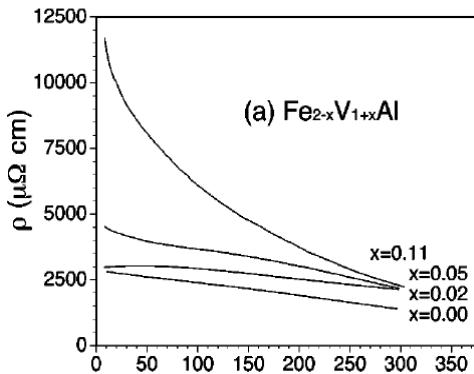
Nishino's group
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Phys. Rev. B 75, 064202 (2007)
Phys. Rev. B 78, 165117 (2008)

Other groups
J. Alloys Compd. 349, 37 (2003)
Phys. Rev. B 77, 224415 (2008)
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Thermoelectric properties of the semimetallic Heusler compounds $\text{Fe}_{2-x}\text{V}_{1+x}M$ ($M=\text{Al, Ga}$)

C. S. Lue & Y. K. Kuo, Phys. Rev. B 66, 085121 (2002)

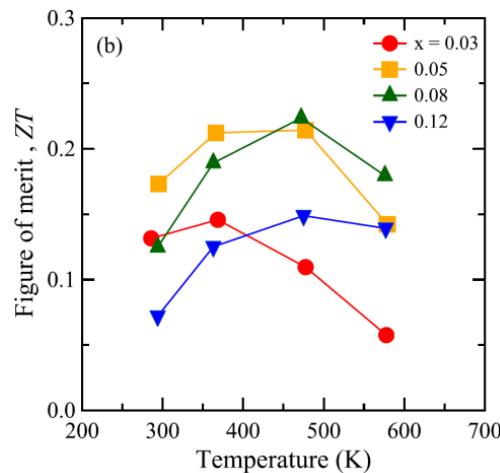
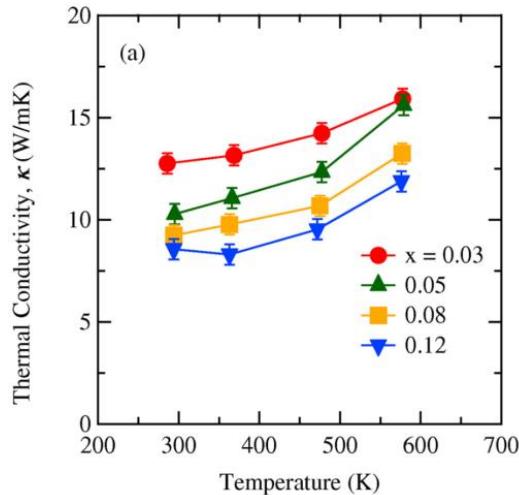
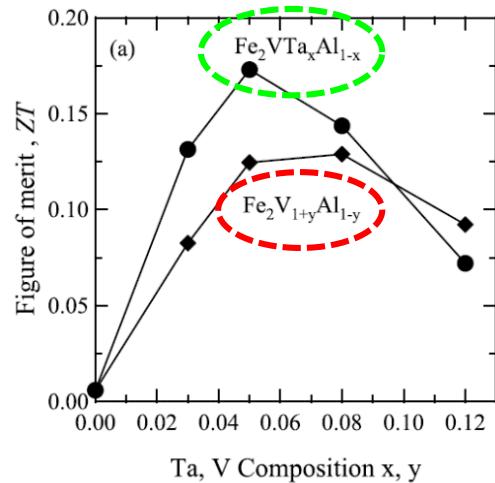
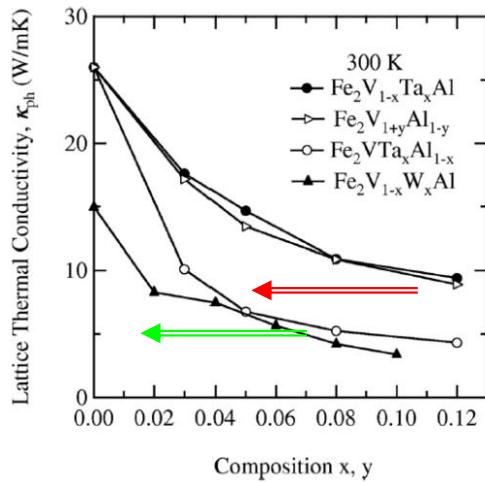


High κ

Thermoelectric studies of Fe_2VAl -based compounds

Thermoelectric properties of the Heusler-type $\text{Fe}_2\text{VTa}_x\text{Al}_{1-x}$ alloys

J. Appl. Phys. 115, 033704 (2014)



Optimized $ZT \sim 0.2$

Thermoelectric studies of half-Heusler compounds with $Z_t = 18$

“Gap at the Fermi level in the intermetallic vacancy system $RNiSn$ ($R=Ti,Zr,Hf$)”,
Z. Phys. B 75, 116 (1989).

“Narrow band in the intermetallic compounds $MNiSn$ ($M=Ti,Zr,Hf$)”,
Z. Phys. B 80, 353 (1990).

“Band gap and stability in the ternary intermetallic compounds $NiSnM$ ($M=Ti,Zr,Hf$):
A first principles study”,
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“Effect of substitutions and defects in half-Heusler $FeVSb$ studied by electron
transport measurements and KKR-CPA electronic structure calculations”,

Phys. Rev. B 70, 184207 (2004).

“Electronic structure and thermoelectric properties of half-Heusler $Zr_{0.5}Hf_{0.5}NiSn$ by
first-principles calculations”,

Appl. Phys. Lett. 113, 193705 (2013).

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PHYSICAL REVIEW B 95, 045202(2017)

Lattice thermal conductivity of $Ti_xZr_yHf_{1-x-y}NiSn$ half-Heusler alloys calculated
from first principles: Key role of nature of phonon modes

“Effect of Ti substitution on the thermoelectric properties of (Zr,Hf)NiSn half-Heusler compounds”,
Appl. Phys. Lett. 86, 082105 (2005).

“Thermoelectric performance of half-Heusler compounds TiNiSn and TiCoSb”,
Appl. Phys. Lett. 105, 013709 (2009).

“Thermoelectric property study of nano-structured p-type half-Heuslers (Hf,Zr,Ti)CoSb_{0.8}Sn_{0.2}”,
Advanced Energy Materials 3, 1195 (2013).

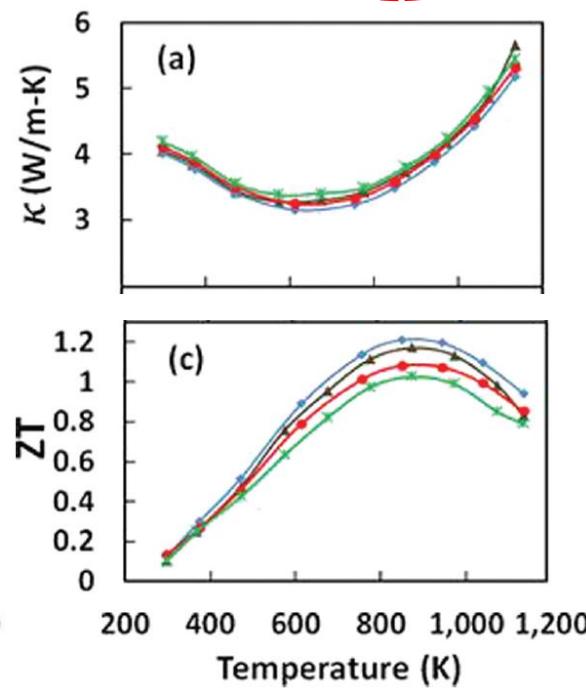
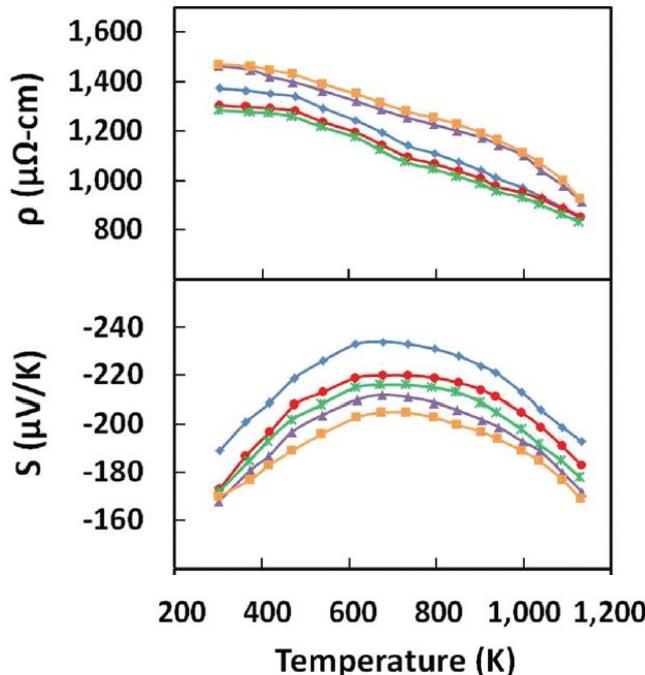
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APPLIED PHYSICS LETTERS 107, 041902 (2015)

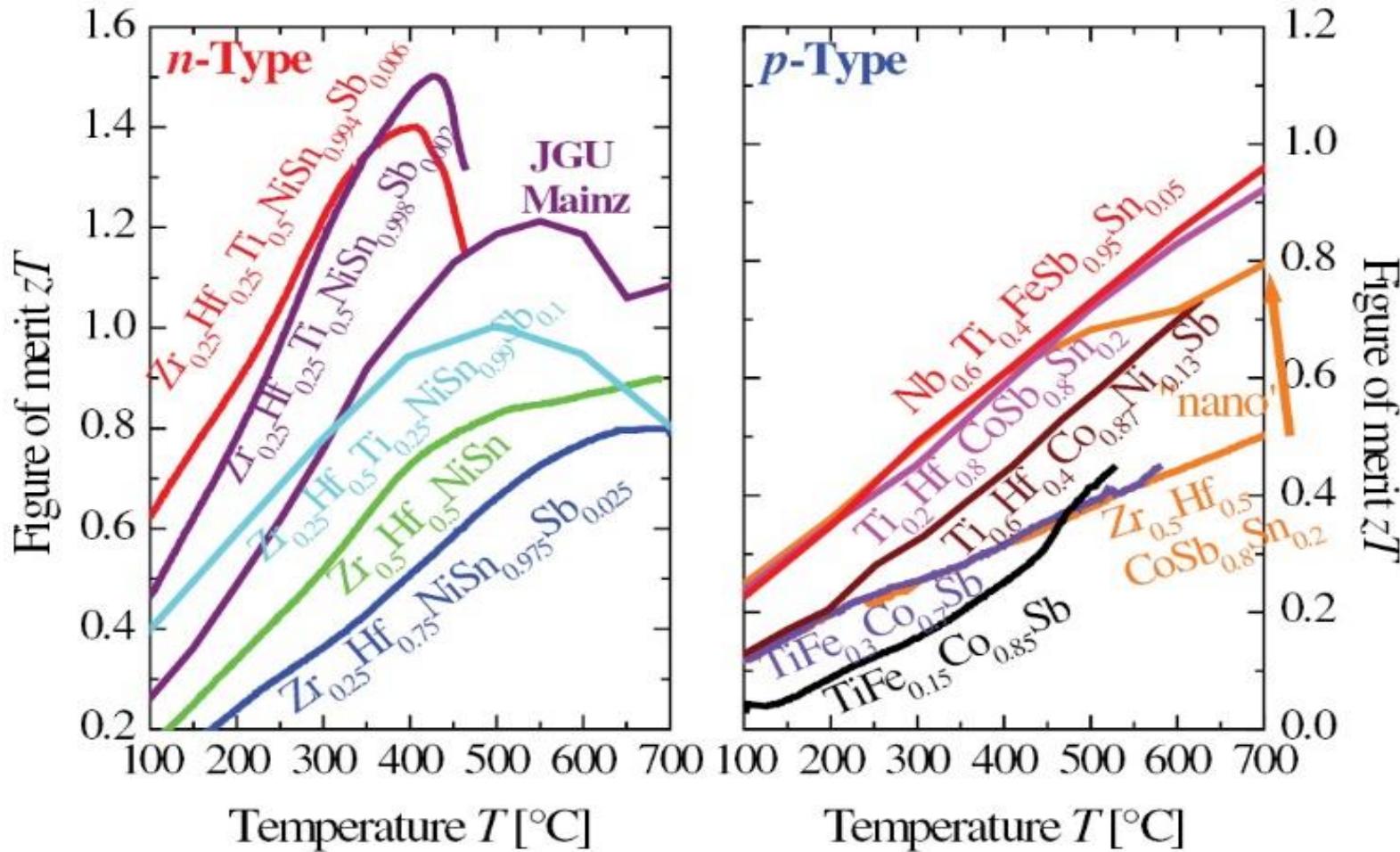


Uncovering high thermoelectric figure of merit in (Hf,Zr)NiSn half-Heusler alloys

L. Chen,¹ S. Gao,¹ X. Zeng,² A. Mehdizadeh Dehkordi,³ T. M. Tritt,^{2,3} and S. J. Poon^{1,4}



Thermoelectric materials based on half-Heusler compounds



Half-metallic Heusler compounds

VOLUME 50, NUMBER 25

PHYSICAL REVIEW LETTERS

20 JUNE 1983

New Class of Materials: Half-Metallic Ferromagnets

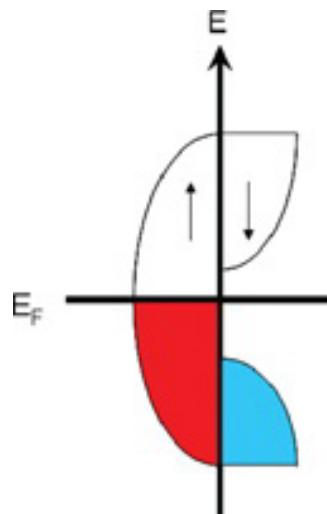
R. A. de Groot and F. M. Mueller

Research Institute for Materials, Faculty of Science, Toernooiveld, 6525 ED Nijmegen, The Netherlands

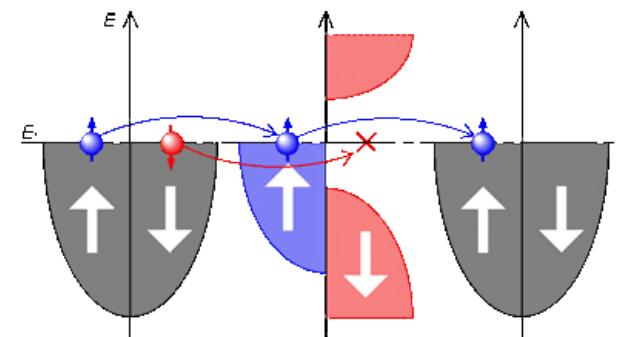
Compound	$N(E)\uparrow$	$N(E)\downarrow$	$n_{3d}^{\text{Mn}\uparrow}$	$n_{3d}^{\text{Mn}\downarrow}$	$\mu_{\text{tot}}^{\text{cal}}$	$\mu_{\text{tot}}^{\text{exp}}$
NiMnSb	9.90	0	4.51	0.87	4.00	3.85
PtMnSb	10.05	0	4.57	0.79	4.00	3.97
PdMnSb	9.04	2.97	4.58	0.71	4.05	3.95
PtMnSn	9.78	19.31	4.40	0.78	3.60	3.42



Half-Heusler



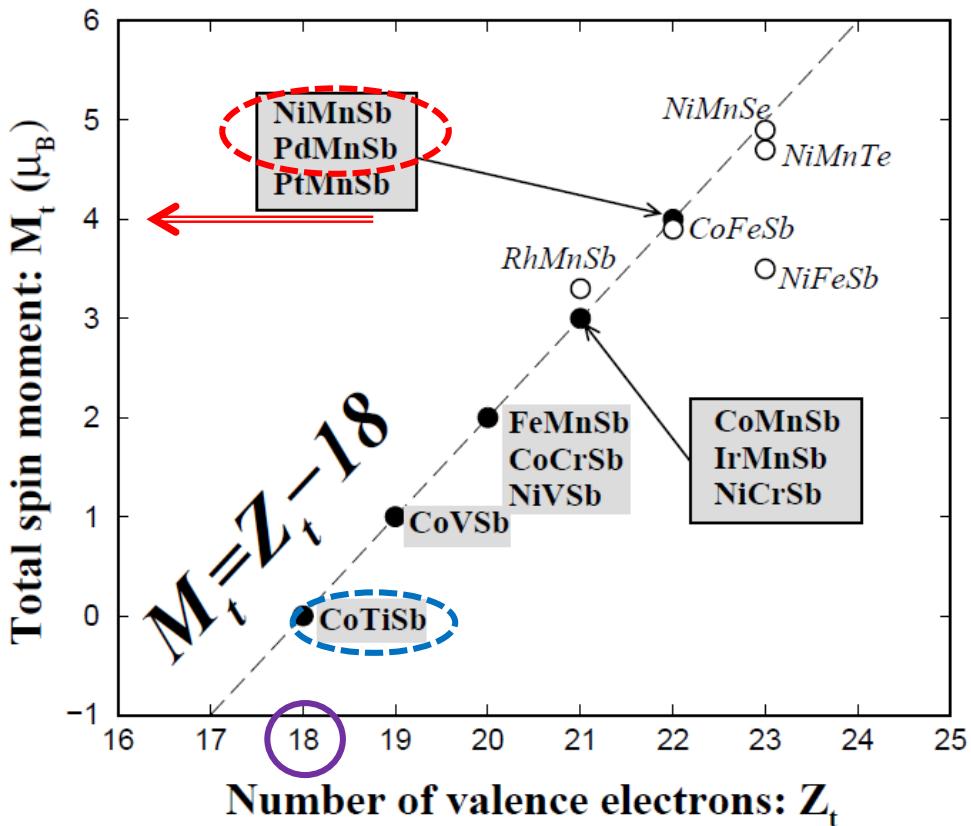
Half-Heusler



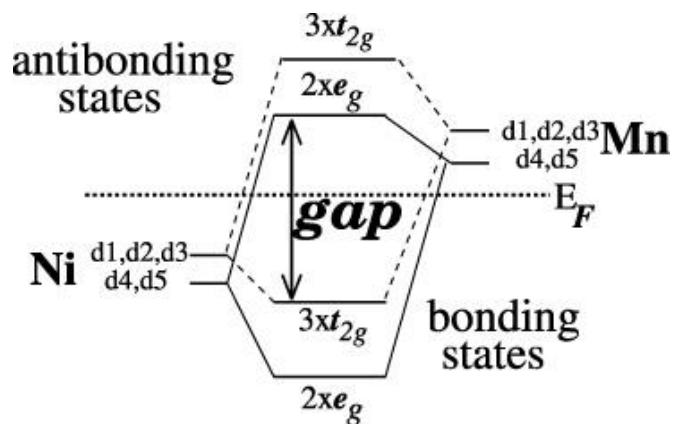
100% polarization

A semi-empirical general rule: Slater-Pauling curve

Half-Heusler compounds



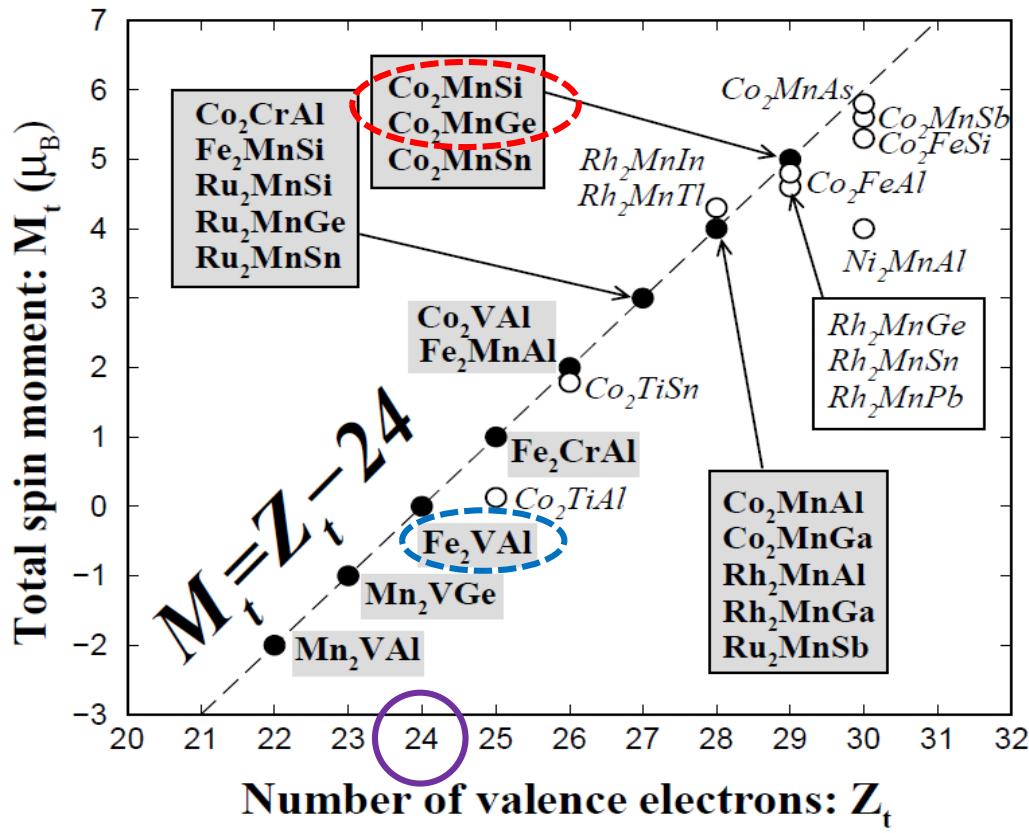
Hybridization between
Ni and Mn in minority
bands in NiMnSb



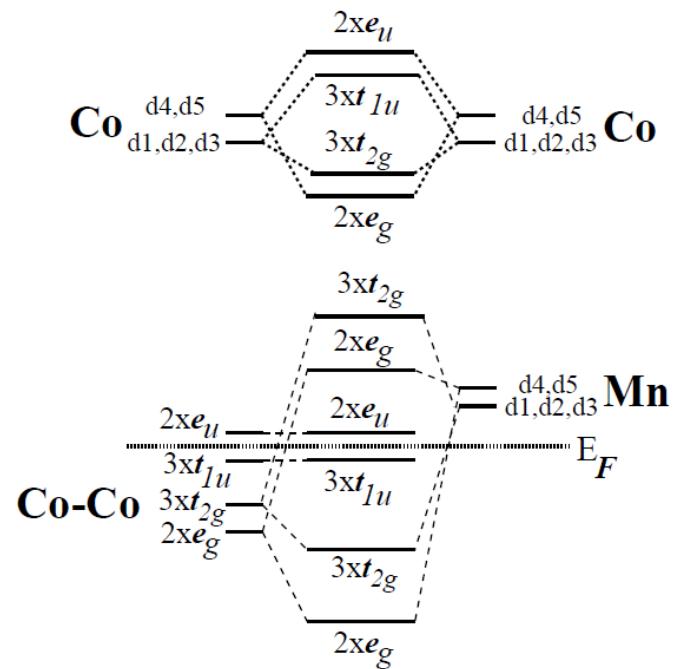
I. Galanakis, P. H. Dederiches, N. Papanikolaou,
Phys. Rev. B **66** 134428 (2002).

Slater-Pauling curve for full-Heusler compounds

Full-Heusler compounds



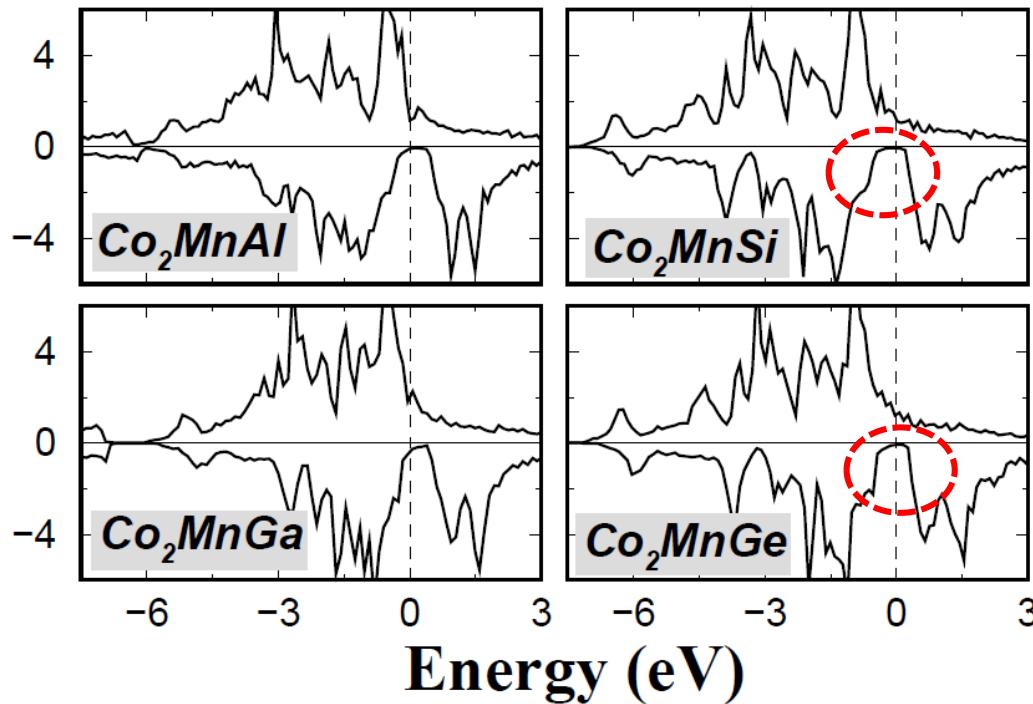
Hybridization between
Co-Co and Mn in minority
bands in $Co_2MnSi(Ge)$



I. Galanakis, P. H. Dederiches, and N. Papanikolaou,
Phys. Rev. B **66** 174429 (2002).

More first-principles calculations

DOS (states/eV)



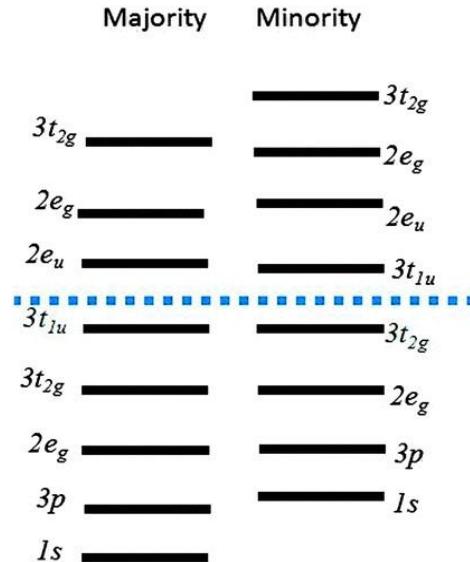
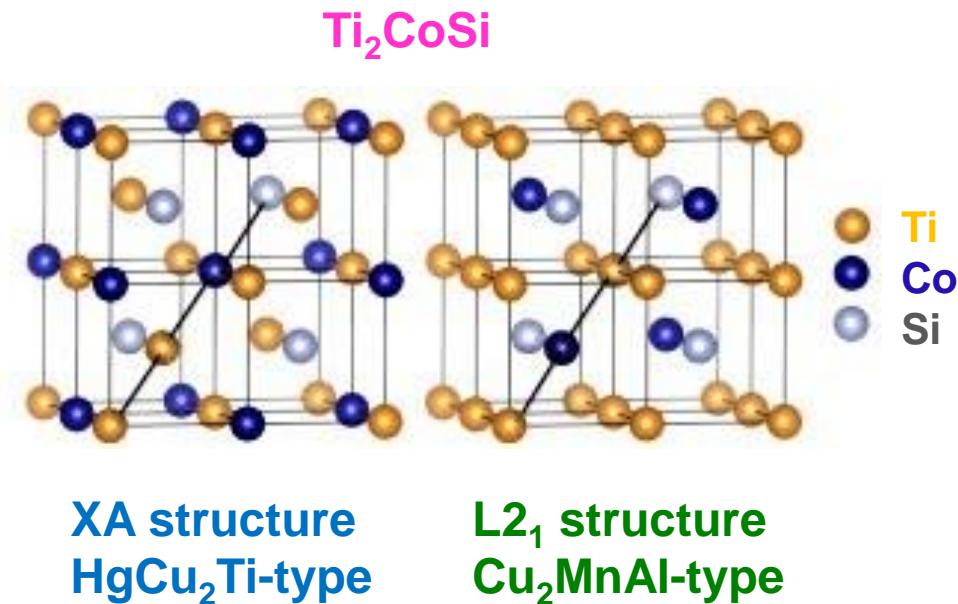
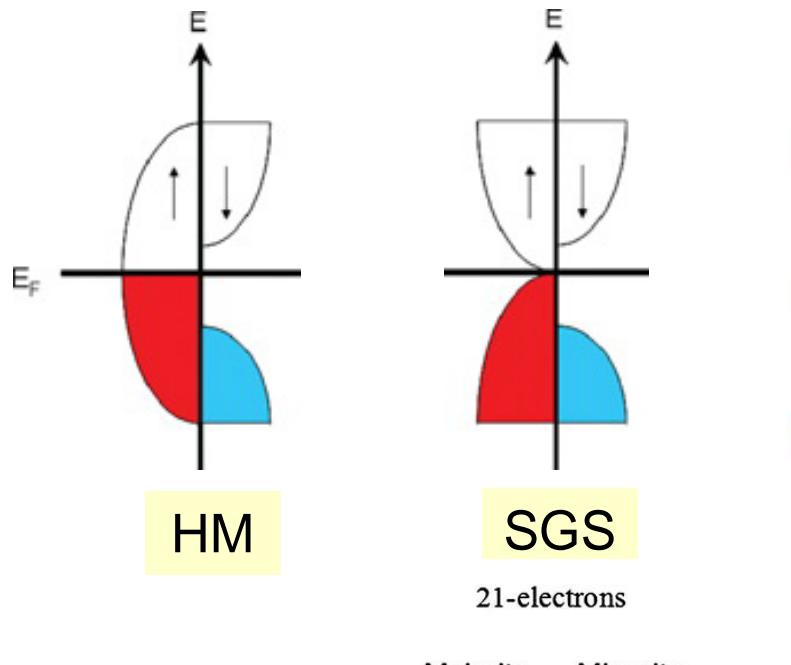
Spin-resolved DOS
for Co_2MnZ

Review article: *J. Phys.: Condens. Matter* **19** 315213 (2007).

“First-principles calculation of the effects of partial alloy disorder on the static and dynamic magnetic properties of Co_2MnSi ”, *Phys. Rev. B* **95**, 094425 (2017).

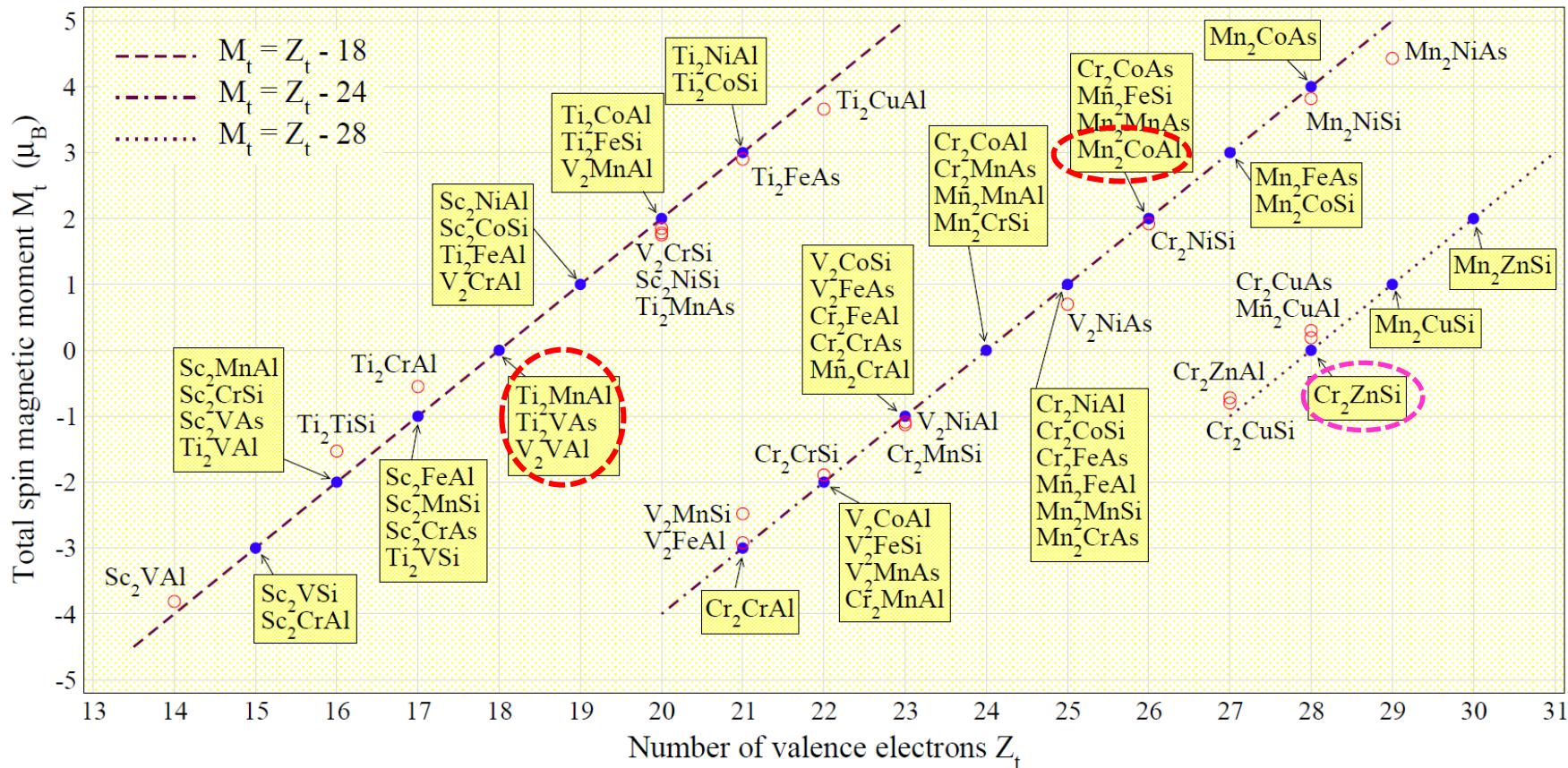
“Computational investigation of half-Heusler compounds for spintronics applications”, *Phys. Rev. B* **95**, 024411 (2017).

Recent advances in the Heusler-based spin gapless semiconductors

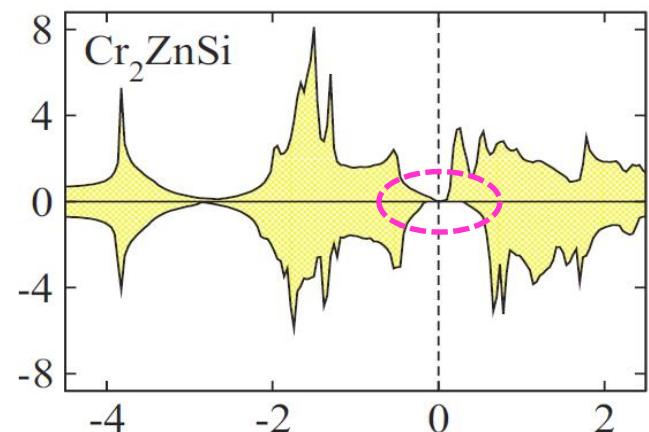


Inverse Heusler

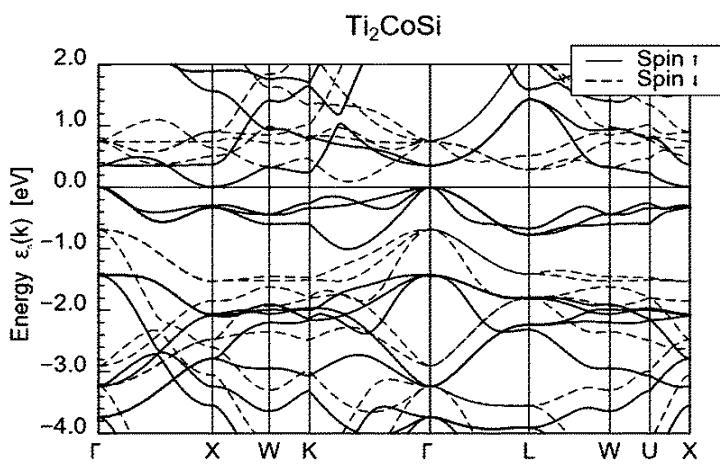
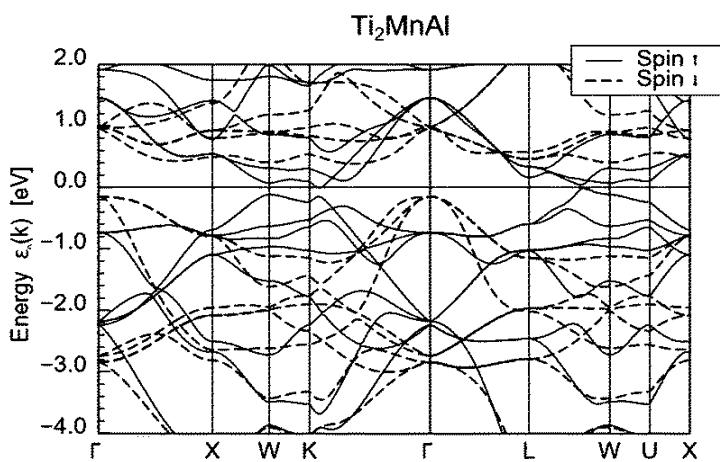
Generalized Slater-Pauling rule for inverse Heusler compounds



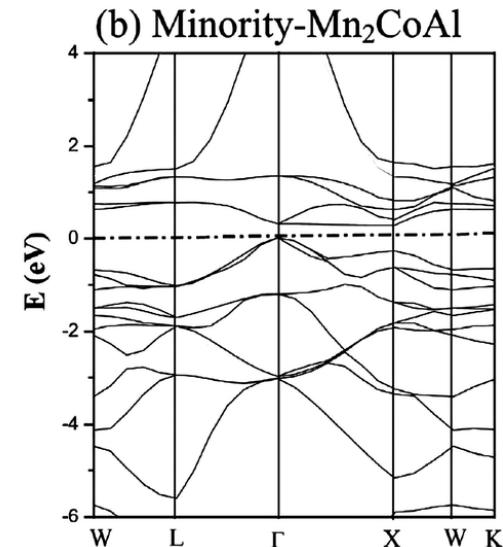
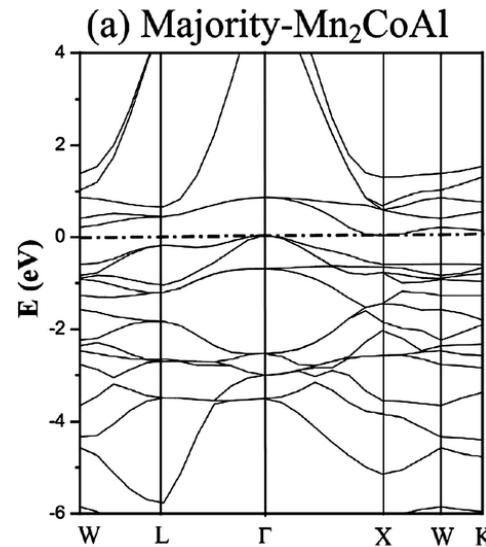
S. Skaftouros, K. Ozdogan, E. Sasioglu,
I. Galanakis, *Phys. Rev. B* **87** 024420 (2013).



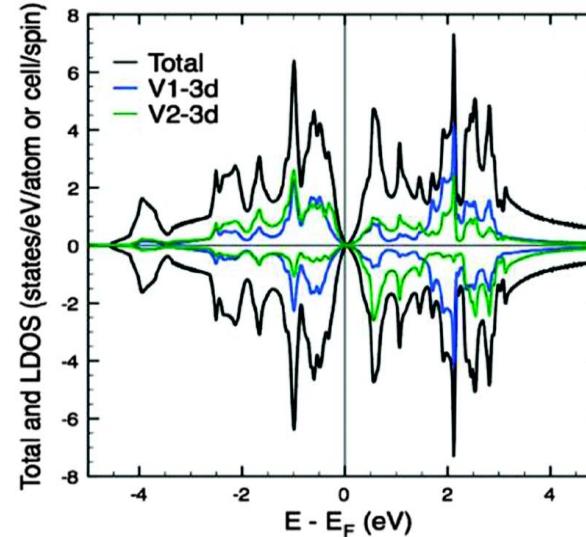
Possible SGs: Theoretical studies



Appl. Phys. Lett. **102** 022402 (2013)



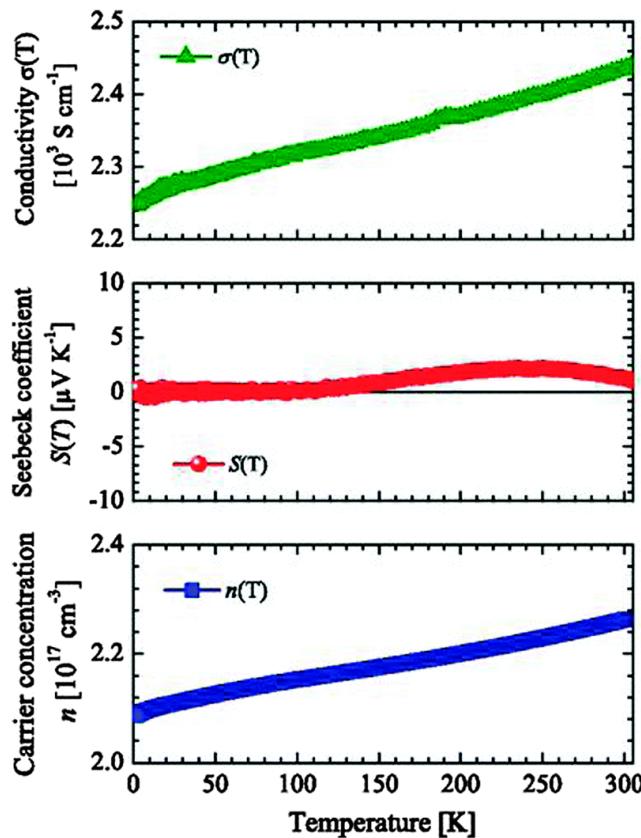
Phys. Rev. B **77** 014427 (2008)



Phys. Rev. B **91** 094409 (2015)

Possible SGSS: Experimental studies

Polycrystalline Mn_2CoAl



Phys. Rev. Lett. **110**, 100401 (2013)

Polycrystalline V_3Al

Phys. Rev. B **91** 094409 (2015)

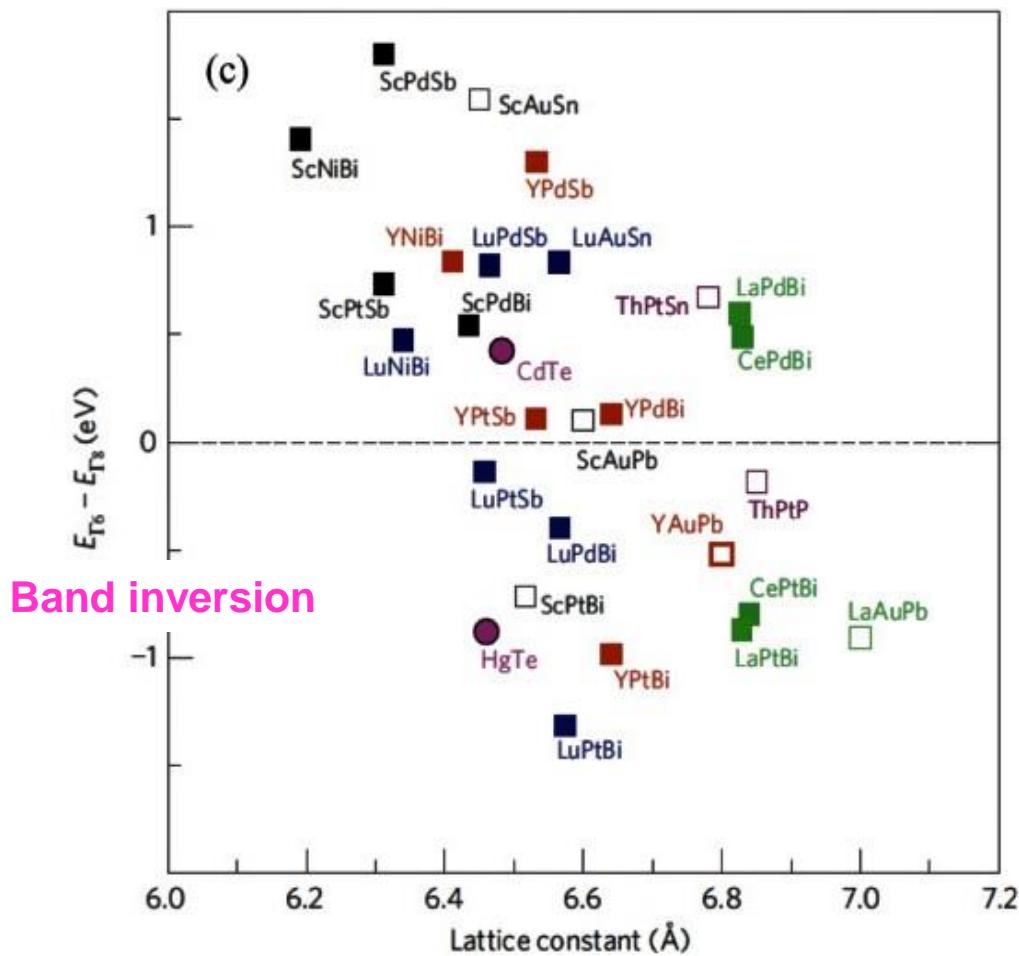
Polycrystalline CrVTiAl

Appl. Phys. Lett. **121** 053903 (2017)

Thin film Ti_2MnAl

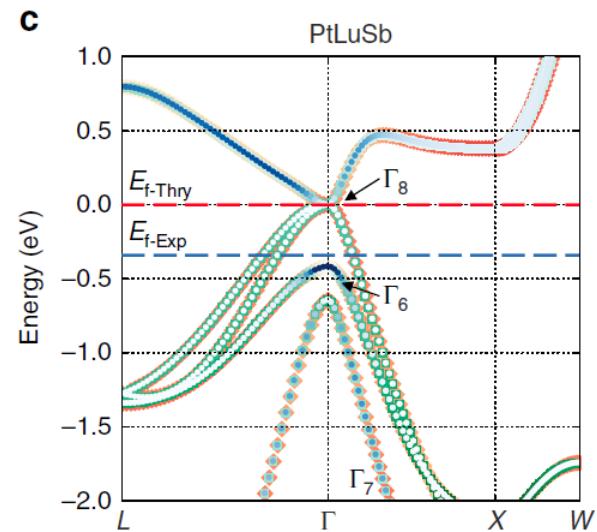
Phys. Status Solidi RRL **9** 641 (2015)

Topological materials in half-Heusler compounds



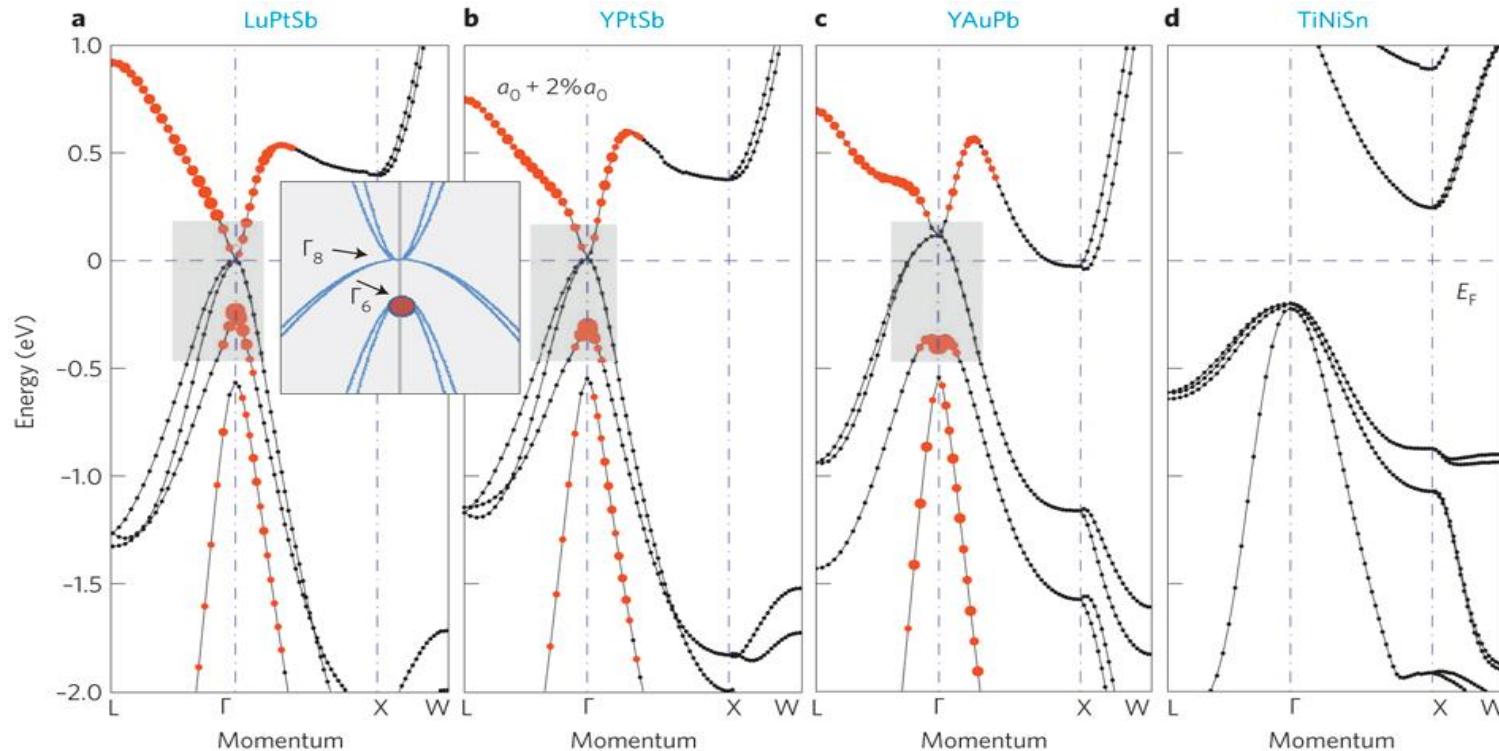
S. Chadov et al., *Nature Materials* **9**, 541 (2010)

Claudia Felser's group



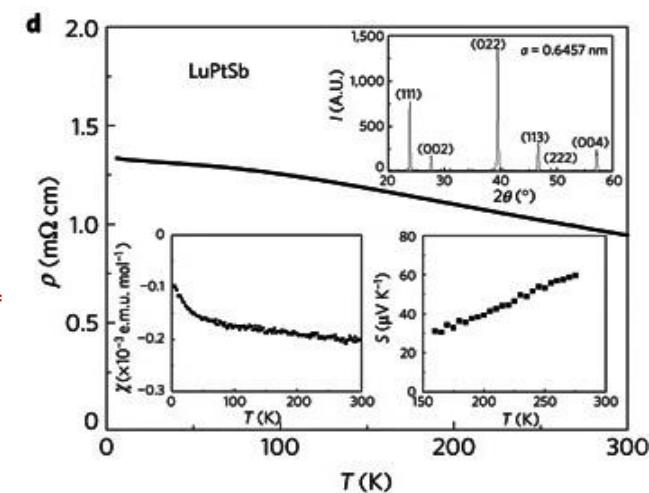
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Topological materials in half-Heusler compounds



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Cava's group



Evidence for topological behavior in half-Heusler compounds

“Observation of a topologically non-trivial surface state in half-Heusler PtLuSb (001) thin films”

J. A. Logan et al., *Nature Communications* **9**, 11993 (2016)

“Observation of unusual topological surface states in half-Heusler compounds LnPtBi (Ln=Lu, Y)”

Z. K. Liu et al., *Nature Communications* **7**, 12924 (2016)

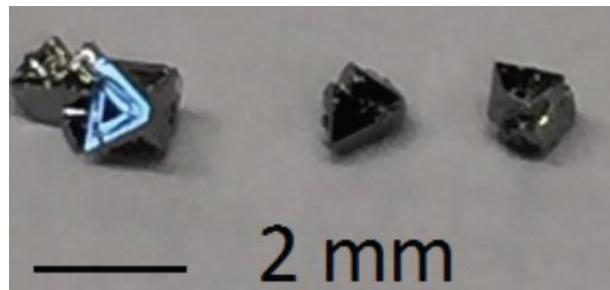
“Large anomalous Hall effect in a half-Heusler antiferromagnet”

T. Suzuki et al., *Nature Physics* **12**, 1119 (2016)

Topological materials in full-Heusler compounds

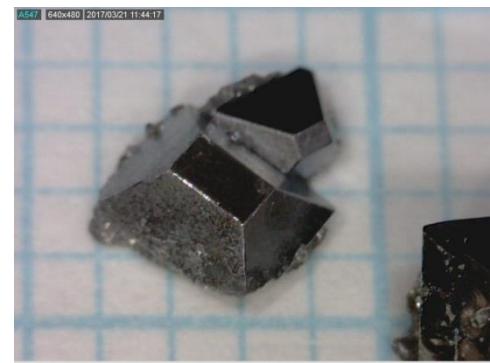
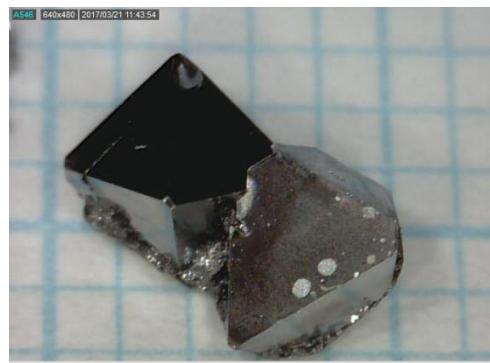
“Room-temperature magnetic topological Weyl fermion and nodal line semimetal states in **half metallic Heusler Co_2TiX ($\text{X}=\text{Si, Ge, or Sn}$)**”
Guoqing Chang et al., Scientific Reports 6, 38839 (2016).

“Time-reversal-breaking Weyl fermions in **magnetic Heusler alloys**”
Zhijun Wang et al., Phys. Rev. Lett. 17, 236401 (2016).



Single crystalline Co_2ZrSn

→ Cava's group



→ Our group

Summary

Theoretical people continue paying attention to Heusler compounds, focusing on their thermoelectric, half-metallic, and topological properties.

Experimental people continue synthesizing novel Heusler compounds and investigating their promising properties for further applications.

Thanks for your attention!