Time-Reversal Breaking Weyl Metals and Non-symmorphically Protected Fermions

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in collaboration with

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Outline

1. Time-Reversal Breaking Weyl Metals

Introduction-Motivation

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Introduction

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Topological Classification

Materials Search

Conclusions

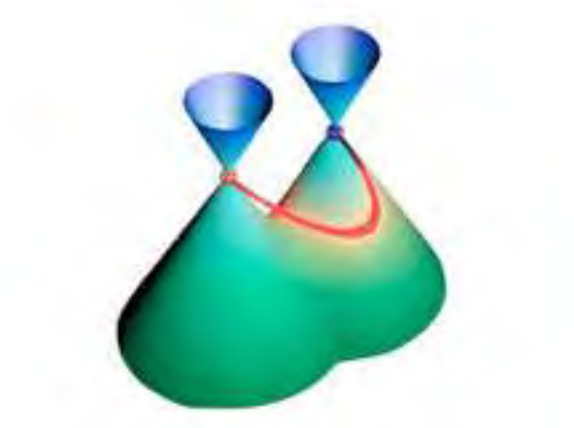
Time-Reversal Breaking Weyls

- Weyls fermions are described by massless Weyl equation with fixed chirality

$$H_D = E_0\mathcal{I} + \mathbf{v_0} \cdot \mathbf{q}\mathcal{I} + \sum_{i=1}^{3} \mathbf{v_i} \cdot \mathbf{q}\sigma_i$$

$$\mathbf{q} = \mathbf{k} - \mathbf{k_0}$$

$$\Delta E = \mathbf{v_0} \cdot \mathbf{q} \pm \sqrt{\sum_{i=1}^{3} (\mathbf{v_i} \cdot \mathbf{q})^2}$$



- We can also assign a chirality: $c = sgn(\mathbf{v_1} \cdot \mathbf{v_2} \times \mathbf{v_3})$

- Stable in 3D: Perturbation can shift the position of the crossing point but it cannot remove it.

- They act like magnetic monopoles in momentum space whose charge is given by the chirality

The Berry connection, is defined as

$$\overrightarrow{A}(\overrightarrow{k}) = \sum_n \langle n\overrightarrow{k}|\overrightarrow{\nabla}_k|n\overrightarrow{k}\rangle$$

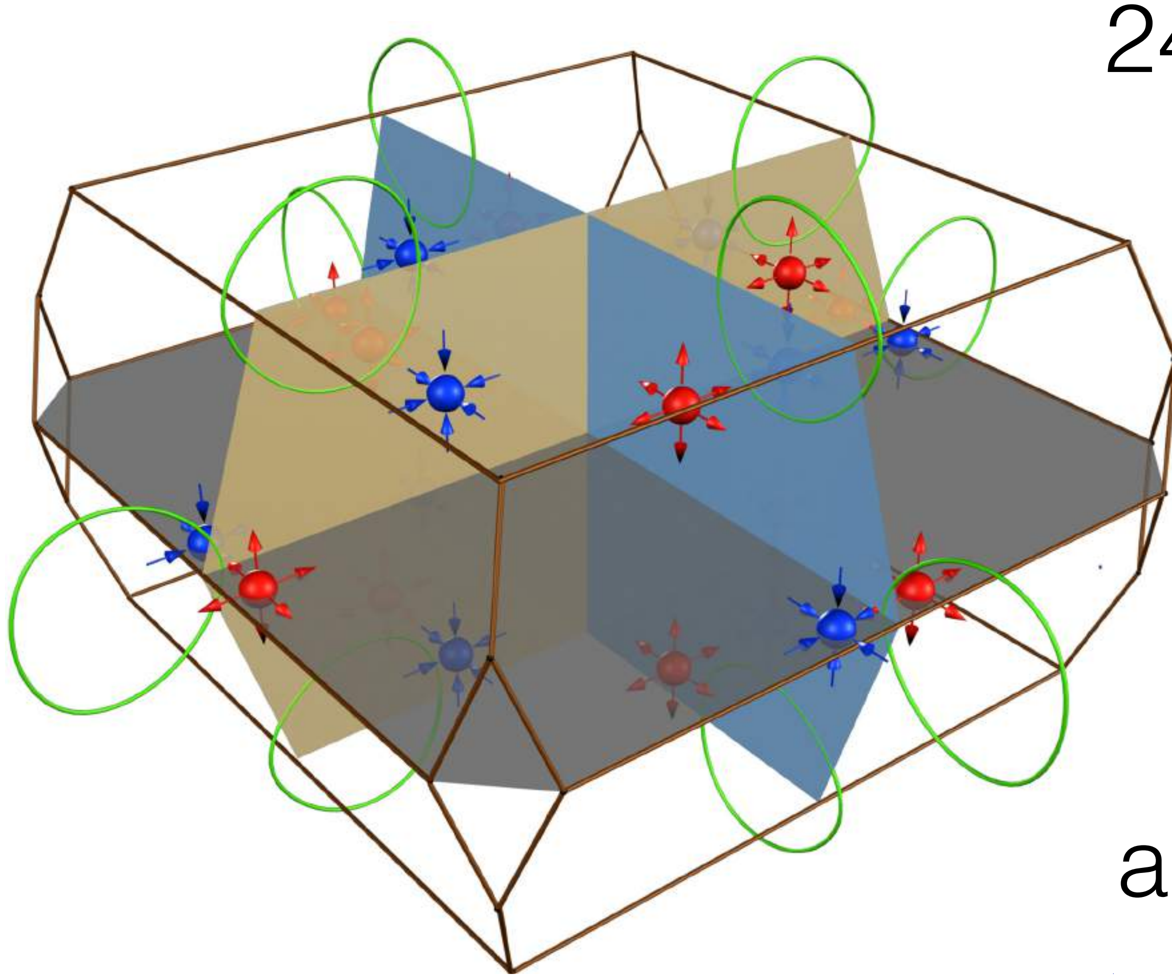
Can be consider as the magnetic field of momentum space

$$\overrightarrow{B}(\overrightarrow{k}) = \overrightarrow{\nabla}_k \times \overrightarrow{A}(\overrightarrow{k})$$

Then these Weyls points are just like magnetic monopoles in momentum space

$$\overrightarrow{\nabla}_k \overrightarrow{B}(\overrightarrow{k}) = \pm\delta(\overrightarrow{k} - \overrightarrow{k}_0)$$

- Weyl nodes appear in multiples of 2, with time reversal symmetry this number raises to 4



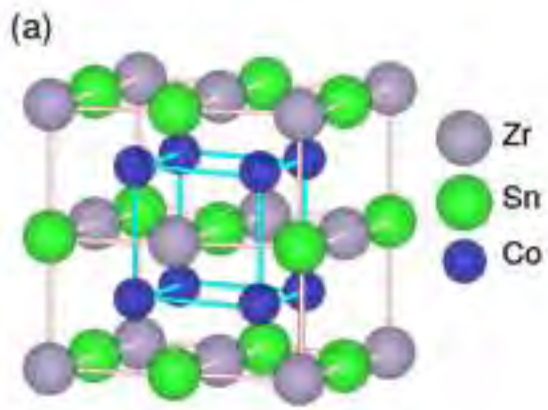
The TaAs family presents 24 Weyl nodes, due to several others mirror symmetries

↓

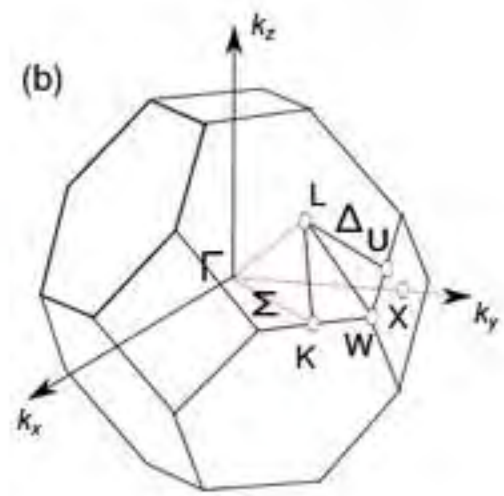
Rise complicated transport and spectroscopic properties

Motivation : Look for Time-Reversal breaking Weyls

- We propose candidates for Weyl metals that are XCo2Z (X=V,Zr,Ti,Nb,Hf; Z=Si,Ge,Sn), VCo2Al and VCo2Ga



sg 225, C_4 and I



Product of inversion eigenvalue

$$\prod_{\mathbf{K}_i=-\mathbf{K}_i} \prod_{E_n(\mathbf{K}_i)<E_f} \zeta_n(\mathbf{K}_i)$$

Γ	+	+	−	−	−	+	+	+	−	−	+	+	+	;	+
			−	−	−	+	+	+	+	+	+	+	+	;	−
X	−	+	−	+	−	−	+	+	+	−	−	−	−	;	+
			−	+	+	−	−	+	+	−	−	−	−	;	+
L	−	−	−	+	+	−	−	−	+	+	+	−	−	;	−
			−	−	−	−	−	−	+	+	+	+	+	;	−
Product														−	
														+	

- They follow the Slater-Pauling rule: $m = N_v - 24$

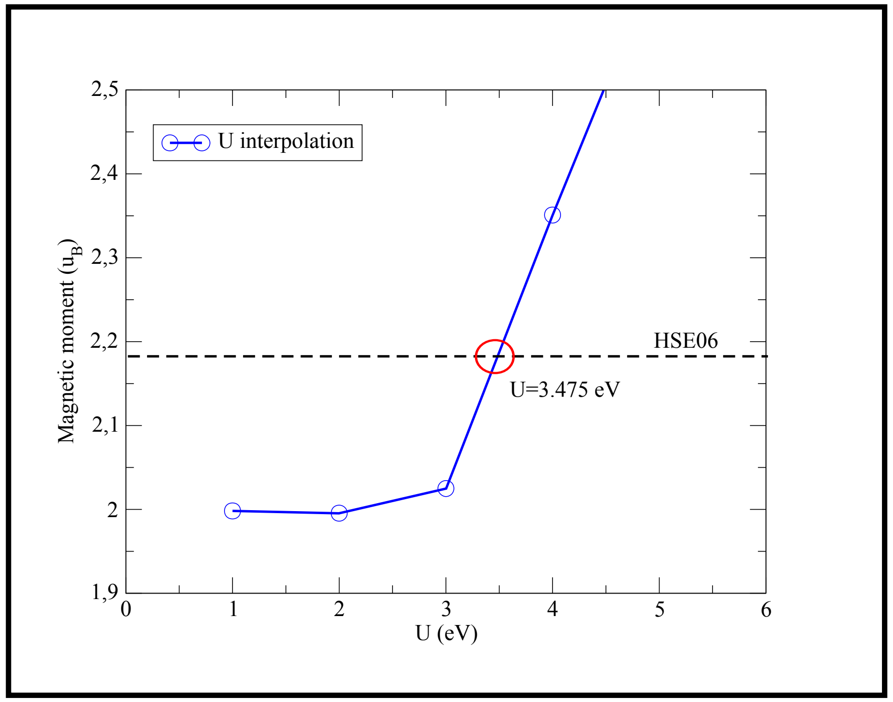
- Half metallic magnetism with 2 u_B per formula unit

- In the following we are gonna focus in ZrCo2Sn that has been synthesized experimentally

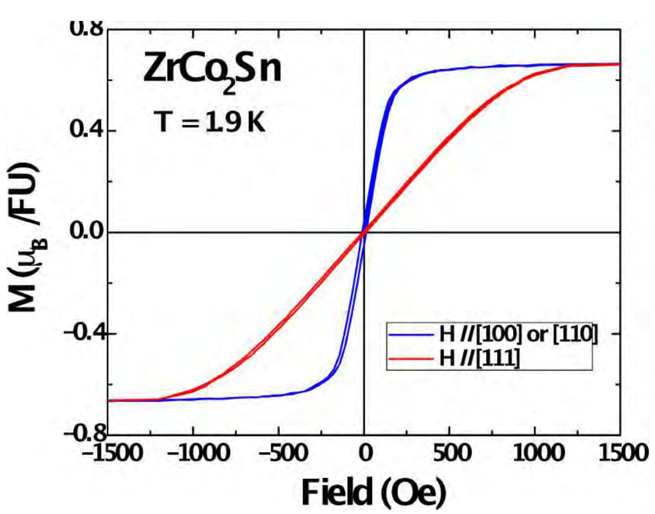
G. H. Fecher, H. C. Kandpal, S.Wurmehl, C. Felser, and G. Schoenhense, Journal of Applied Physics 99,08J106 (2006).

Electronic structure:

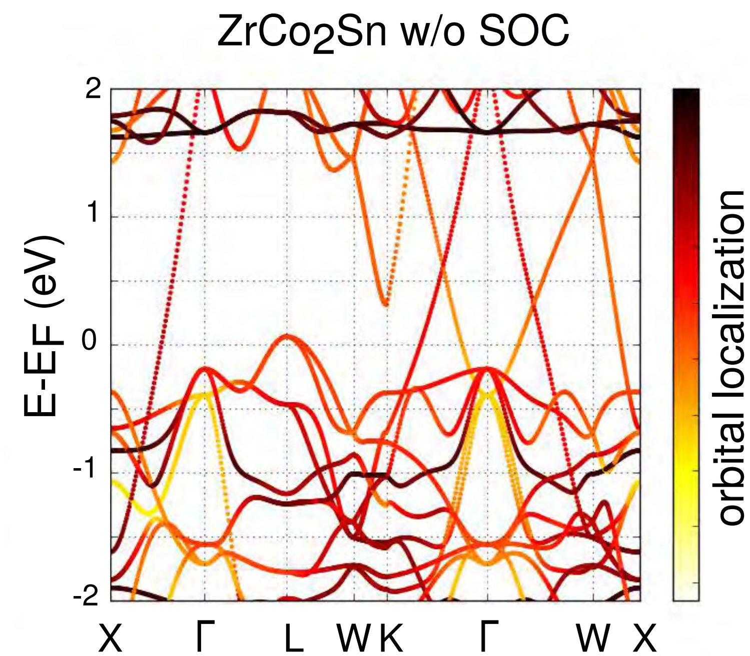
(1) On site Coulomb interaction

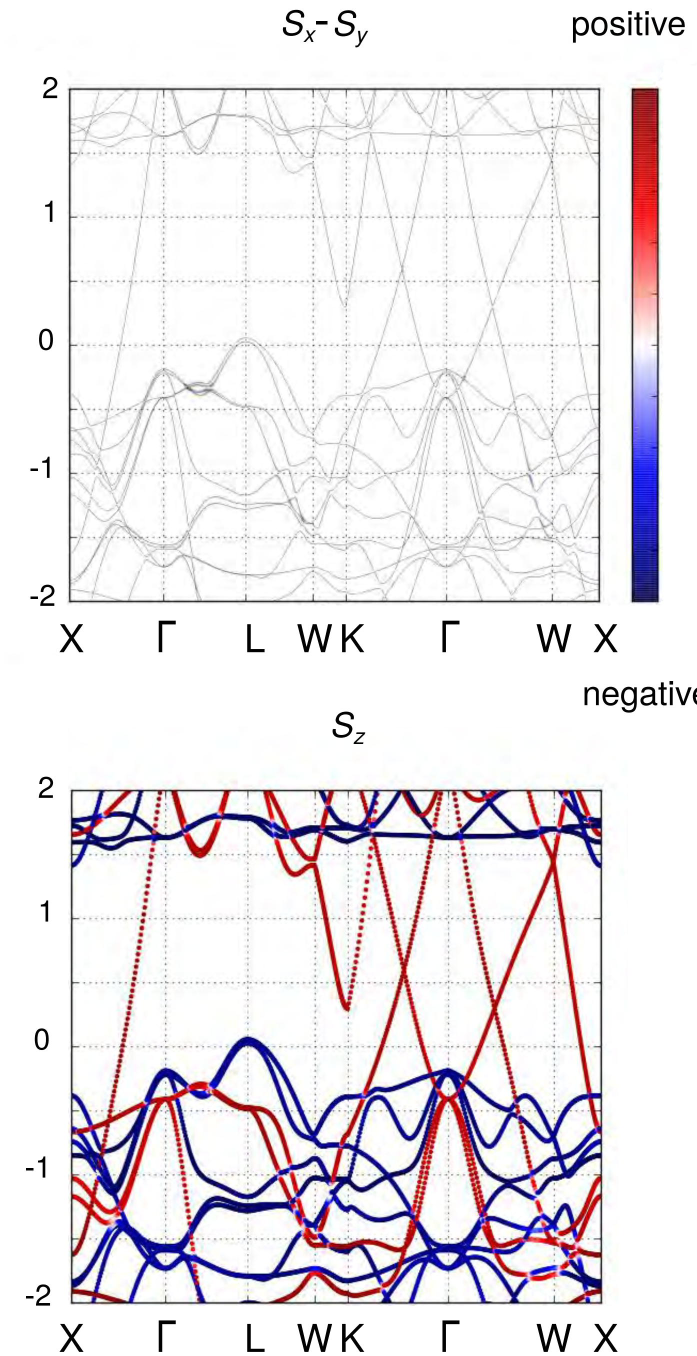


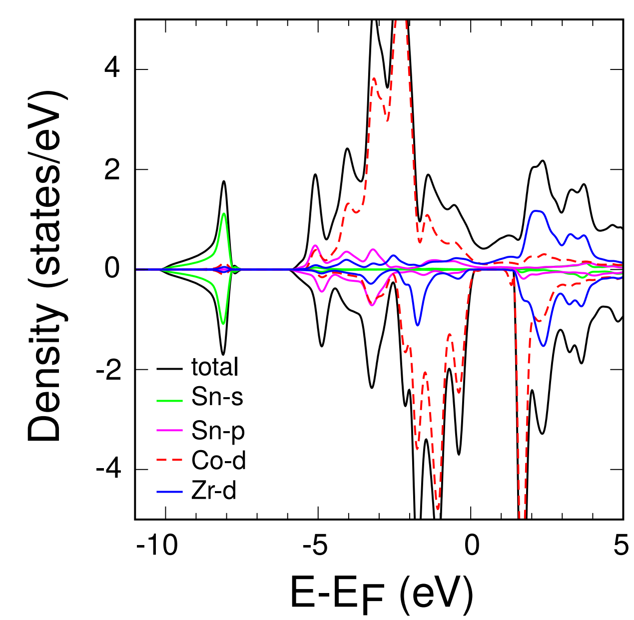
ANISOTROPY
easy axis [110]



(2) SOC vs NSOC



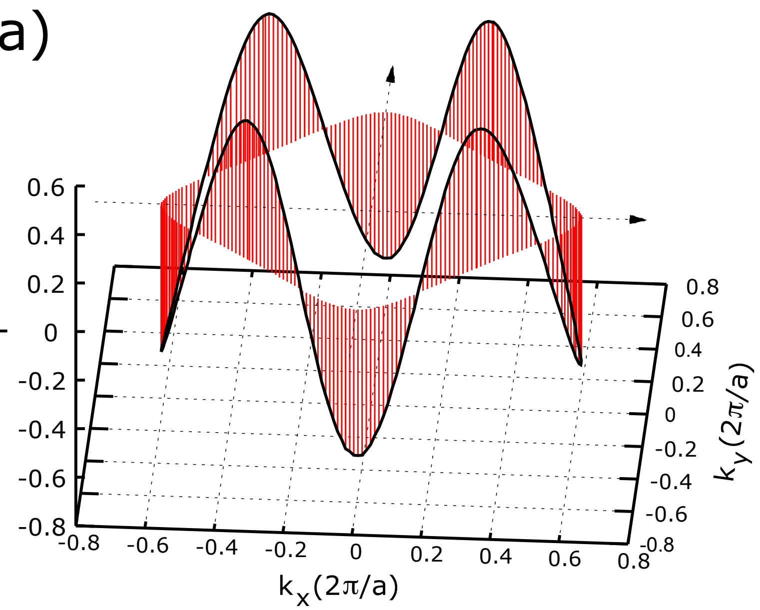




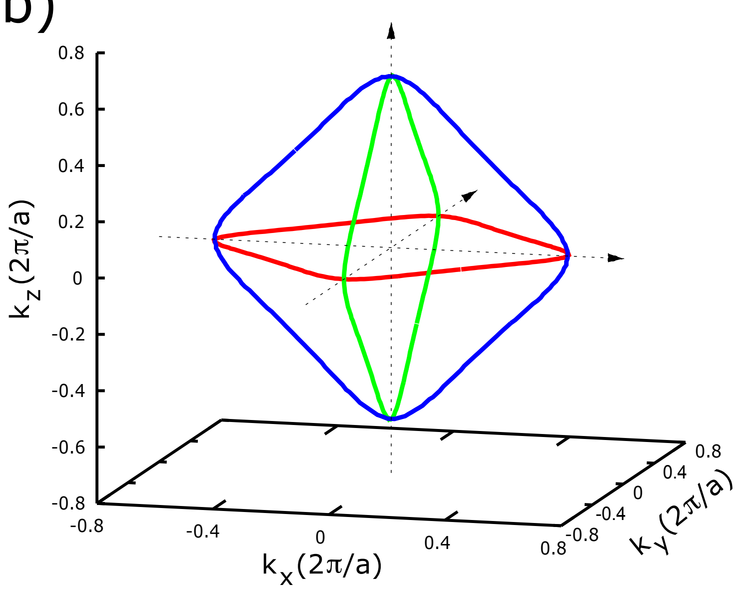
GGA+U PBE

Symmetry analysis and Weyls physics

(a)

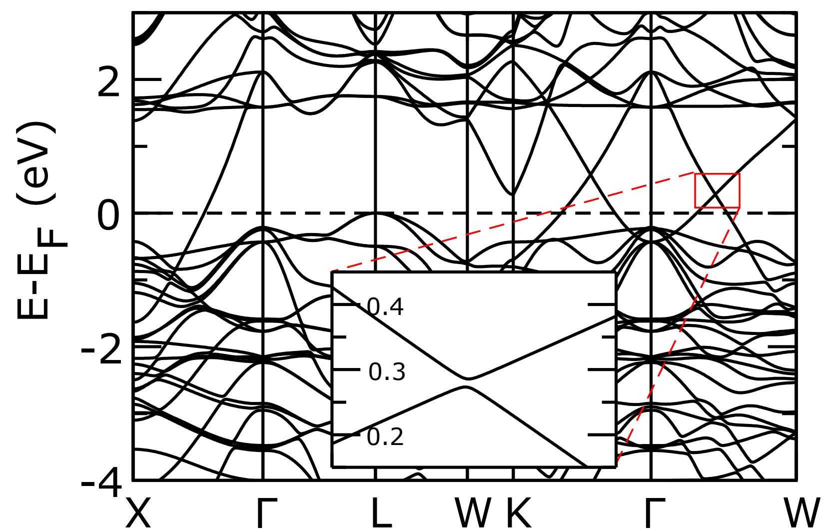


(b)

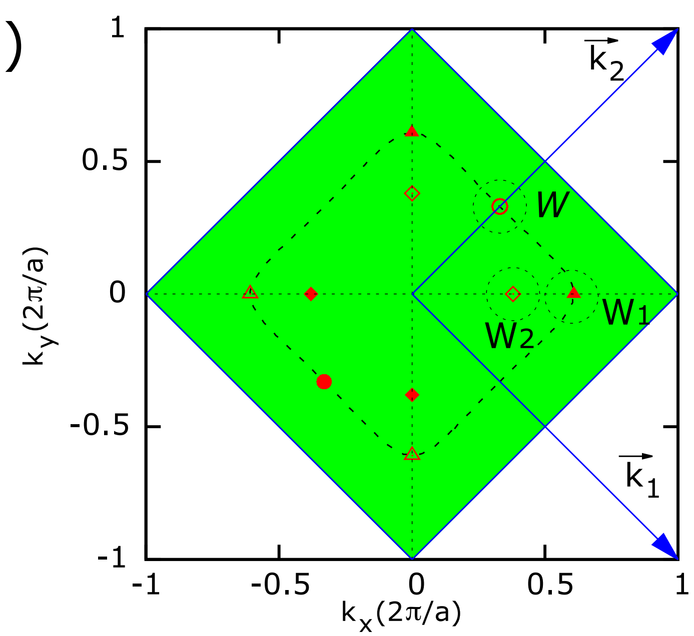


NSOC:M_x,M_y,M_z

(c)



(d)



SOC

Weyl points	coordinates $(k_x\frac{2\pi}{a}, k_y\frac{2\pi}{a}, k_z\frac{2\pi}{a})$	Chern number	$E-E_{\mathrm{F}}$ (eV)
W	$(0.334, 0.334, 0)$	-1	$+0.6$
W_1	$(0.58, -0.0005, 0)$	$+1$	-0.6
W_2	$(0.40, 0.001, \pm 0.28)$	-1	$+0.3$

Chern number of (1,-1,0) plane =3

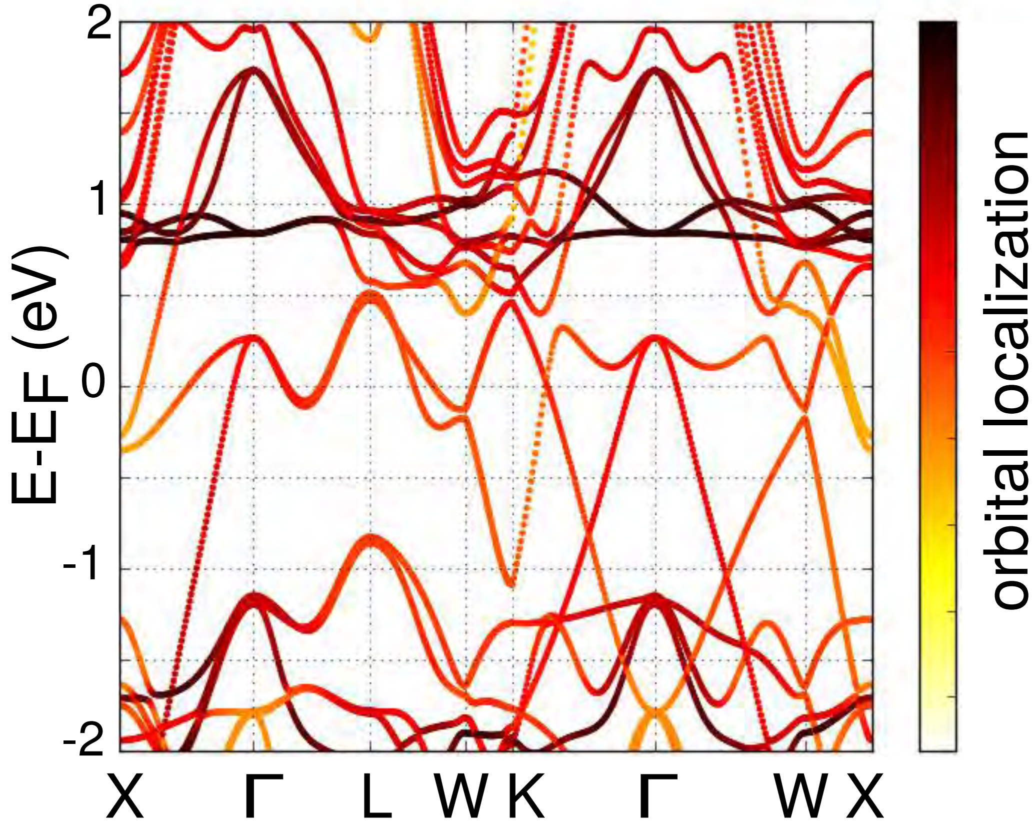
W:$C2_{110}$

W_1:I and $C2_{110}$

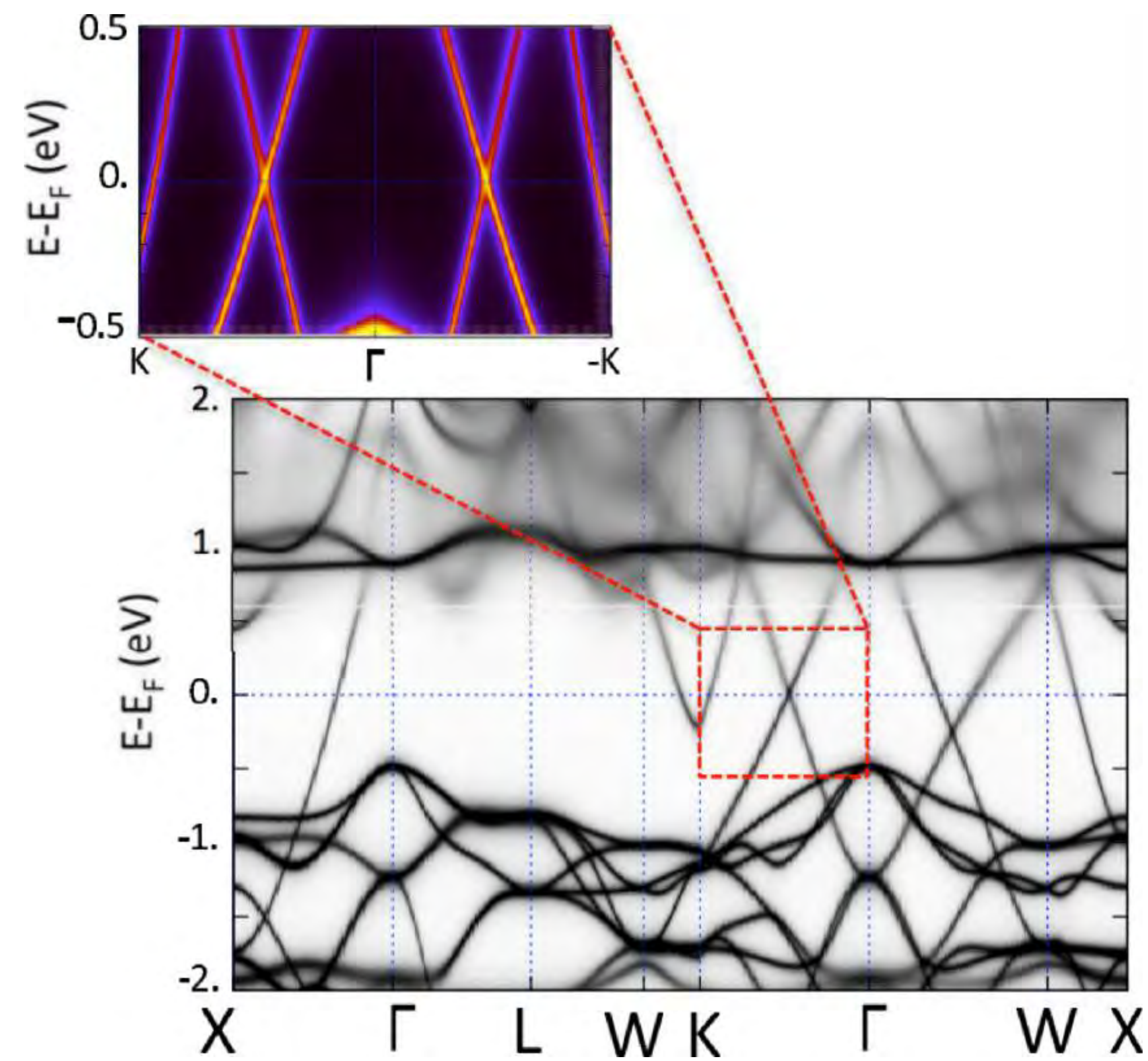
W_2:generic

(no stable)

$NbCo_2Sn$ SOC



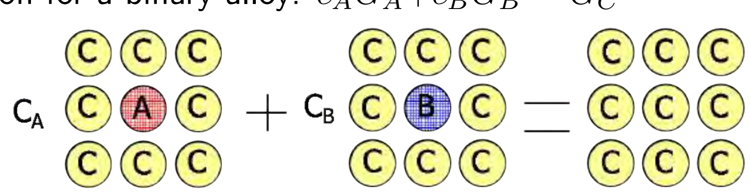
$Zr_{0.725}Nb_{0.275}Co_2Sn$



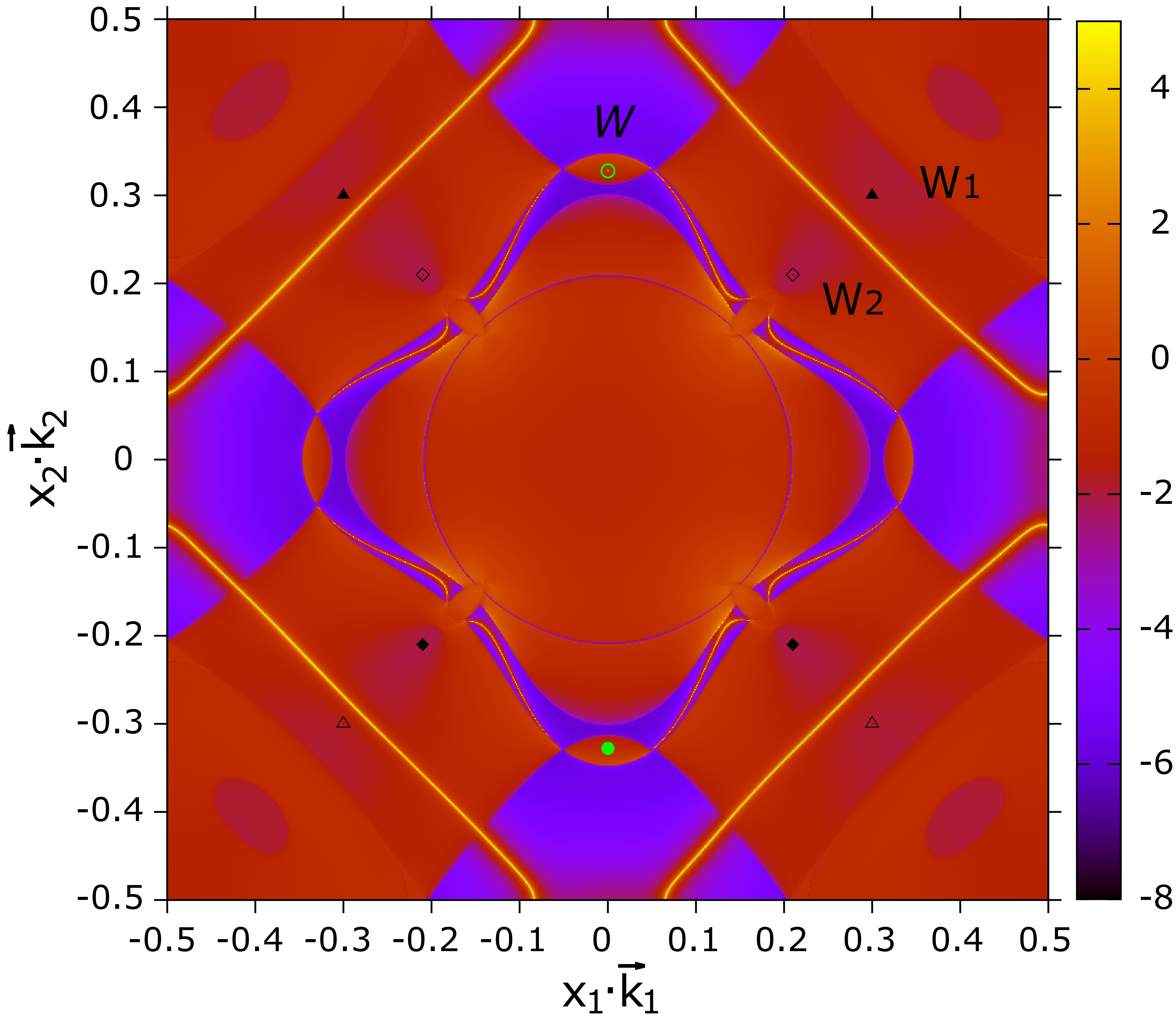
Coherent Potential Approximation

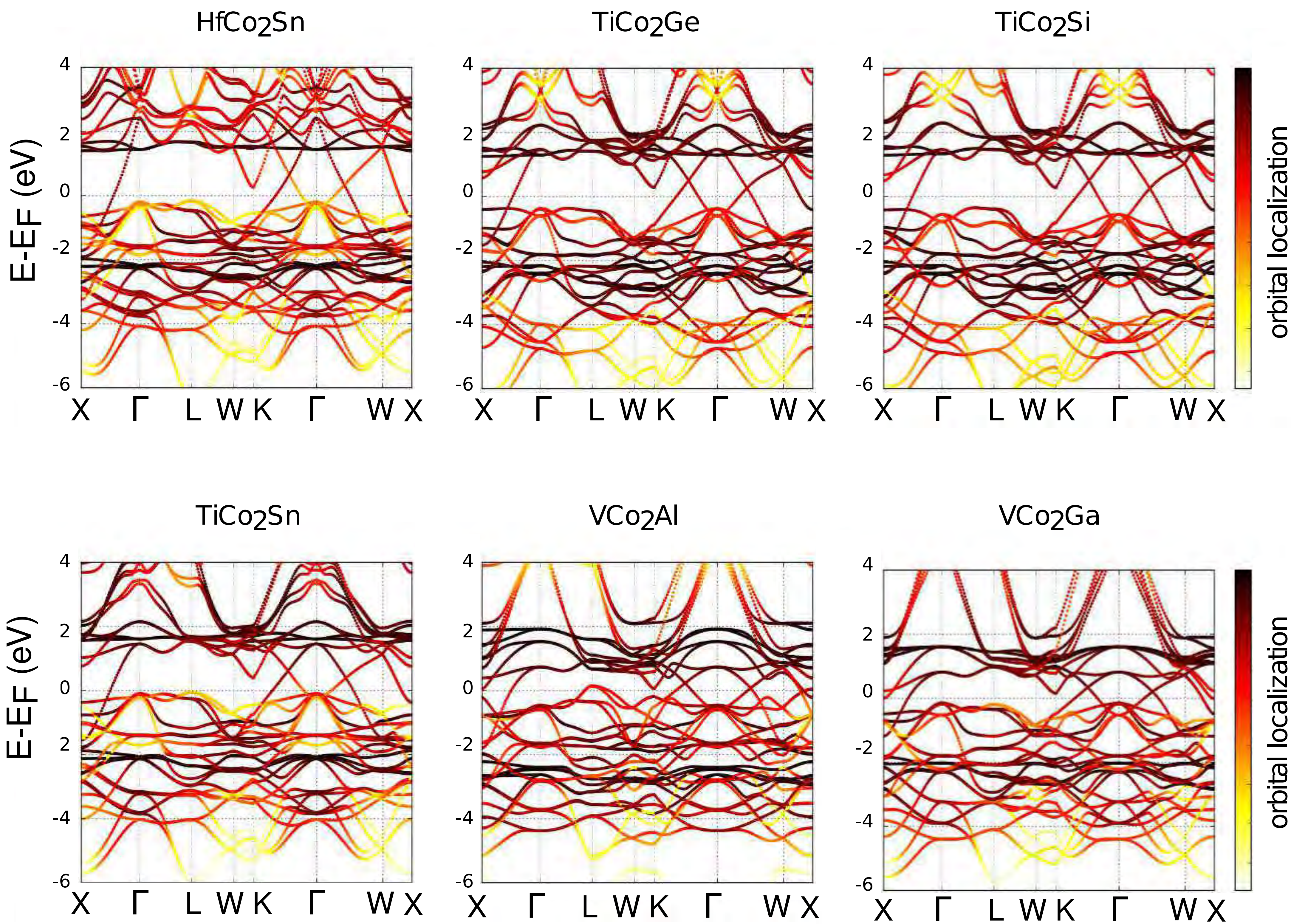
Based on scattering theory $$T_C(E) = \sum_i c_i T_i(E).$$

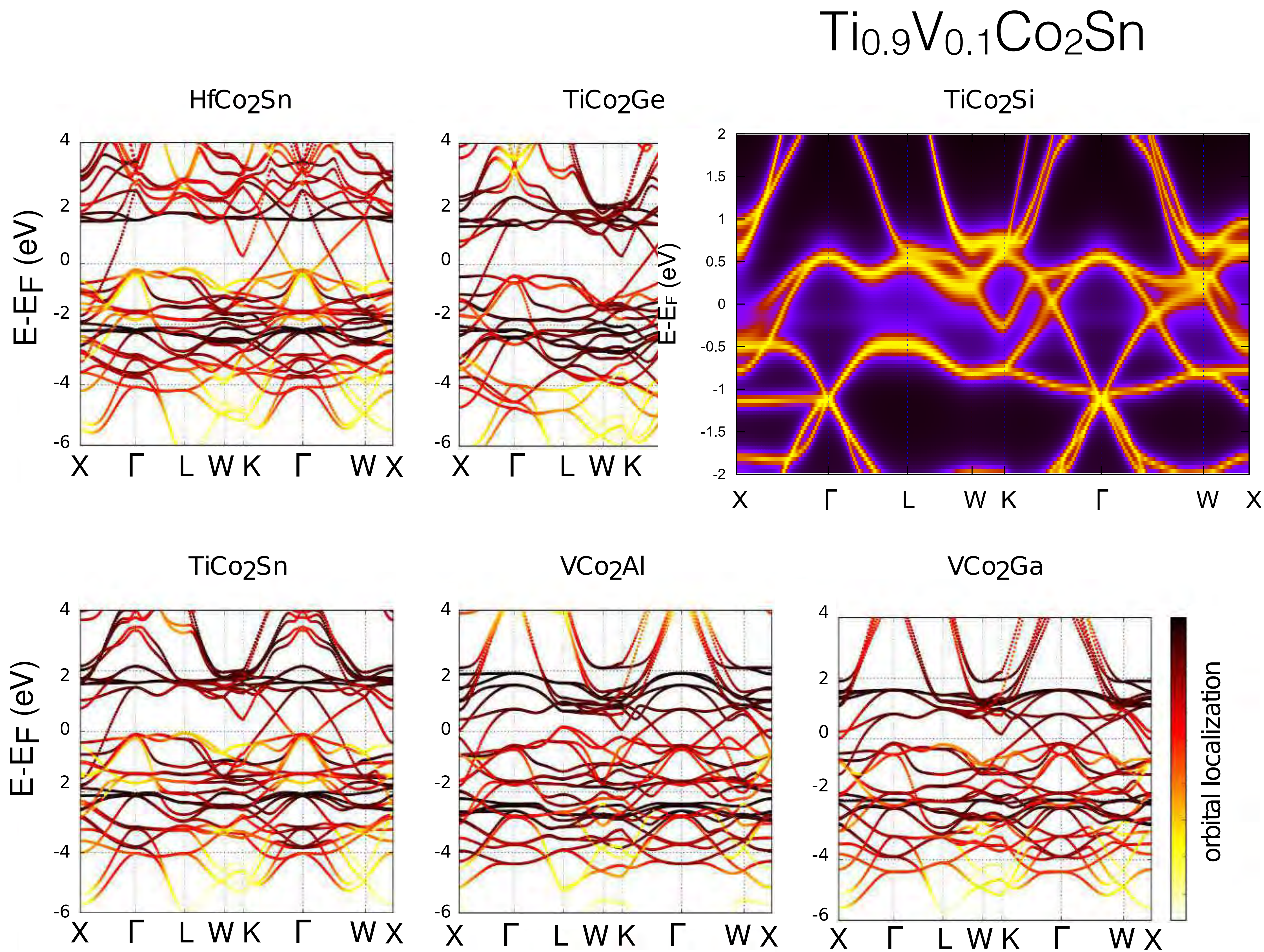
CPA equation for a binary alloy: $c_A G_A + c_B G_B = G_C$



(001 surface) Fermi Arcs




HfCo2Sn
TiCo2Ge
TiCo2Si
TiCo2Sn
VCo2Al
VCo2Ga
E-EF (eV)
orbital localization
X Γ L W K Γ W X
4
2
0
-2
-4
-6


Ti0.9V0.1Co2Sn
HfCo2Sn
TiCo2Ge
TiCo2Si
TiCo2Sn
VCo2Al
VCo2Ga
E-EF (eV)
X Γ L W K Γ W X
orbital localization

Conclusions

- We have predicted theoretically that a new family of Co-base Heuslers realize Weyls systems
- By means of ab initio calculations we have determined the easy axis of $ZrCo_2Sn$ to be [110]
- Symmetry analysis shows there are 2 Weyls separated in momentum space of the order of 2π
- We doped the compound to shift the Weyls to Fermi level
- We have also obtained the Fermi arc structure of this materials

arXiv:1603.00479v1

see also Chandra Shekhar et al. arXiv:1604.01641

Non-symmorphically protected fermions

1. The existence of 3fold and higher degeneracies has been known from band theory

The Mathematical Theory of Symmetry in Solids
Irreducible representations in space groups

2. The topological classification of these degeneracies is still missing

3. We will look for irreducible representations at high symmetry points, being the dimension of these irreps the number of bands that meet at high symmetry-point.

SG	La	k	d	Generators
198	cP	R	6	$\{C^-_{3,111}\|010\}, \{C_{2x}\|\frac{1}{2}\frac{3}{2}0\}, \{C_{2y}\|0\frac{3}{2}\frac{1}{2}\}$
199	cB	P	3	$\{C^-_{3,111}\|101\}, \{C_{2x}\|\bar{\frac{1}{2}}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\bar{\frac{1}{2}}\}$
205	cP	R	6	$\{C^-_{3,111}\|010\}, \{C_{2x}\|\frac{1}{2}\frac{3}{2}0\}, \{C_{2y}\|0\frac{3}{2}\frac{1}{2}\}, \{I\|000\}$
206	cB	P	6	$\{C^-_{3,111}\|101\}, \{C_{2x}\|\bar{\frac{1}{2}}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\bar{\frac{1}{2}}\}$
212	cP	R	6	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C^-_{3,111}\|000\},\{C_{2,1\bar{1}0}\|\frac{1}{4}\frac{1}{4}\frac{1}{4}\}$
213	cP	R	6	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C^-_{3,111}\|000\},\{C_{2,1\bar{1}0}\|\frac{3}{4}\frac{3}{4}\frac{3}{4}\}$
214	cB	P	3	$\{C^-_{3,111}\|101\}, \{C_{2x}\|\bar{\frac{1}{2}}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\bar{\frac{1}{2}}\}$
220	cB	P	3	$\{C_{3,\bar{1}\bar{1}1}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2x}\|\frac{3}{2}\frac{3}{2}0\},\{IC^-_{4x}\|\frac{1}{2}11\}$
230	cB	P	6	$\{C_{3,\bar{1}\bar{1}1}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2x}\|\frac{3}{2}\frac{3}{2}0\},\{IC^-_{4x}\|\frac{1}{2}11\}$
130	tP	A	8	$\{C_{4z}\|000\}, \{\sigma_{\bar{x}y}\|00\frac{1}{2}\}, \{I\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
135	tP	A	8	$\{C_{4z}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{\sigma_{\bar{x}y}\|00\frac{1}{2}\}, \{I\|000\}$
218	cP	R	8	$\{C_{2x}\|001\}, \{C_{2y}\|000\}, \{C^-_{3,111}\|001\}, \{\sigma_{\bar{x}y}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
220	cB	H	8	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\frac{3}{2}\}, \{C^-_{3,111}\|001\}, \{\sigma_{\bar{x}y}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
222	cP	R	8	$\{C^-_{4z}\|000\}, \{C_{2x}\|000\}, \{C^-_{3,111}\|010\}, \{I\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
223	cP	R	8	$\{C^-_{4z}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{C_{2x}\|000\}, \{C^-_{3,111}\|010\}, \{I\|000\}$
230	cB	H	8	$\{C_{4z}\|0\frac{1}{2}0\}, \{C_{2y}\|1\frac{1}{2}\frac{1}{2}\}, \{C_{3,111}\|111\}, \{I\|000\}$

All space groups include non-symmorphic generators

cP: cubic primitive
cB: cubic body-centered
tP: tetragonal primitive

Bravais lattice	Lattice vectors	Reciprocal lattice vectors
Primitive cubic	$(a,0,0),(0,a,0),(0,0,a)$	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{a}(0,0,1)$
Body-centered cubic	$\frac{a}{2}(-1,1,1), \frac{a}{2}(1,-1,1), \frac{a}{2}(1,1,-1)$	$\frac{2\pi}{a}(0,1,1), \frac{2\pi}{a}(1,0,1), \frac{2\pi}{a}(1,1,0)$
Primitive tetragonal	$(a,0,0),(0,a,0),(0,0,c)$	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{c}(0,0,1)$

TABLE I. Lattice and reciprocal lattice vectors

SG	La	k	d	Generators
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205	cP	R	6	$\{C^-_{3,111}\|010\}, \{C_{2x}\|\tfrac{1}{2}\tfrac{3}{2}0\}, \{C_{2y}\|0\tfrac{3}{2}\tfrac{1}{2}\}, \{I\|000\}$
206	cB	P	6	$\{C^-_{3,111}\|101\}, \{C_{2x}\|\tfrac{1}{2}\tfrac{1}{2}0\}, \{C_{2y}\|0\tfrac{1}{2}\tfrac{1}{2}\}$
212	cP	R	6	$\{C_{2x}\|\tfrac{1}{2}\tfrac{1}{2}0\},\{C_{2y}\|0\tfrac{1}{2}\tfrac{1}{2}\},\{C^-_{3,111}\|000\},\{C_{2,1\bar{1}0}\|\tfrac{1}{4}\tfrac{1}{4}\tfrac{1}{4}\}$
213	cP	R	6	$\{C_{2x}\|\tfrac{1}{2}\tfrac{1}{2}0\},\{C_{2y}\|0\tfrac{1}{2}\tfrac{1}{2}\},\{C^-_{3,111}\|000\},\{C_{2,1\bar{1}0}\|\tfrac{3}{4}\tfrac{3}{4}\tfrac{3}{4}\}$
214	cB	P	3	$\{C^-_{3,111}\|101\}, \{C_{2x}\|\tfrac{1}{2}\tfrac{1}{2}0\}, \{C_{2y}\|0\tfrac{1}{2}\tfrac{1}{2}\}$
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230	cB	P	6	$\{C_{3,\bar{1}\bar{1}1}\|0\tfrac{1}{2}\tfrac{1}{2}\},\{C_{2y}\|0\tfrac{1}{2}\tfrac{1}{2}\},\{C_{2x}\|\tfrac{3}{2}\tfrac{3}{2}0\},\{IC^-_{4x}\|\tfrac{1}{2}11\}$
130	tP	A	8	$\{C_{4z}\|000\}, \{\sigma_{\bar{x}y}\|00\tfrac{1}{2}\}, \{I\|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\}$
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218	cP	R	8	$\{C_{2x}\|001\}, \{C_{2y}\|000\}, \{C^-_{3,111}\|001\}, \{\sigma_{\bar{x}y}\|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\}$
220	cB	H	8	$\{C_{2x}\|\tfrac{1}{2}\tfrac{1}{2}0\}, \{C_{2y}\|0\tfrac{1}{2}\tfrac{3}{2}\}, \{C^-_{3,111}\|001\}, \{\sigma_{\bar{x}y}\|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\}$
222	cP	R	8	$\{C^-_{4z}\|000\}, \{C_{2x}\|000\}, \{C^-_{3,111}\|010\}, \{I\|\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\}$
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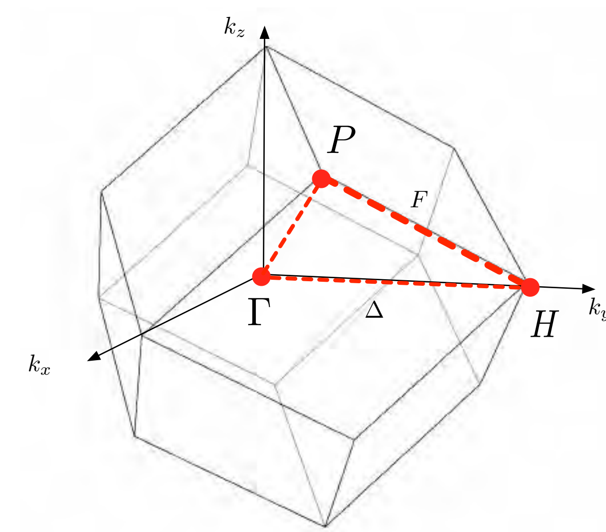
230	cB	H	8	$\{C_{4z}\|0\tfrac{1}{2}0\}, \{C_{2y}\|1\tfrac{1}{2}\tfrac{1}{2}\}, \{C_{3,111}\|111\}, \{I\|000\}$

- 3-fold degeneracies at P point in BZ

- P is non TR invariant

- 3fold at -P



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Primitive tetragonal	$(a,0,0),(0,a,0),(0,0,c)$	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{c}(0,0,1)$

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- 3-fold +TR = 6fold

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198	cP	R	6	$\{C^-_{3,111}\vert 010\}, \{C_{2x}\vert \frac{1}{2}\frac{3}{2}0\}, \{C_{2y}\vert 0\frac{3}{2}\frac{1}{2}\}$
199	cB	P	3	$\{C^-_{3,111}\vert 101\}, \{C_{2x}\vert \frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\}$
205	cP	R	6	$\{C^-_{3,111}\vert 010\}, \{C_{2x}\vert \frac{1}{2}\frac{3}{2}0\}, \{C_{2y}\vert 0\frac{3}{2}\frac{1}{2}\}, \{I\vert 000\}$
206	cB	P	6	$\{C^-_{3,111}\vert 101\}, \{C_{2x}\vert \frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\}$
212	cP	R	6	$\{C_{2x}\vert \frac{1}{2}\frac{1}{2}0\},\{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\},\{C^-_{3,111}\vert 000\},\{C_{2,1\bar{1}0}\vert \frac{1}{4}\frac{1}{4}\frac{1}{4}\}$
213	cP	R	6	$\{C_{2x}\vert \frac{1}{2}\frac{1}{2}0\},\{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\},\{C^-_{3,111}\vert 000\},\{C_{2,1\bar{1}0}\vert \frac{3}{4}\frac{3}{4}\frac{3}{4}\}$
214	cB	P	3	$\{C^-_{3,111}\vert 101\}, \{C_{2x}\vert \frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\}$
220	cB	P	3	$\{C_{3,\bar{1}\bar{1}1}\vert 0\frac{1}{2}\frac{1}{2}\},\{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\},\{C_{2x}\vert \frac{3}{2}\frac{3}{2}0\},\{IC^-_{4x}\vert \frac{1}{2}11\}$
230	cB	P	6	$\{C_{3,\bar{1}\bar{1}1}\vert 0\frac{1}{2}\frac{1}{2}\},\{C_{2y}\vert 0\frac{1}{2}\frac{1}{2}\},\{C_{2x}\vert \frac{3}{2}\frac{3}{2}0\},\{IC^-_{4x}\vert \frac{1}{2}11\}$
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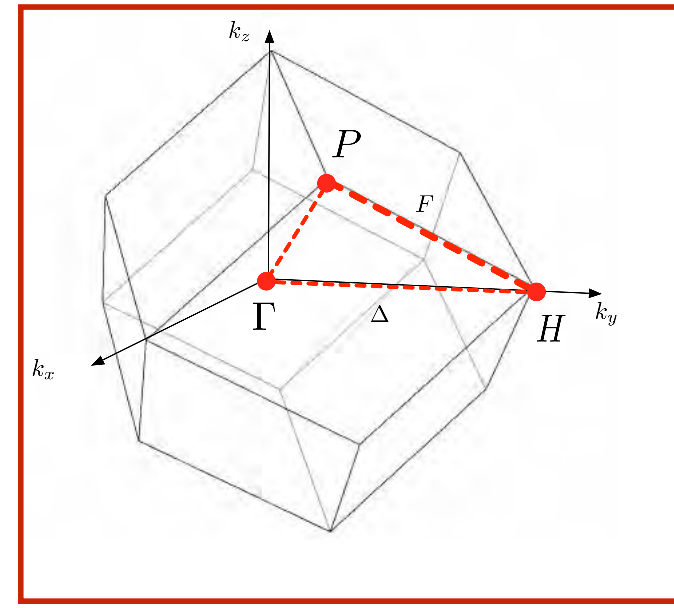
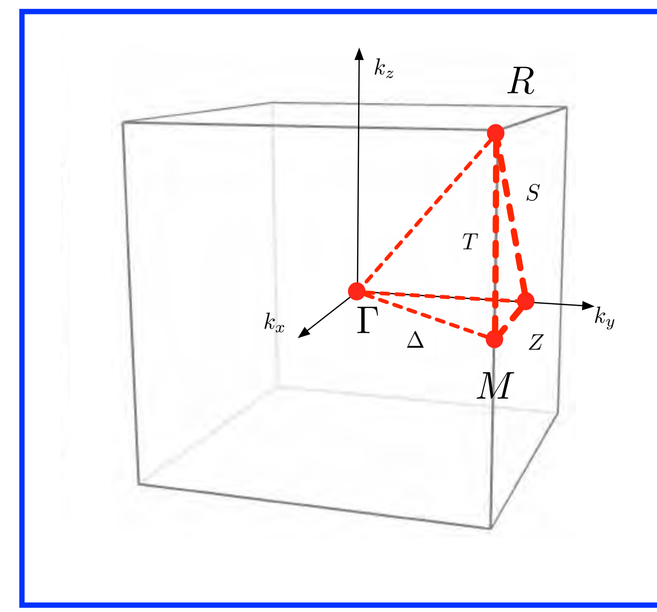
135	tP	A	8	$\{C_{4z}\vert \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{\sigma_{\bar{x}y}\vert 00\frac{1}{2}\}, \{I\vert 000\}$
218	cP	R	8	$\{C_{2x}\vert 001\}, \{C_{2y}\vert 000\}, \{C^-_{3,111}\vert 001\}, \{\sigma_{\bar{x}y}\vert \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
220	cB	H	8	$\{C_{2x}\vert \frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\vert 0\frac{1}{2}\frac{3}{2}\}, \{C^-_{3,111}\vert 001\}, \{\sigma_{\bar{x}y}\vert \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
222	cP	R	8	$\{C^-_{4z}\vert 000\}, \{C_{2x}\vert 000\}, \{C^-_{3,111}\vert 010\}, \{I\vert \frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
223	cP	R	8	$\{C^-_{4z}\vert \frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{C_{2x}\vert 000\}, \{C^-_{3,111}\vert 010\}, \{I\vert 000\}$
230	cB	H	8	$\{C_{4z}\vert 0\frac{1}{2}0\}, \{C_{2y}\vert 1\frac{1}{2}\frac{1}{2}\}, \{C_{3,111}\vert 111\}, \{I\vert 000\}$





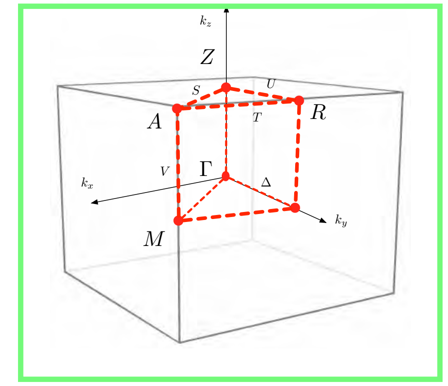
cP: cubic primitive
cB: cubic body-centered
tP: tetragonal primitive

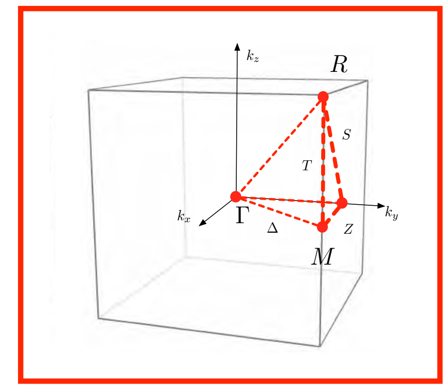
Bravais lattice	Lattice vectors	Reciprocal lattice vectors
Primitive cubic	$(a,0,0),(0,a,0),(0,0,a)$	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{a}(0,0,1)$
Body-centered cubic	$\frac{a}{2}(-1,1,1), \frac{a}{2}(1,-1,1), \frac{a}{2}(1,1,-1)$	$\frac{2\pi}{a}(0,1,1), \frac{2\pi}{a}(1,0,1), \frac{2\pi}{a}(1,1,0)$
Primitive tetragonal	$(a,0,0),(0,a,0),(0,0,c)$	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{c}(0,0,1)$

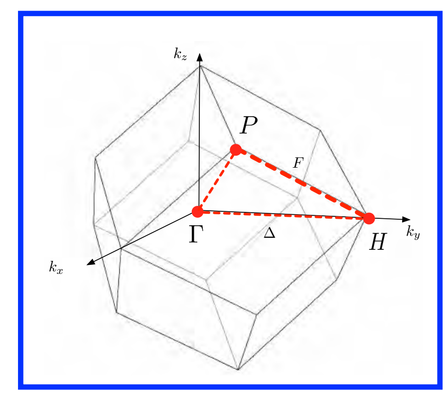
TABLE I. Lattice and reciprocal lattice vectors

SG	La	k	d	Generators
198	cP	R	6	$\{C^{-}_{3,111}\|010\}, \{C_{2x}\|\frac{1}{2}\frac{3}{2}0\}, \{C_{2y}\|0\frac{3}{2}\frac{1}{2}\}$
199	cB	P	3	$\{C^{-}_{3,111}\|101\}, \{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$
205	cP	R	6	$\{C^{-}_{3,111}\|010\}, \{C_{2x}\|\frac{1}{2}\frac{3}{2}0\}, \{C_{2y}\|0\frac{3}{2}\frac{1}{2}\}, \{I\|000\}$
206	cB	P	6	$\{C^{-}_{3,111}\|101\}, \{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$
212	cP	R	6	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C^{-}_{3,111}\|000\},\{C_{2,1\bar{1}0}\|\frac{1}{4}\frac{1}{4}\frac{1}{4}\}$
213	cP	R	6	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C^{-}_{3,111}\|000\},\{C_{2,1\bar{1}0}\|\frac{3}{4}\frac{3}{4}\frac{3}{4}\}$
214	cB	P	3	$\{C^{-}_{3,111}\|101\}, \{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\frac{1}{2}\}$
220	cB	P	3	$\{C_{3,\bar{1}\bar{1}1}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2x}\|\frac{3}{2}\frac{3}{2}0\},\{IC^{-}_{4x}\|\frac{1}{2}11\}$
230	cB	P	6	$\{C_{3,\bar{1}\bar{1}1}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2y}\|0\frac{1}{2}\frac{1}{2}\},\{C_{2x}\|\frac{3}{2}\frac{3}{2}0\},\{IC^{-}_{4x}\|\frac{1}{2}11\}$
130	tP	A	8	$\{C_{4z}\|000\}, \{\sigma_{\bar{x}y}\|00\frac{1}{2}\}, \{I\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
135	tP	A	8	$\{C_{4z}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{\sigma_{\bar{x}y}\|00\frac{1}{2}\}, \{I\|000\}$
218	cP	R	8	$\{C_{2x}\|001\}, \{C_{2y}\|000\}, \{C^{-}_{3,111}\|001\}, \{\sigma_{\bar{x}y}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
220	cB	H	8	$\{C_{2x}\|\frac{1}{2}\frac{1}{2}0\}, \{C_{2y}\|0\frac{1}{2}\frac{3}{2}\}, \{C^{-}_{3,111}\|001\}, \{\sigma_{\bar{x}y}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
222	cP	R	8	$\{C^{-}_{4z}\|000\}, \{C_{2x}\|000\}, \{C^{-}_{3,111}\|010\}, \{I\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}$
223	cP	R	8	$\{C^{-}_{4z}\|\frac{1}{2}\frac{1}{2}\frac{1}{2}\}, \{C_{2x}\|000\}, \{C^{-}_{3,111}\|010\}, \{I\|000\}$
230	cB	H	8	$\{C_{4z}\|0\frac{1}{2}0\}, \{C_{2y}\|1\frac{1}{2}\frac{1}{2}\}, \{C_{3,111}\|111\}, \{I\|000\}$

8fold







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Body-centered cubic	$\frac{a}{2}(-1,1,1)$, $\frac{a}{2}(1,-1,1)$, $\frac{a}{2}(1,1,-1)$	$\frac{2\pi}{a}(0,1,1)$, $\frac{2\pi}{a}(1,0,1)$, $\frac{2\pi}{a}(1,1,0)$
Primitive tetragonal	$(a,0,0),(0,a,0),(0,0,c)$	$\frac{2\pi}{a}(1,0,0)$, $\frac{2\pi}{a}(0,1,0)$, $\frac{2\pi}{c}(0,0,1)$

TABLE I. Lattice and reciprocal lattice vectors

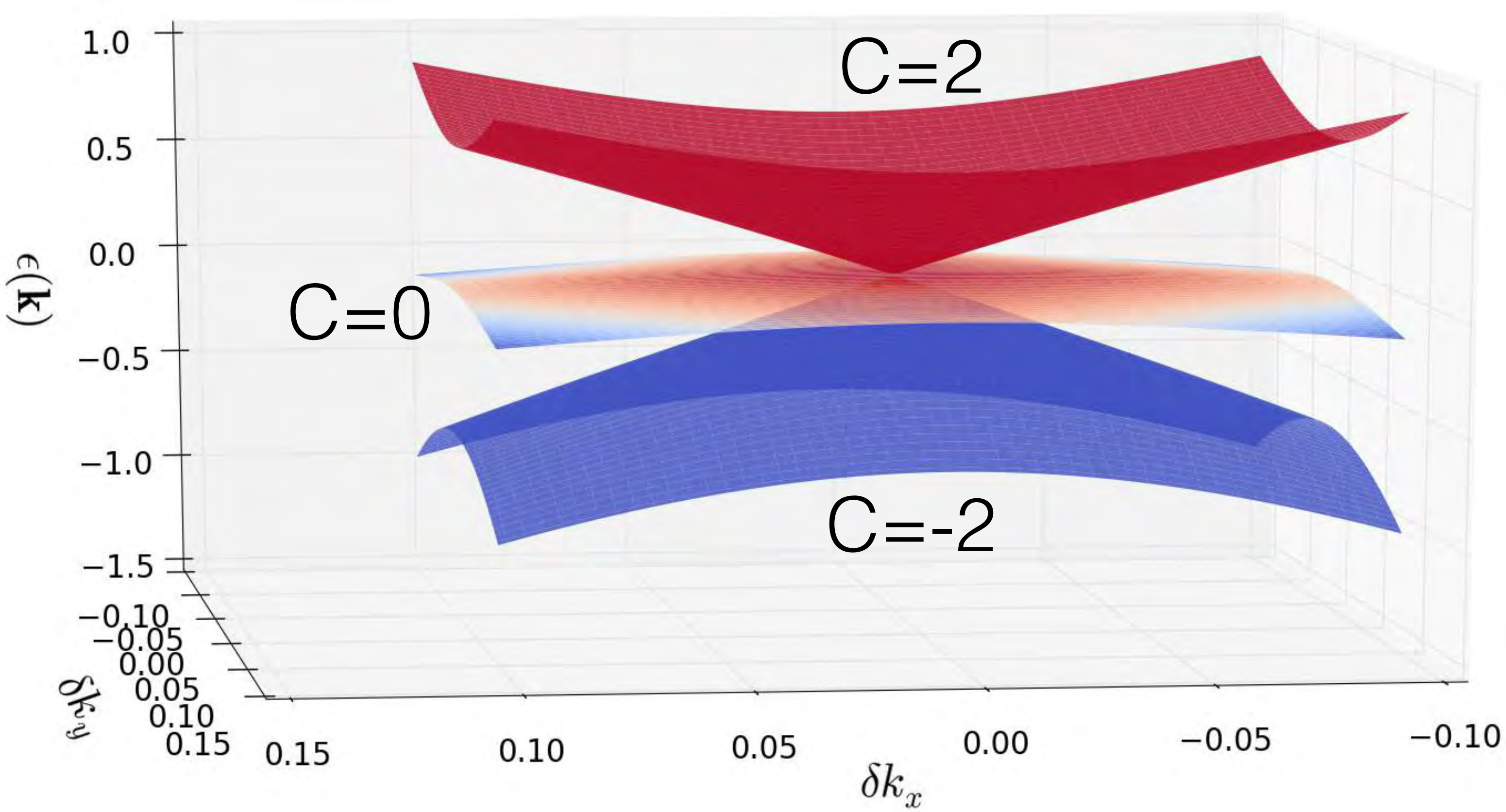
Low-energy effective Hamiltonians consistent with the symmetries of the little group

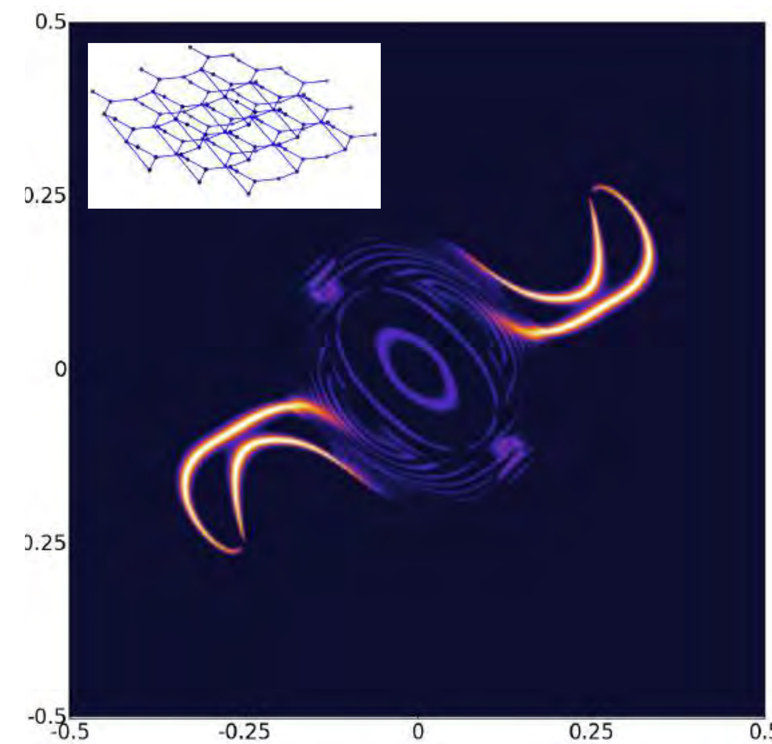
A special case: 3-fold Degeneracy (in several symmetry groups)

$$\boxed{\vec{k} \cdot \vec{S}}$$

Spin 1 matrices

In SPG-214 not needed to stabilize the fermion: New Chiral Anomaly and anomalous transport





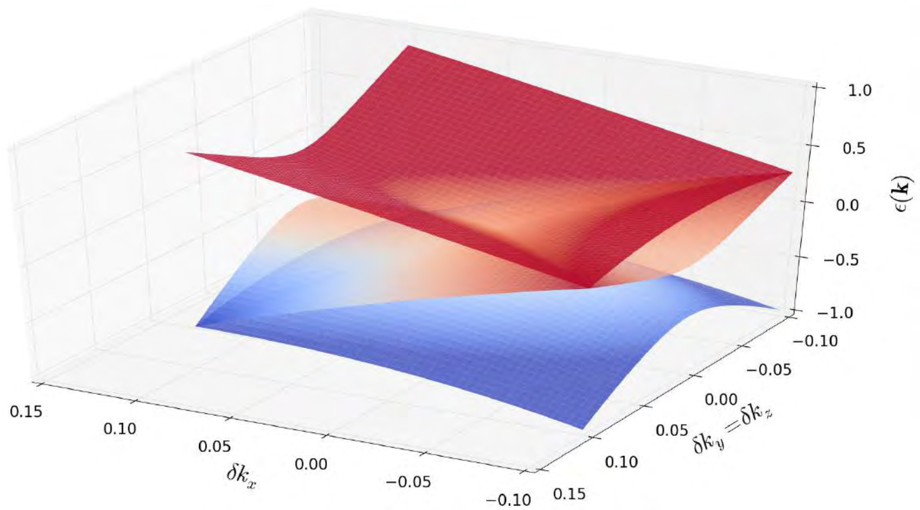
(a) SGs 199 and 214

Leslie M. Schoop, Mazhar N. Ali, Carola Straßer, Viola Duppel, Stuart S. P. Parkin, Bettina V. Lotsch, Christian R. Ast, Nat. Comm. (2016)

3-fold, 6-fold, 8-fold Crossings: All Different Fermions

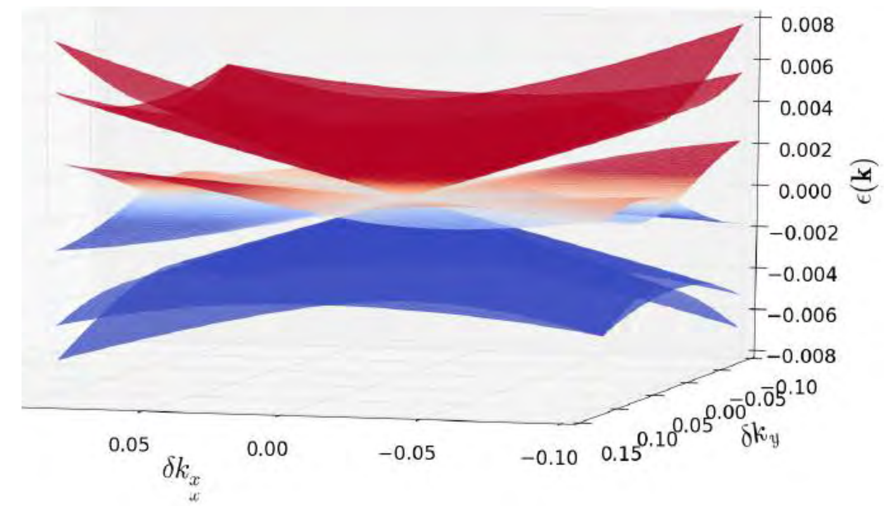
For 8-fold see also Benjamin J. Wieder, Youngkuk Kim, A. M. Rappe, C. L. Kane, arXiv:1512.00074

k dot p models



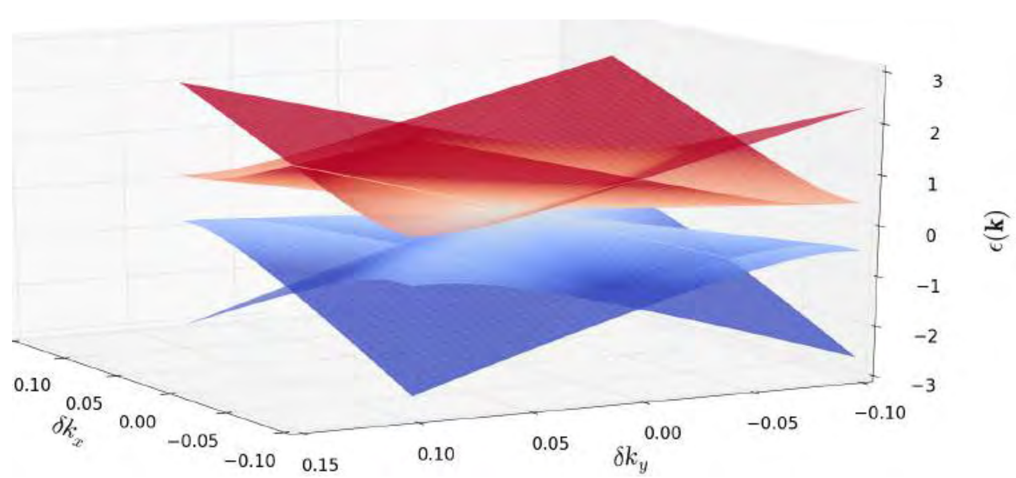
(b) SG 220

3-fold degeneracy,
Line-nodes on $|\delta k_x| = |\delta k_y| = |\delta k_z$



(c) SGs 198, 212 and 213

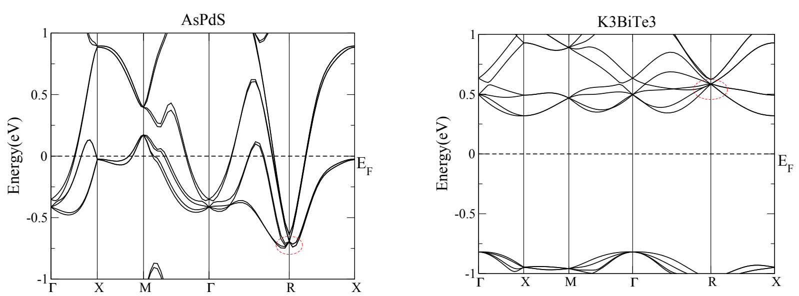
6-fold degeneracy,
Surface-nodes on $\delta k_i = 0$ of the BZ



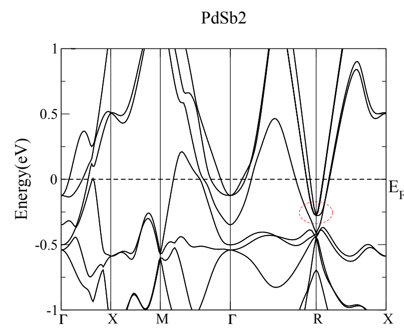
(a) SGs 130 and 135

4-fold degenerate at corner of BZ:
Dirac Line Nodes

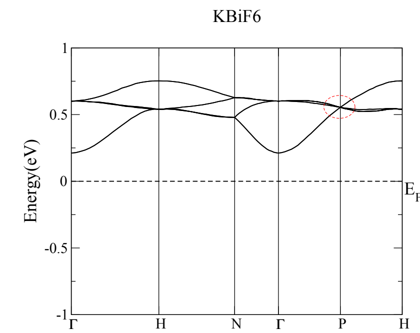
The Different Classes of New Fermions: 3,6, 8 Fold



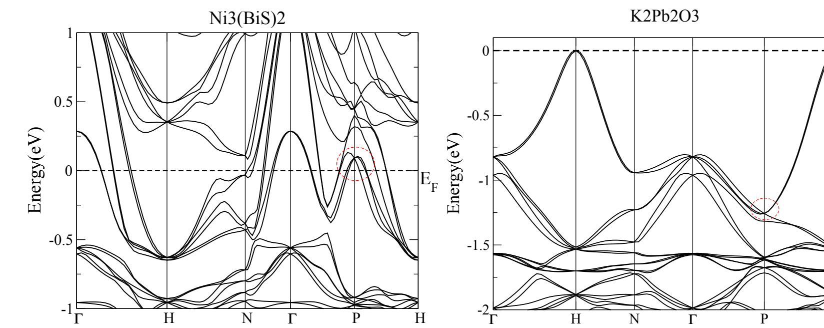
A 6-fold fermion can occur at the R point in the dashed circle. *SG 198*



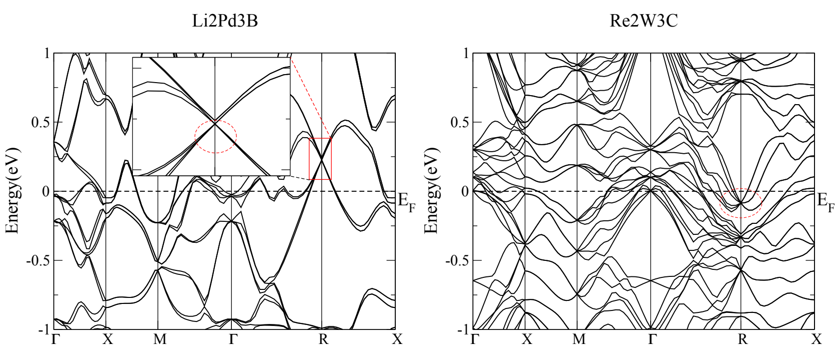
6-fold fermion occur below E_F at the R point *SG 205*



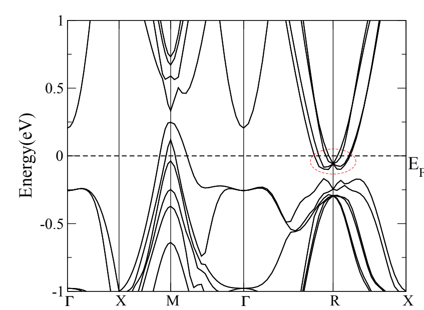
A 6-fold fermion occur above E_F at the P point *SG 206*



A 3-fold fermion can occur at the P point. *SG 199*



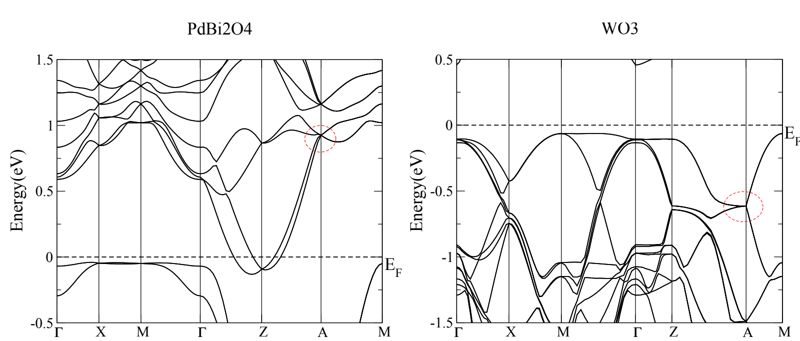
A 6-fold fermion can occur at the R point *SGs 212 and 213*



(a) Ta_3Sb (SG 223)

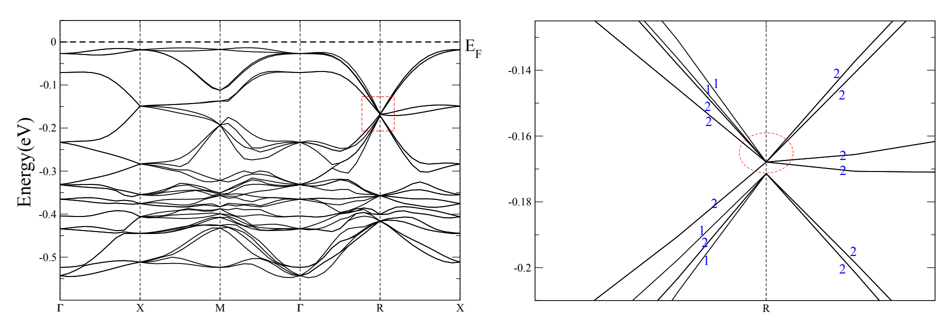
AsPdS,
K3BiTe3
M3(XS)2 where M= Ni,Pd, X= Pb, Bi
A2 B2 O3 (A=K, Rb, B= Ge, Sn, Pb)
PdSb2

FeS2
PtP2
KBiF6
Li2(Pd/Pt)3B
Re2(W/Mo)3C
La3PbI3

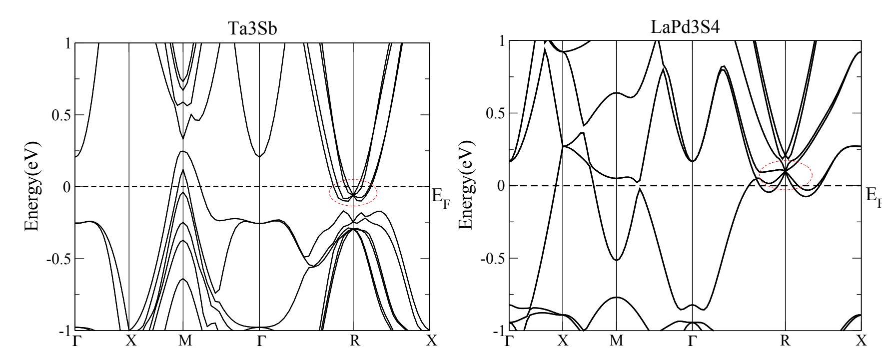


8-Fold Fermions at the A-point *SGs 130 and 135*

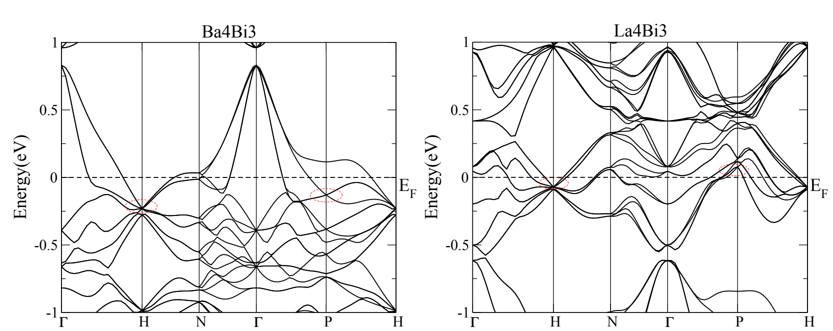
CsSn



An 8-fold fermion can occur at the R point *SGs 218*



An 8-fold) fermion can occur at the R point. *SGs 222 and 223*



A 3-fold (resp. 8-fold) fermion can occur at the P (resp. H) point. *SG 220*

A4Pn3 where A= Ca, Sr, Ba, Eu and R= La, Ce and
Pn = pnictogen (As, Sb, Bi)
MPd3S4 where M= rare earth (see La very close to
the Fermi level)
X3Y where X=Nb,Ta and Y= A-IV; A-V (Sb for ex)
Th3P4, PdBi2O4, AuBi2O5, WO3, CsSn, CsSi

Conclusions

- We have given al possible non-symmorphic space groups where 3fold, 6fold and 8 fold degeneracies can occur
- We have also given some possible experimental signatures
- A list of potential candidates displaying these properties has been reported.

arXiv:1603.03093v2