Weyl Semimetal Type II classification.

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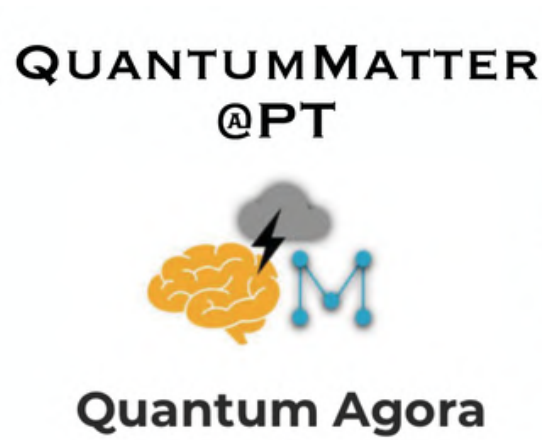
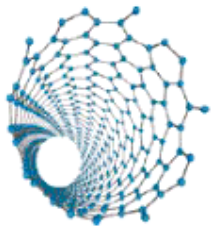
November 18, 2021





Overview

- Weyl semimetal WSMs.
- WSMs notoble properties.
- Type-I and type-II WSMs classification.
- Transition Metal Dichalcogenide-TMDs

  WTe_2 and $MoTe_2$.
- Janus-TMDs family $\rightarrow$ topological classification.

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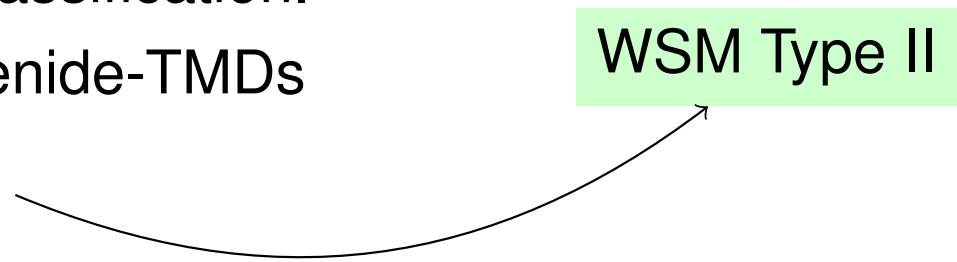
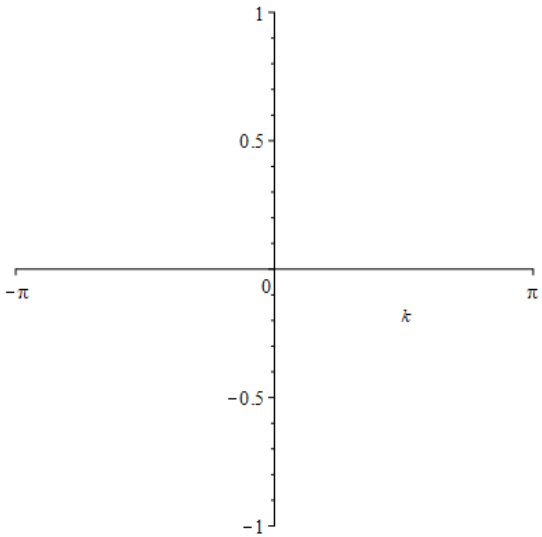
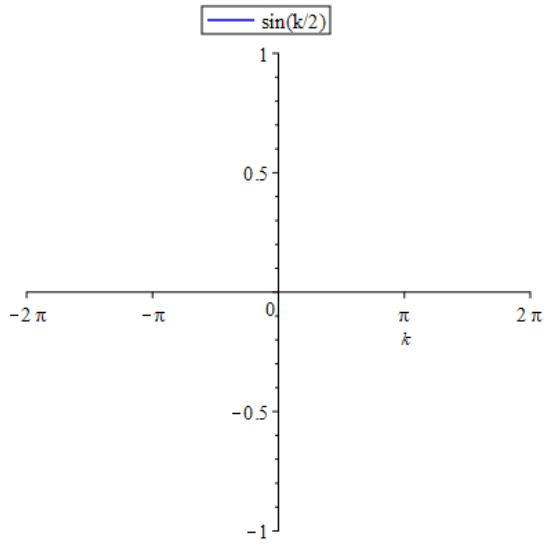


Nielsen-Ninomiya theorem

One Right-moving Fermion



On a Lattice: Crystals



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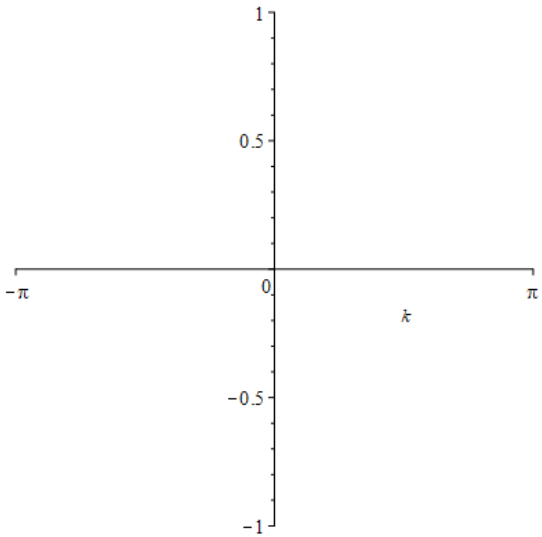

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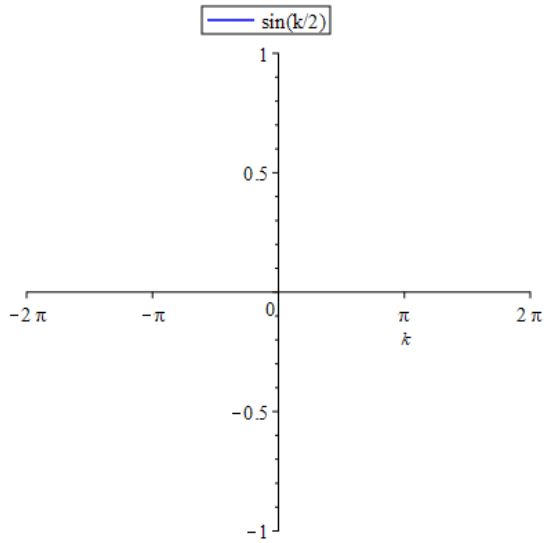
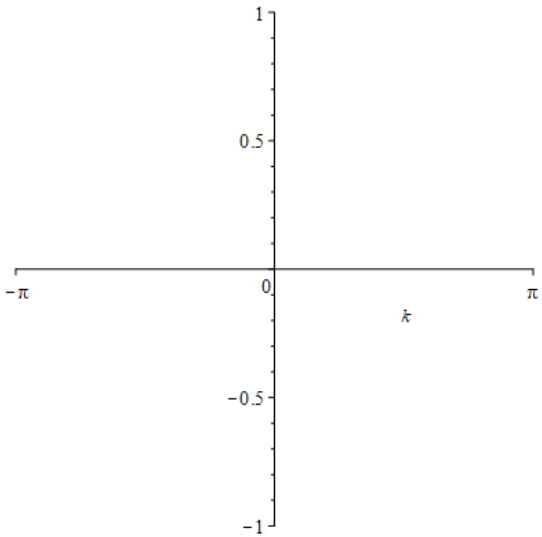


double fermion

left-moving state

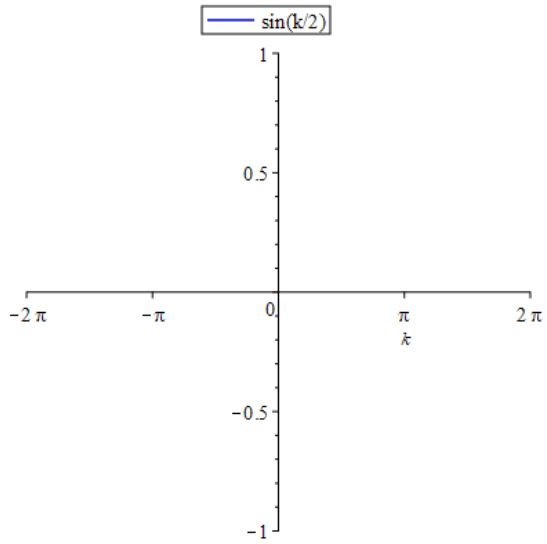
Nielsen-Ninomiya theorem

One Right-moving Fermion



- Dimension?
- Symmetry?

On a Lattice: Crystals



double fermion

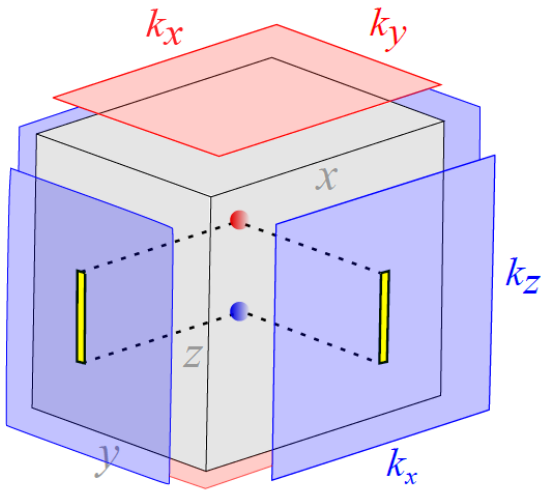
left-moving state

Wyel Semimetal: notoble properties

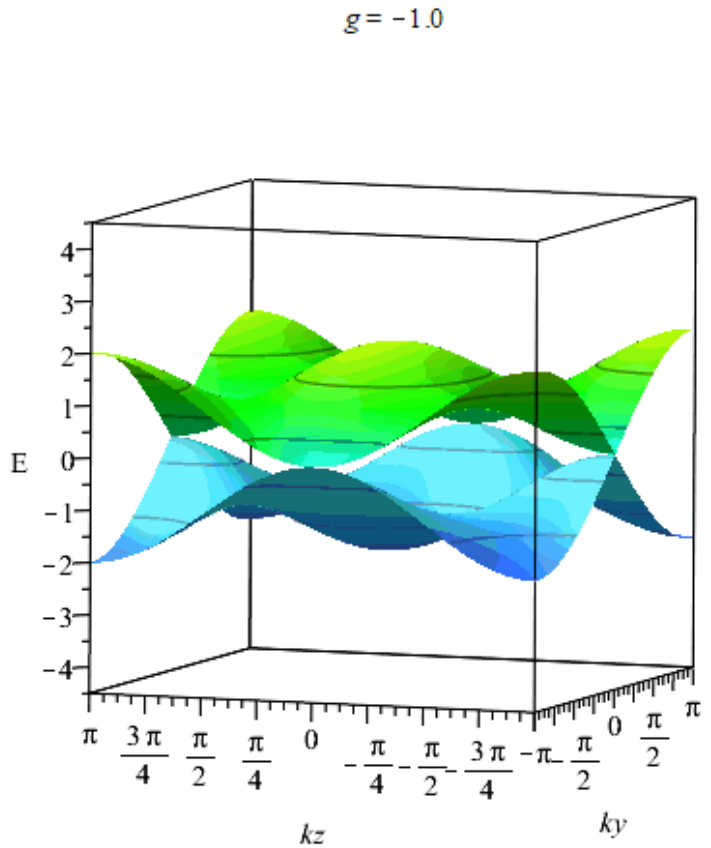
Broken symmetry mecanism

- Time-reversal symmetry-TRS.
- Inversion Symmetry.

- Fermi arcs.
- Chiral anomaly
- negative magnetoresistence.



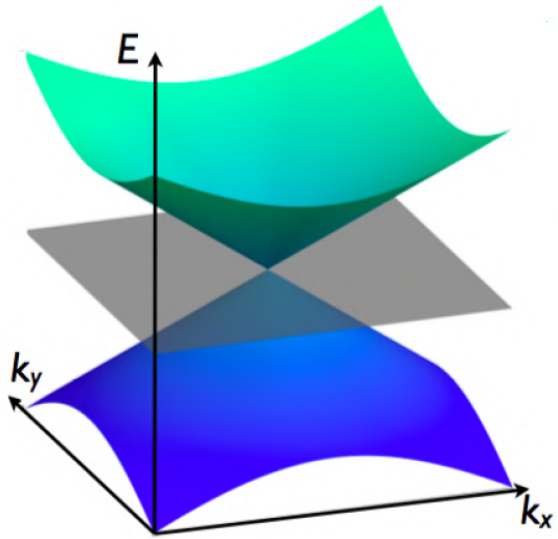
T-broken symmetry



Type I and type II Weyl semimetal

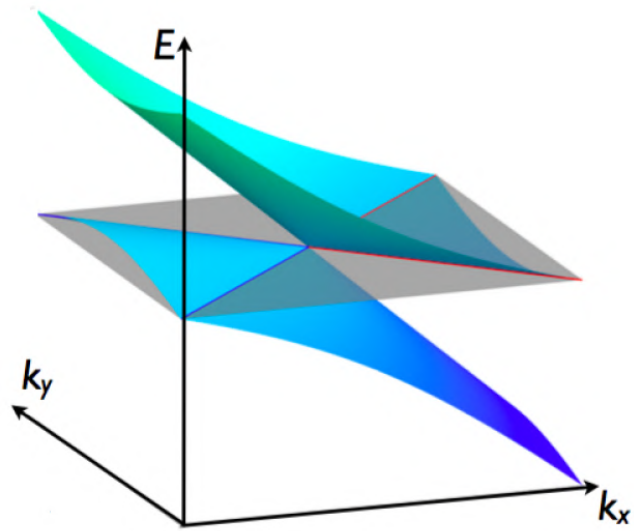
Type I WSM

- Weyl cones exhibit linear crossing bands.
- Lorentz symmetry.
- point-like Fermi surface cross-section.



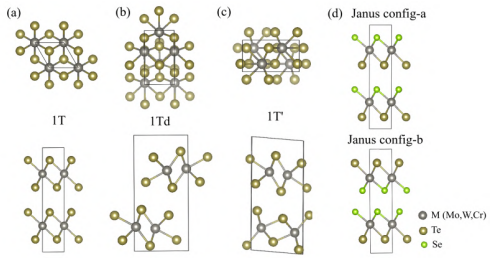
Type II WSM

- Weyl cones are tilted about the energy axis.
- Broken Lorentz symmetry.
- non-point-like Fermi surface cross-section.

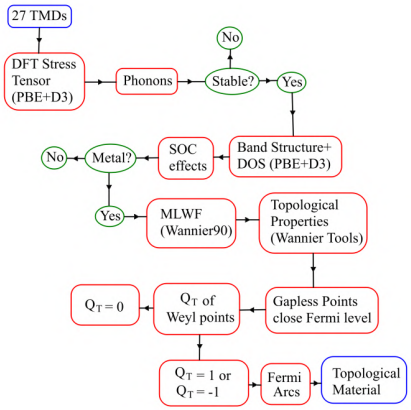


Transition Metal Diacholgenides-TMDs WTe_2 and $MoTe_2$ → WSM Type II

Janus-TMDs



Workflow



Enhancing topological Weyl Semimetals by Janus Transition Metal Dichalcogenides structures

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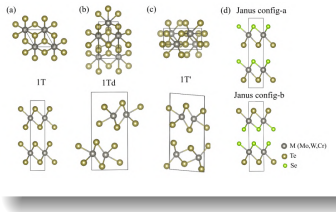
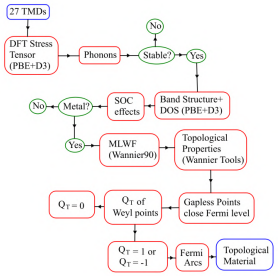
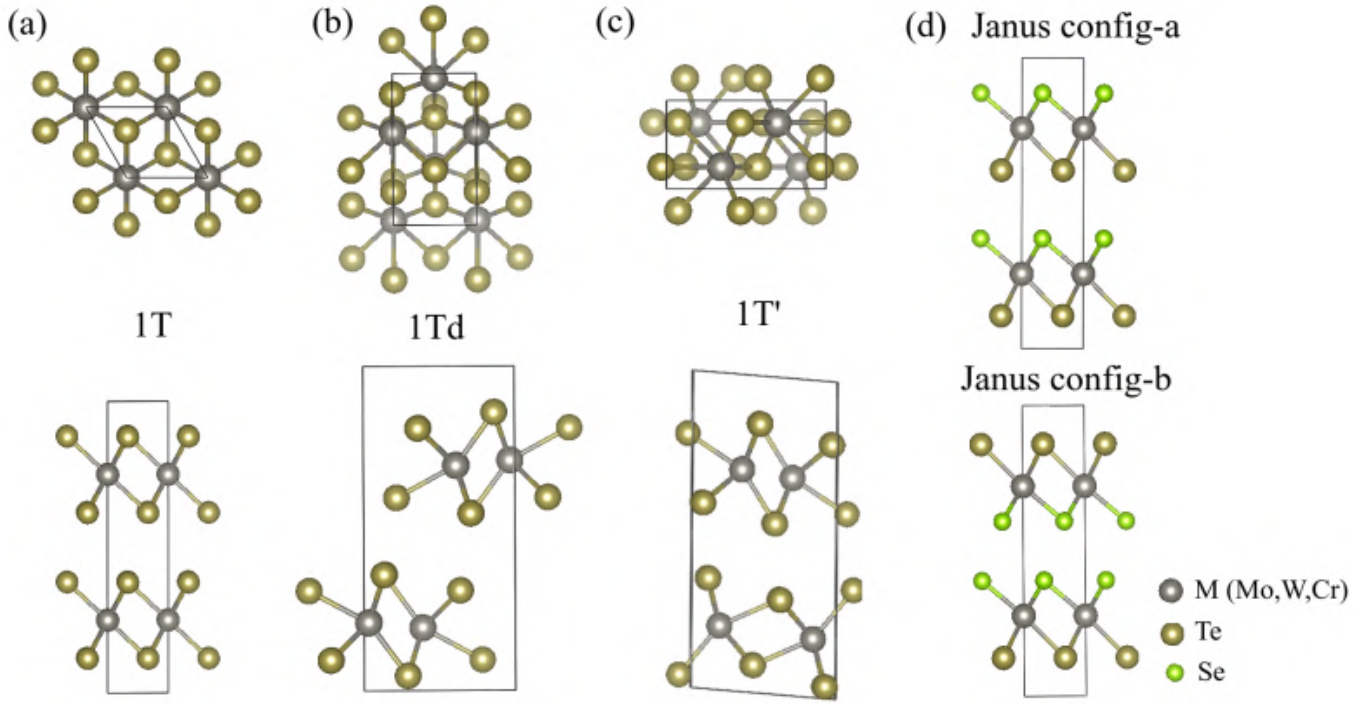
Transition Metal Diacholgenides-TMDs WTe_2 and $MoTe_2$ → WSM Type II

WSM Type II



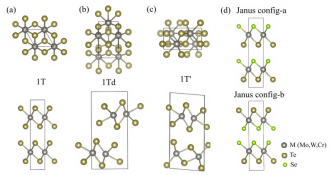
Workflow



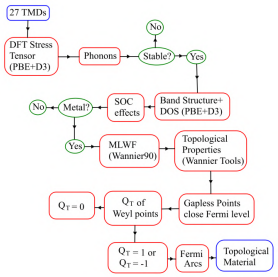


Transition Metal Diacholgenides-TMDs WTe_2 and $MoTe_2$ → WSM Type II

WSM Type II

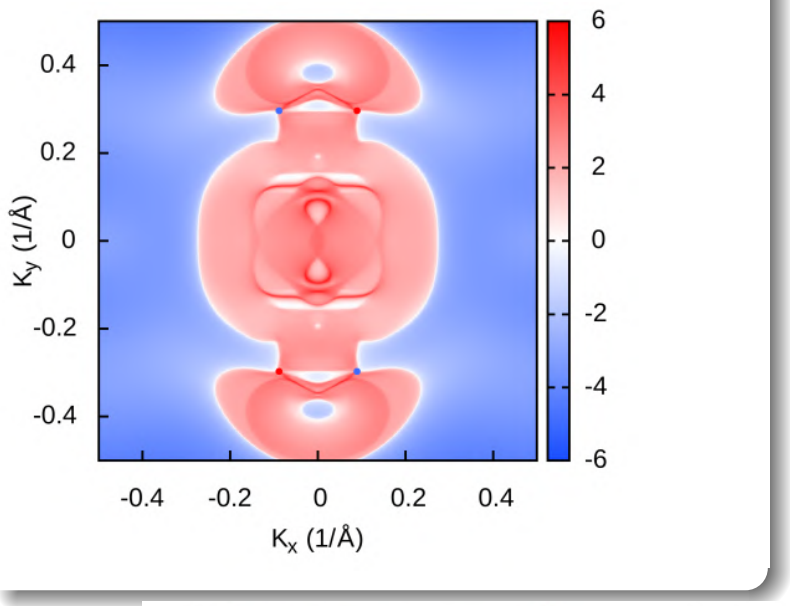


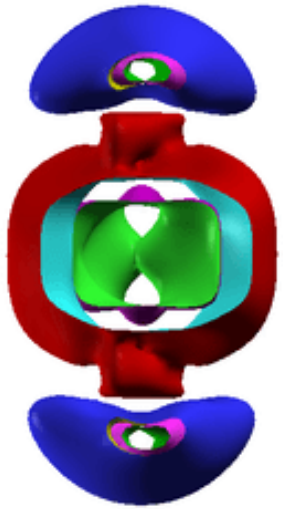
Workflow

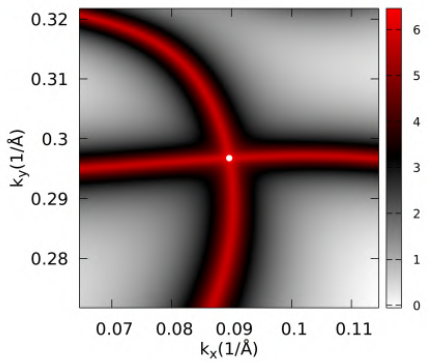


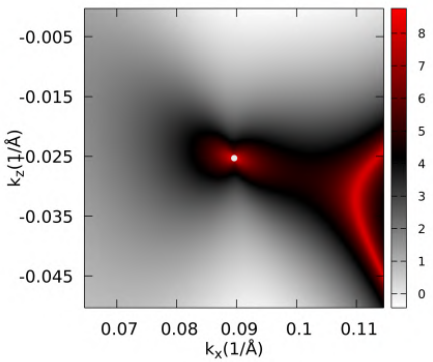
3D Fermi Surface: WTeSe-XX $1T'$

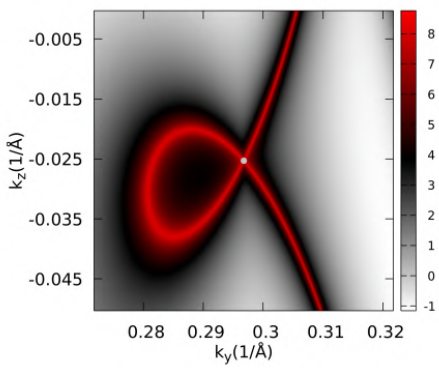
Surface States









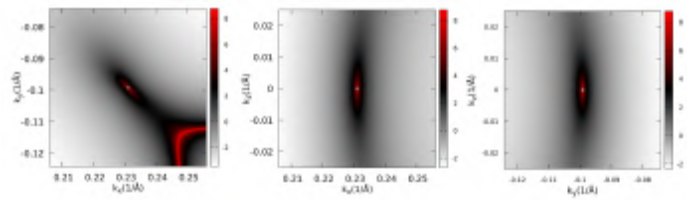


Janus-TMDs Topological classification

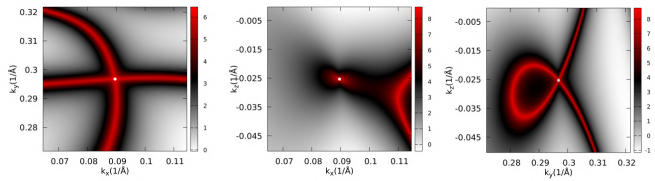
Table 3 Stable Janus topological classification.

Material	Topological Classification
WTeSe-XY-1T_d	strong Type II
WTeSe-XX-1T'	weak Type II
WTeSe-XX-1T_d	Type I
MoTeSe-XY-1T_d	strong Type II
MoTeSe-XX-1T_d	weak Type II
CrTeSe-XY-1T'	weak Type II
CrTeSe-XY-1T_d	strong Type II
CrTeSe-XX-1T_d	weak Type II

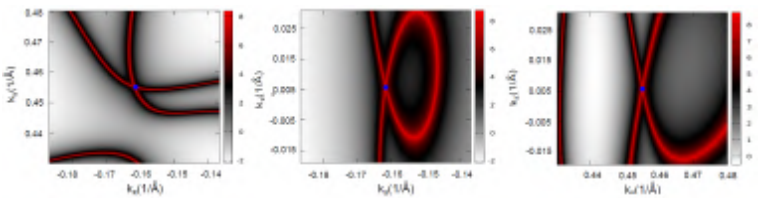
Type I - WTeSe-XX $1T_d$



Weak Type II - WTeSe-XX $1T'$

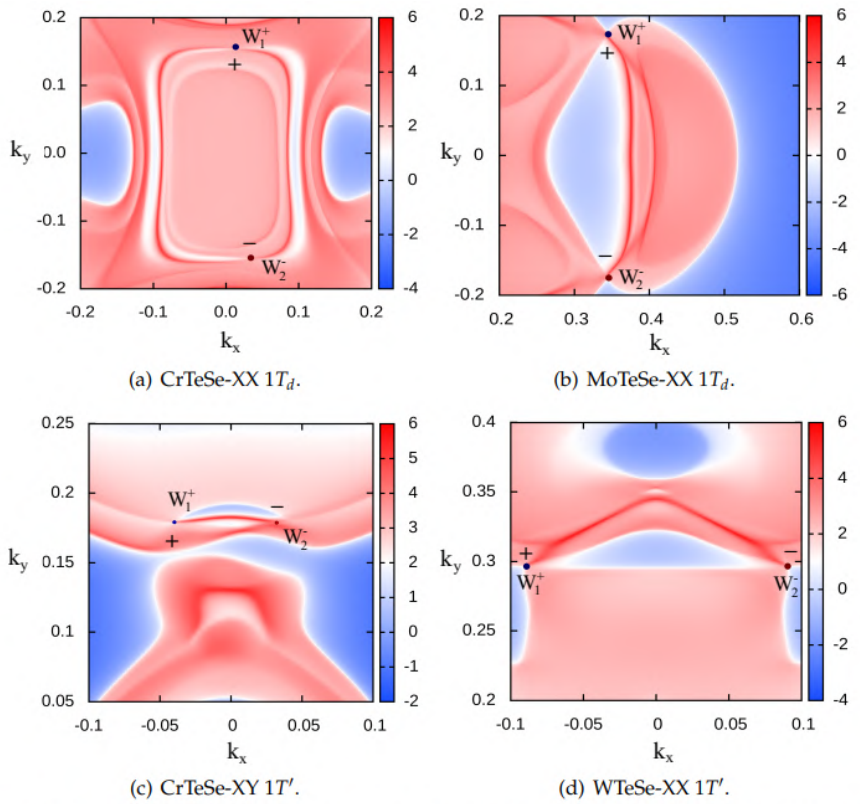


Strong Type II - CrTeSe-XY $1T_d$



Difficults...

Fermi arcs and Weyl points

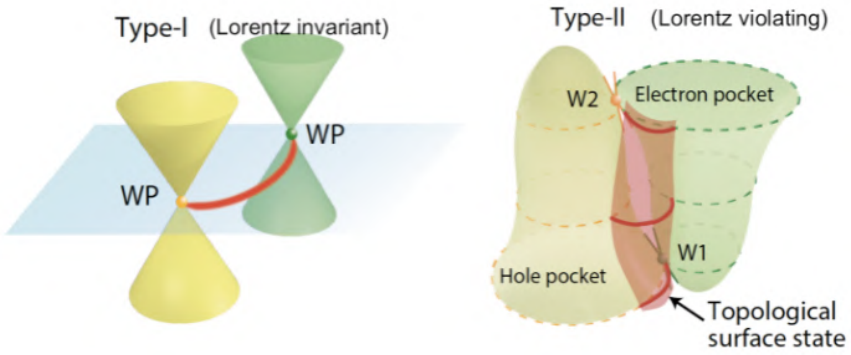


(a) CrTeSe-XX $1T_d$. (b) MoTeSe-XX $1T_d$.

(c) CrTeSe-XY $1T'$. (d) WTeSe-XX $1T'$.

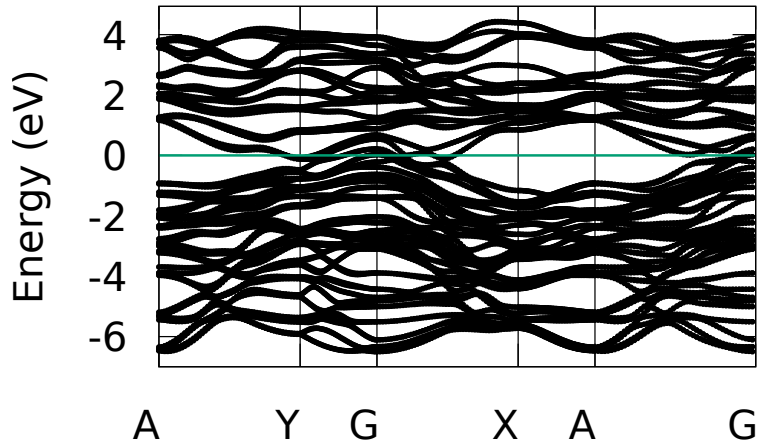
Figure 5 (Color online) Theoretical constant surface (001) energy contour plots for different compounds and energies. a) CrTeSe-XX $1T_d$ with $E = -3$ meV, b) MoTeSe-XX $1T_d$ with $E = -18$ meV. c) CrTeSe-XY $1T'$ with $E = -60$meV and d) WTeSe-XX $1T'$ with $E = -18$ meV.

Type II Weyl semimetal

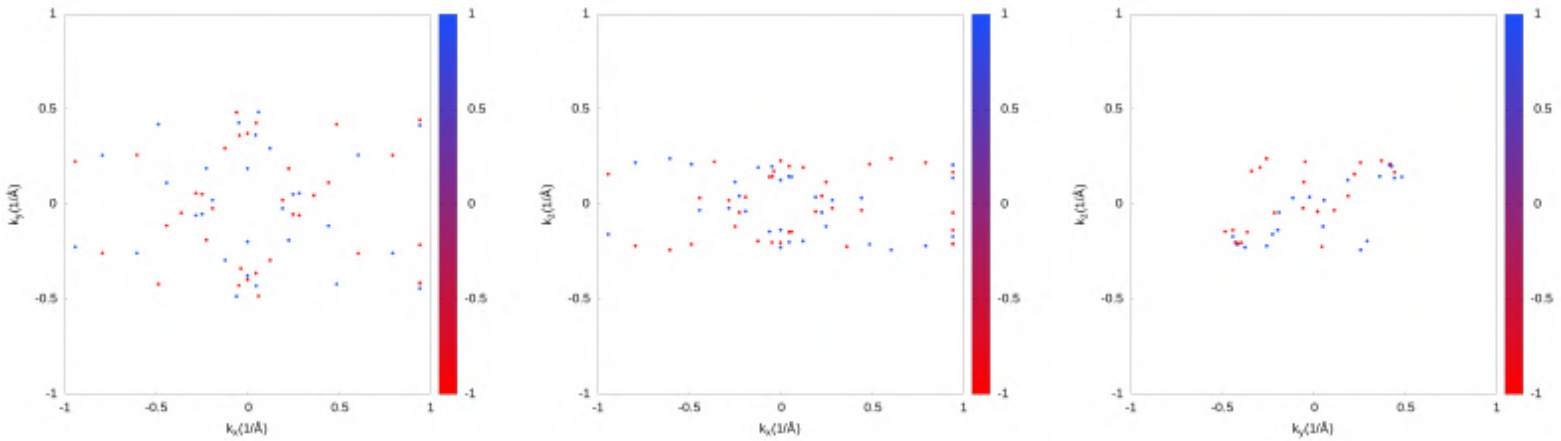


Protocol: MoTeSe-XY $1T_d$

Bulk bands

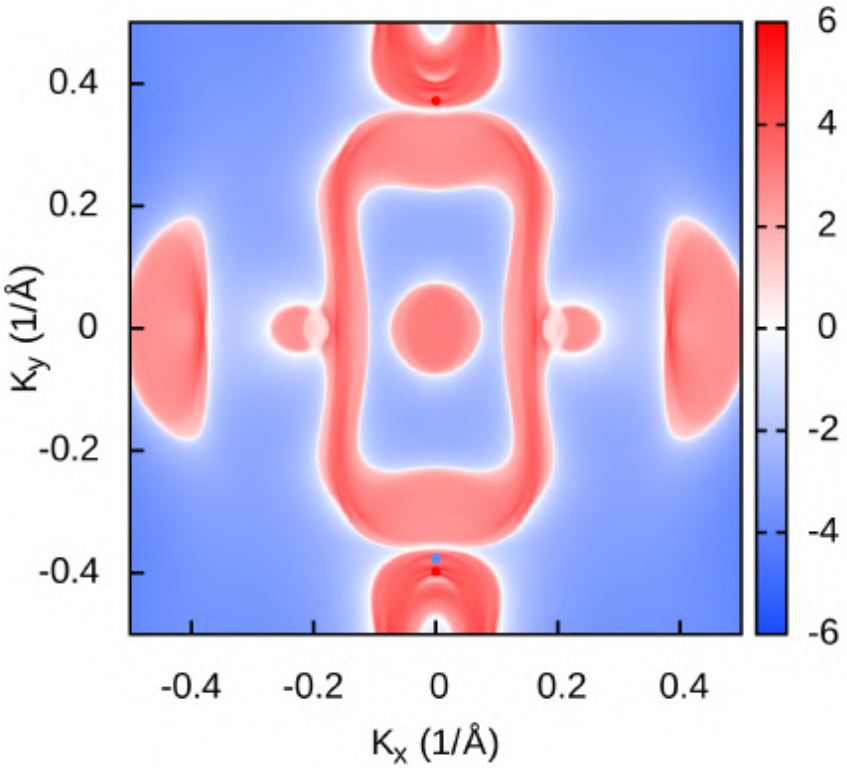


Topological charge

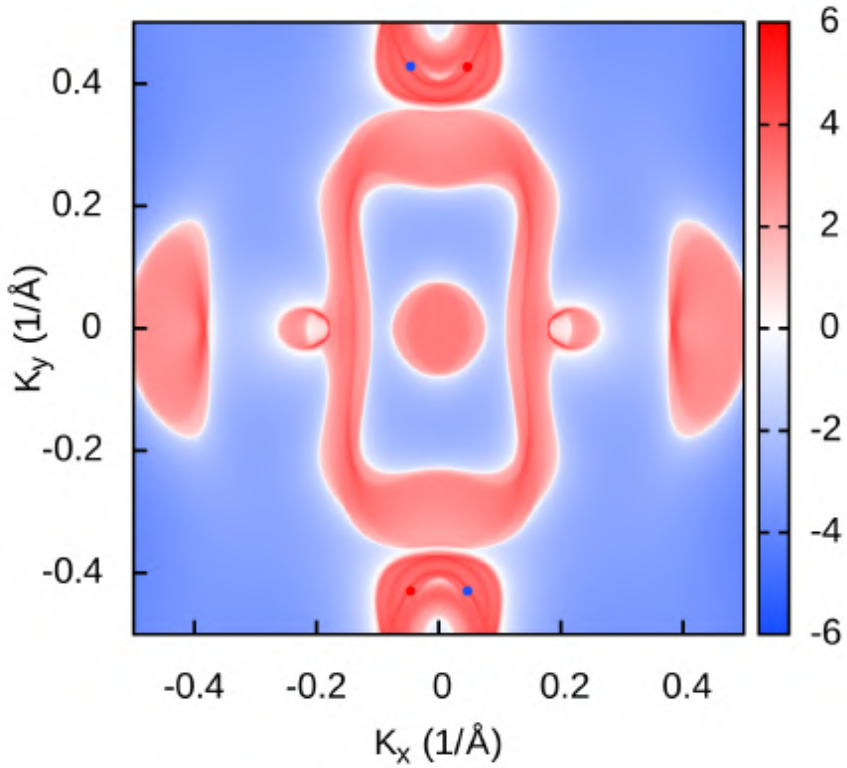


Protocol: MoTeSe-XY $1T_d$

candidate 1: E=-0.0197eV

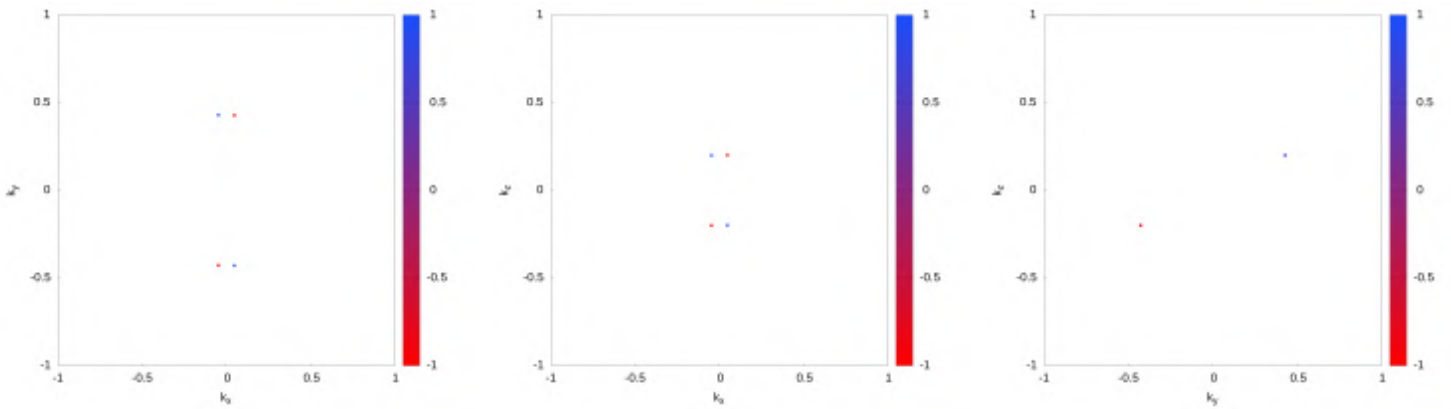


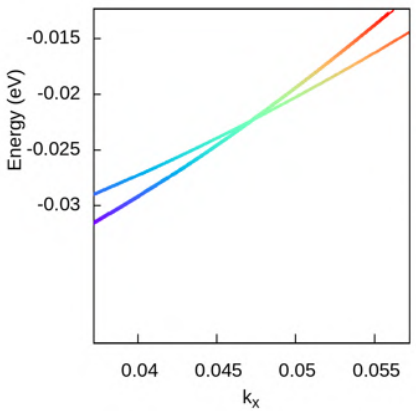
candidate 2: E=-0.0226eV

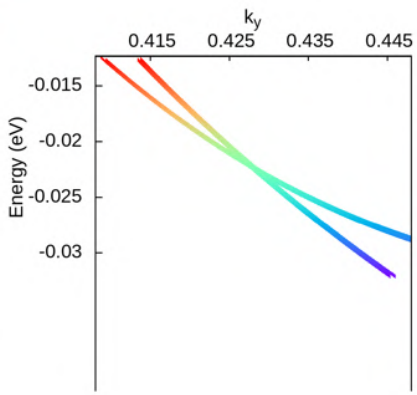


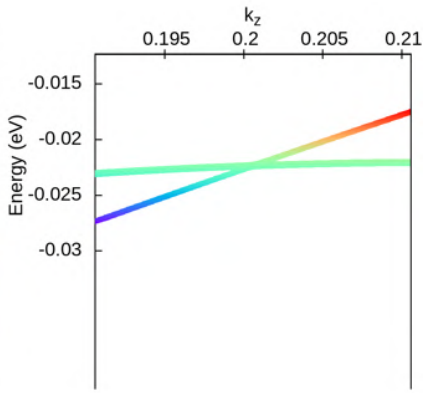
Protocol: MoTeSe-XY $1T_d$

cadidate 2: E=-0.0226; Weyls projection;Energy crossing









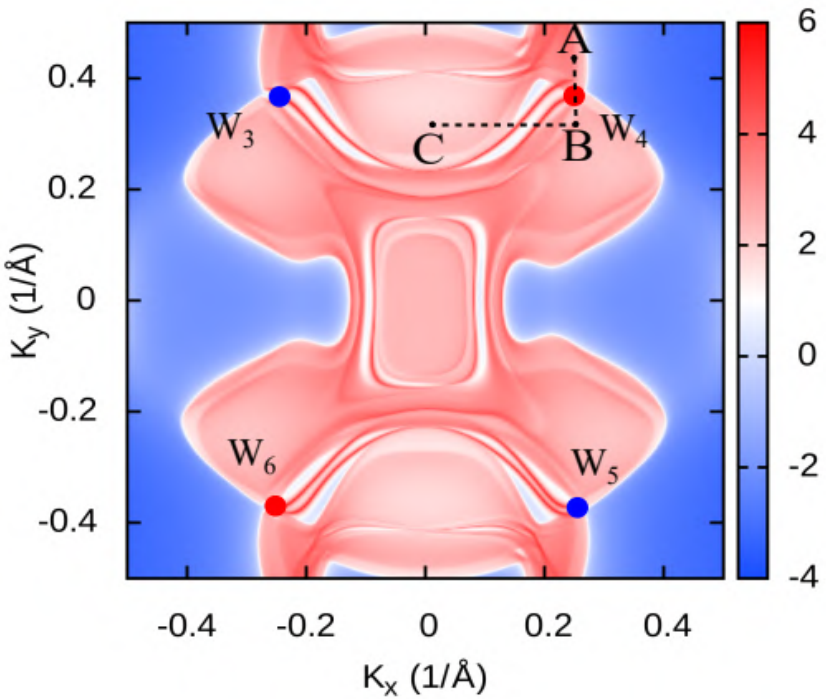
Janus-TMDs Topological classification

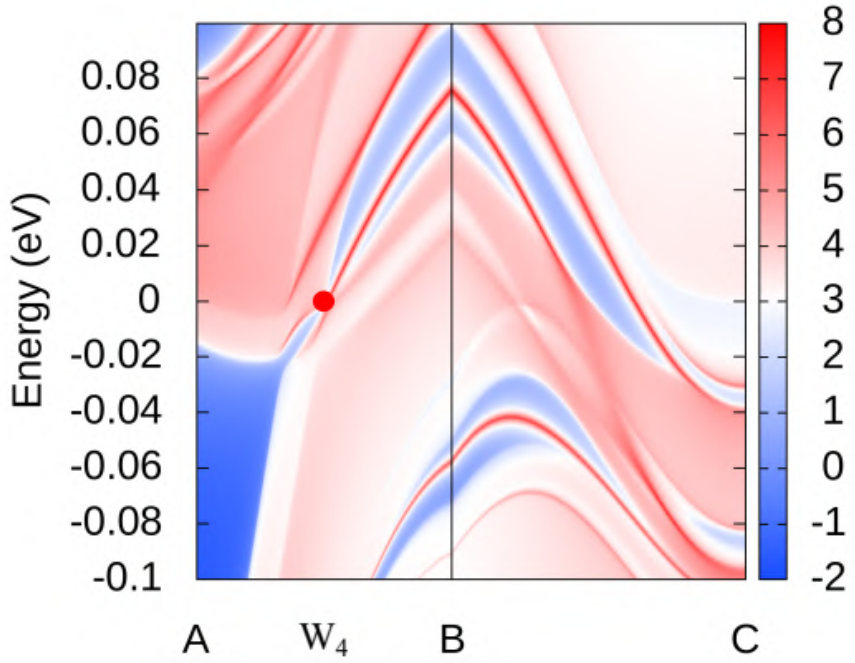
Topological charge and Weyl energies

Material	P. Group	$\vec{k}_{W_1^+}(\text{Å}^{-1})$	$\vec{k}_{W_2^-}(\text{Å}^{-1})$	$\Delta_k\ (\text{Å}^{-1})$	$(E_{W_1^+}, E_{W_2^-})$ eV
WTe_2-1T_d	4[C_s]	(0.219,-0.045,0.000)	(0.219,0.045,0.000)	0.090	(0.056,0.056)
$MoTe_2$-1T_d	4[C_s]	(0.185,0.0539,0.000)	(0.187,-0.053,0.000)	0.100	(0.062,0.062)
WTeSe-XY$-1T_d$	4[C_s]	(-0.400,0.146,-0.072)	(-0.400,-0.145,0.072)	0.324	(-0.011,-0.012)
WTeSe$-XX$-1T'	4[C_s]	(-0.089,0.296,0.025)	(0.089,0.296,-0.025)	0.184	(-0.018,-0.018)
WTeSe$-XX$-1T_d	7[C_{2v}]	(0.231,-0.099,0.000)	(0.230,0.099,0,000)	0.139	(-0.016,-0.016)
MoTeSe$-XY$-1T_d	4[C_s]	(-0.047,0.429,0.200)	(0.047,0.428,0.200)	0.094	(-0.022,-0.022)
MoTeSe$-XX$-1T_d	7[C_{2v}]	(0.344,0.174,0.013)	(0.344,-0.174,-0.013)	0.348	(-0.045,0.045)
CrTeSe$-XY$-1T'	4[C_s]	(0.041,0.177,-0.030)	(-0.039,0.182,0.035)	0.103	(-0.060,-0.070)
CrTeSe$-XY$-1T_d	4[C_s]	(0.085,-0.501,-0.135)	(-0.053,-0.507,-0.162)	0.140	(-0.050,-0.058)
CrTeSe$-XX$-1T_d	7[C_{2v}]	(0.014,0.157, 0.218)	(0.034,-0.154,-0.231)	0.310	(-0.003, 0.001)
CrTeSe$-XX$-1T_d	7[C_{2v}]	(-0.245,0.369, -0.003)	(0.245,0.371,0.005)	0.490	(0.003,-0.001)

Janus-TMDs: CrTeSe – XX $1T_d$

Material	P. Group	$\vec{k}_{W_1^+}(\text{Å}^{-1})$	$\vec{k}_{W_2^-}(\text{Å}^{-1})$	$\Delta_k\,(\text{Å}^{-1})$	$(E_{W_1^+}, E_{W_2^-})$ eV
CrTeSe$-XX$-1T_d	7$[C_{2v}]$	(-0.245,0.369, -0.003)	(0.245,0.371,0.005)	0.490	(0.003,-0.001)





Review

Weyl semimetal

- Janus-TMDs.
- Topological classification.

Review

Weyl semimetal

- Janus-TMDs.
- Topological classification.

Thank you!

References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website www.wanniertools.org.