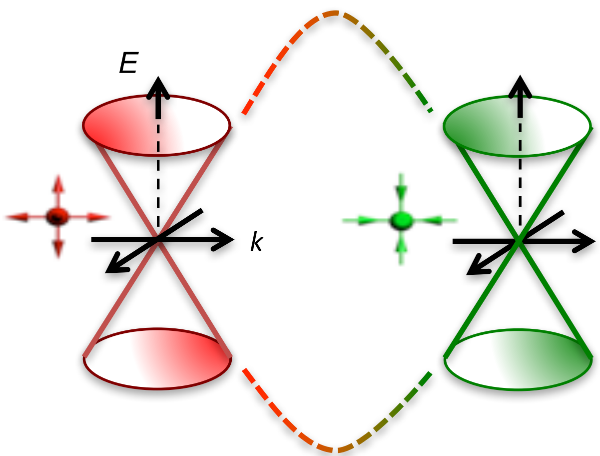
Berry curvature dipole in Weyl materials



Binghai Yan
Weizmann Institute of Science, Israel
www.weizmann.ac.il/condmat/Yan/

arXiv:1708.08589.

Topological insulators and topological metals

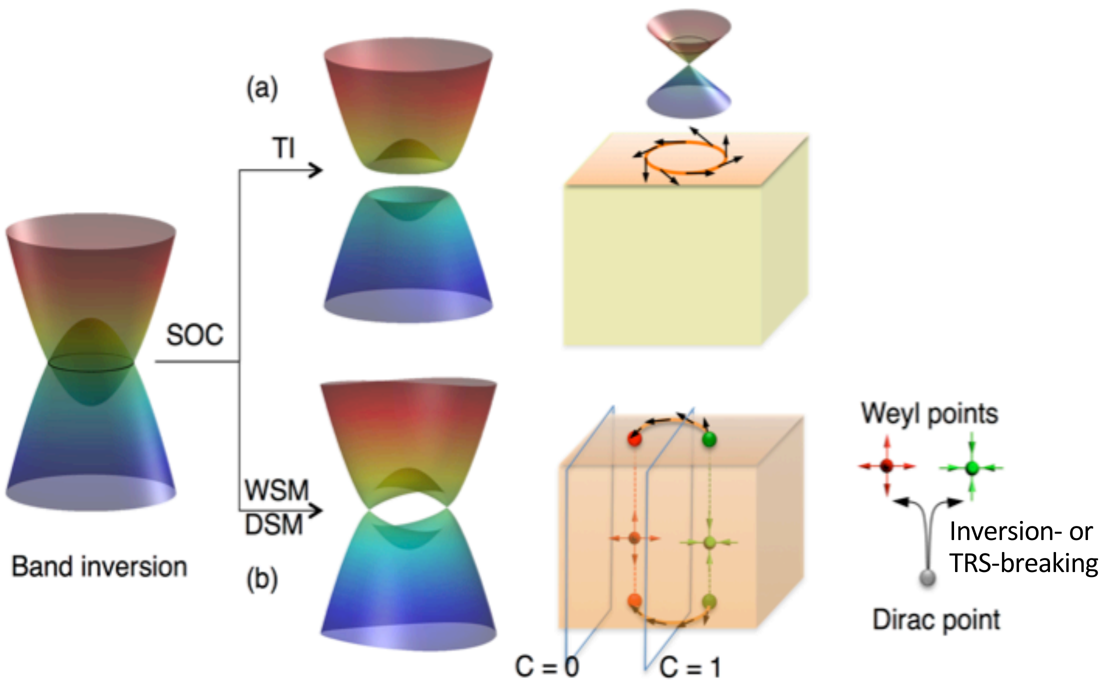
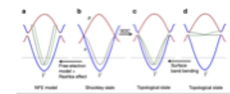
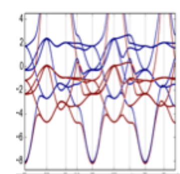
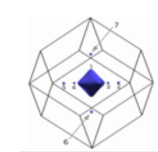


Figure from Annu. Rev. Condens. Matter Phys. 8, 337-354 (2017)



Topological surface states on Gold (111)
Yan 15’





Wey points in *bcc* Fe
Vanderbilt 15’

More commonly existing in materials than thought.

Weyl SemiMetal (WSM)

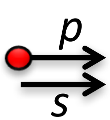
$$\left(\beta mc^2 + c\left(\sum_{n=1}^{3}\alpha_n p_n\right)\right)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

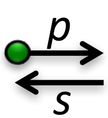
m = 0

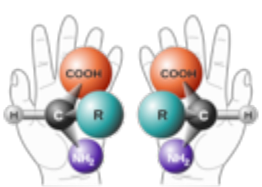
$$i\,\frac{\partial\psi}{\partial t} = \pm\, c\,\vec{p}.\vec{\sigma}\,\psi$$

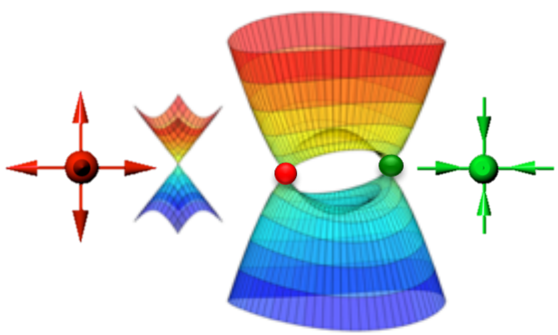
Hermann Weyl
1929’

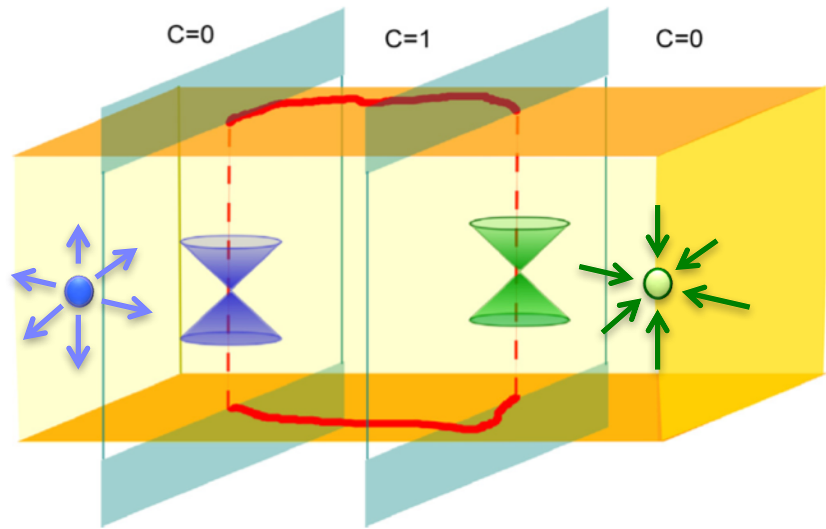
$H = \pm\, \sigma \cdot p$





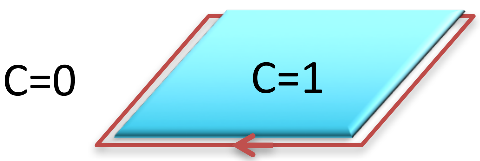


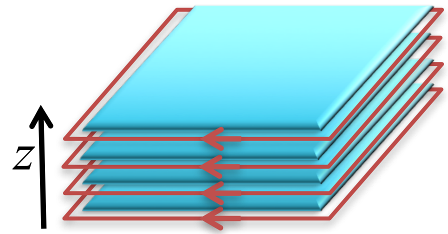


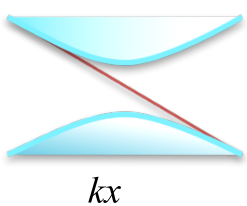


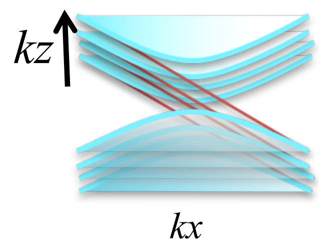
X. Wan et al PRB 83, 205101 (2011).
S. Murakami, New Journal of Physics **10**, 029802 (2008).
G. E. Volovik, *The Universe in A Helium Droplet* (Clarendon Press, Oxford, 2003).

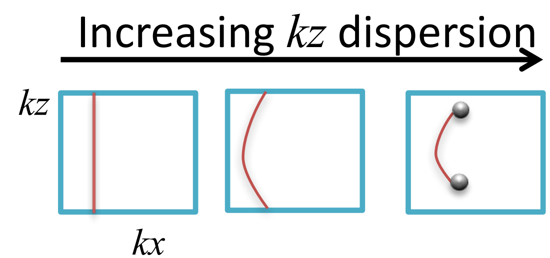
Quantum Hall effect or Chern insulator

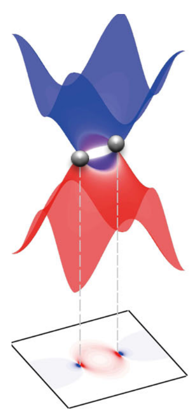








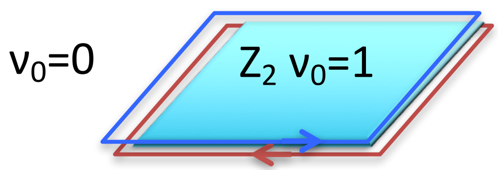


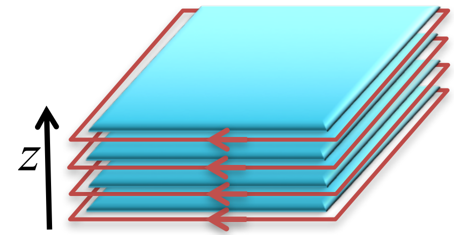


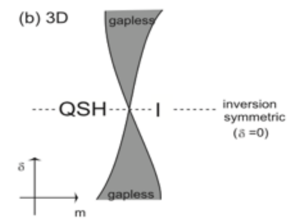
$$AHE = \frac{k_z}{\pi} G_0$$

$$SHE = \frac{k_z}{\pi} G_0 \frac{\hbar}{2e}$$

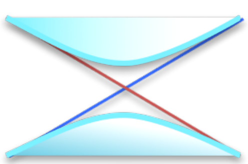
Topological Insulator



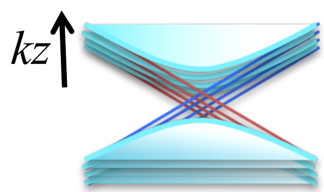


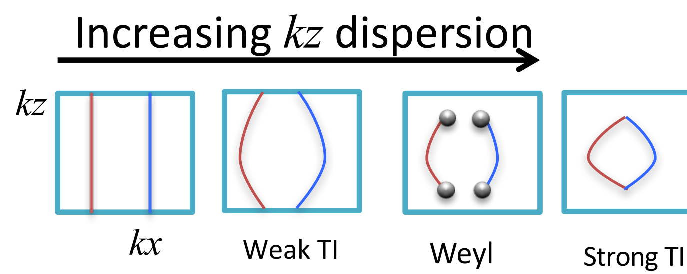


Murakami 2008'.

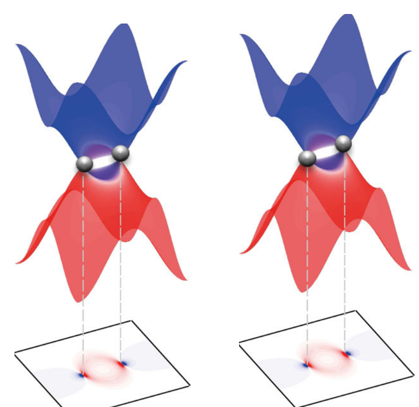


kx





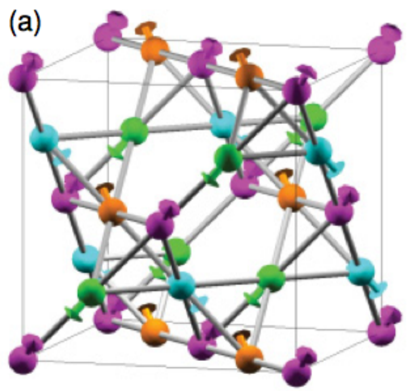
Time-Reversal Symmetry (TRS)



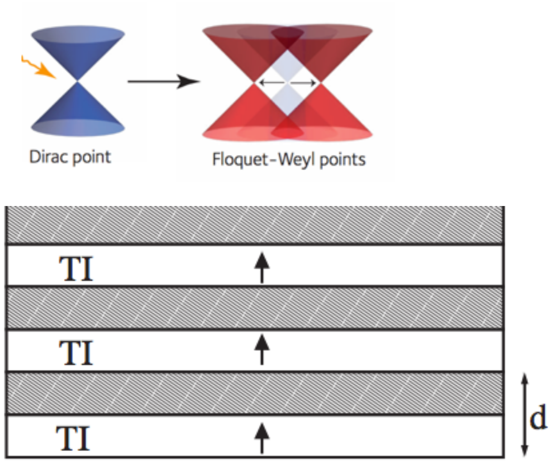
$$AHE = 0$$

$$SHE = \frac{k_z}{\pi} G_0 \frac{\hbar}{2e} \times 2$$

WSM materials

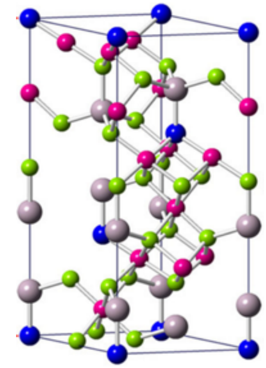


Pyrochclore $Y_2Ir_2O_7$
(noncollinear AFM)
X. Wan, et al.
PRB **83**, 205101 (2011).



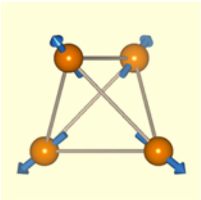
Super lattice: TI + FM

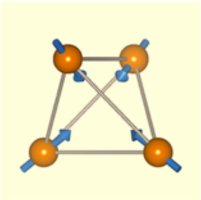
A. Burkov and L. Balents,
PRL **107**, 127205 (2011).



$HgCr_2Se_4$ (FM)

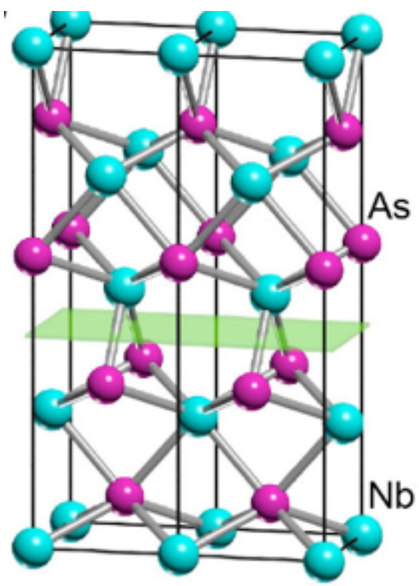
G. Xu et al.
PRL **107,** 186806 (2011).

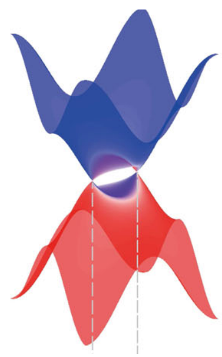




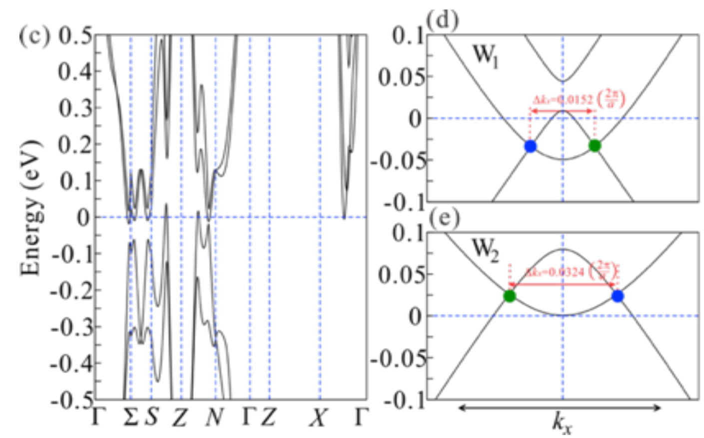
Physically interesting,
Chemically more interesting!

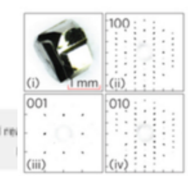
WSM materials





Dream → Reality

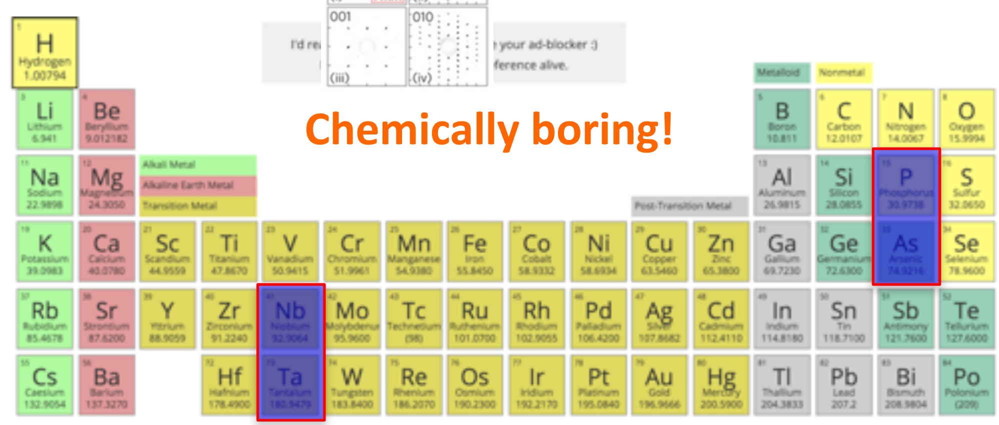




TaAs, TaP, NbAs, NbP

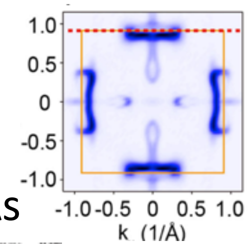
H.M. Weng *et al*. *Phys. Rev. X* **5,** 011029 (2015).
S. M. Huang *et al. Nature Commun.* **6,** 7373 (2015).

B. Q. Lv *et al.*, *Phys. Rev. X* **5**, 031013 (2015).
S.-Y. Xu *et al.*, *Science* **349**, 613 (2015).
L.X. Yang et al. *Nature Physics* **11**, 728 (2015).



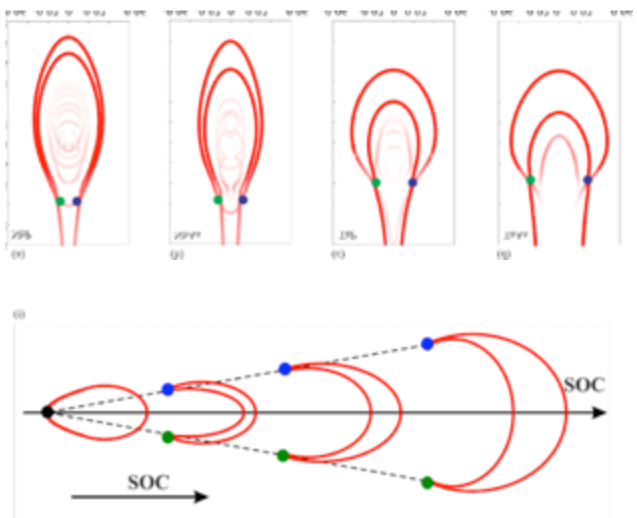
Chemically boring!

A family photo of four compounds

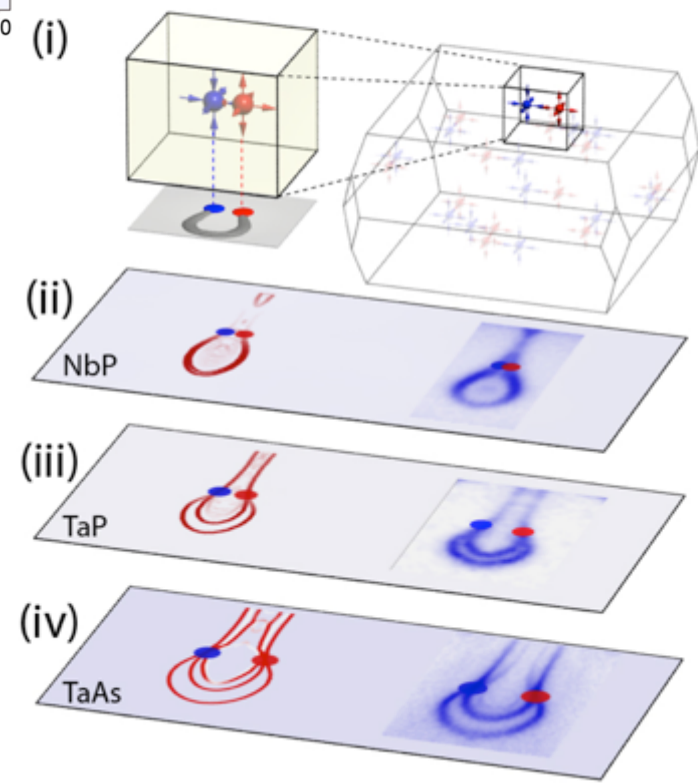


Theory

NbP NbAs TaP TaAs



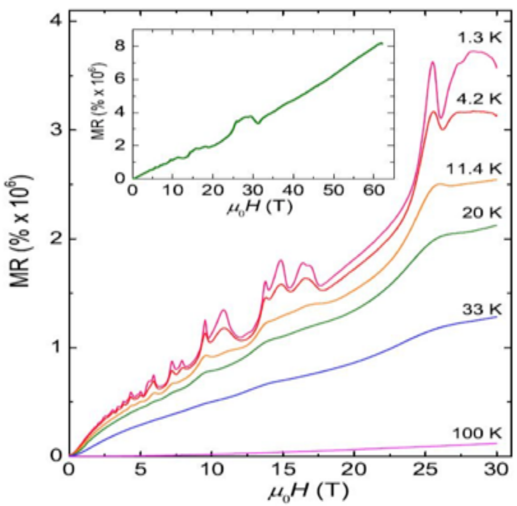
ARPES



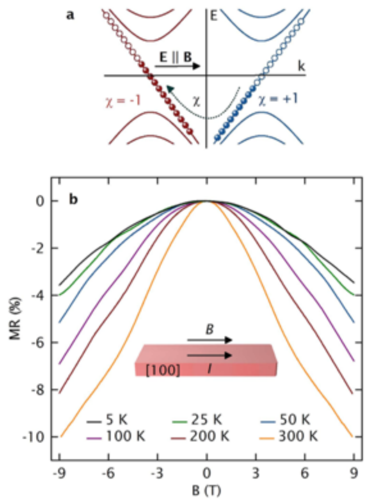
Y. Sun, S.-C. Wu, B. Yan, PRB 92, 115428 (2015)

Z. K. Liu, et al Nature Mater.15,27 (2016)

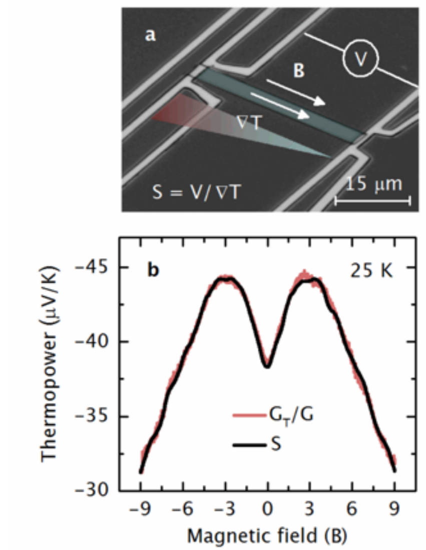
Magneto-transport of WSMs



Large MR and high mobility in NbP

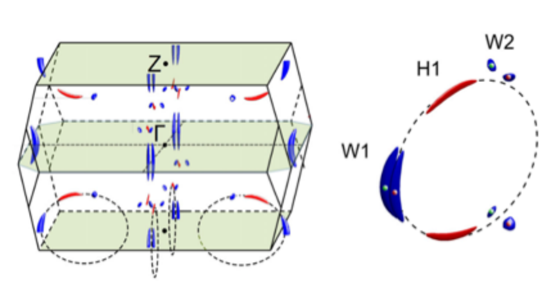


Chiral anomaly,
Negative LMR in TaP, NbP

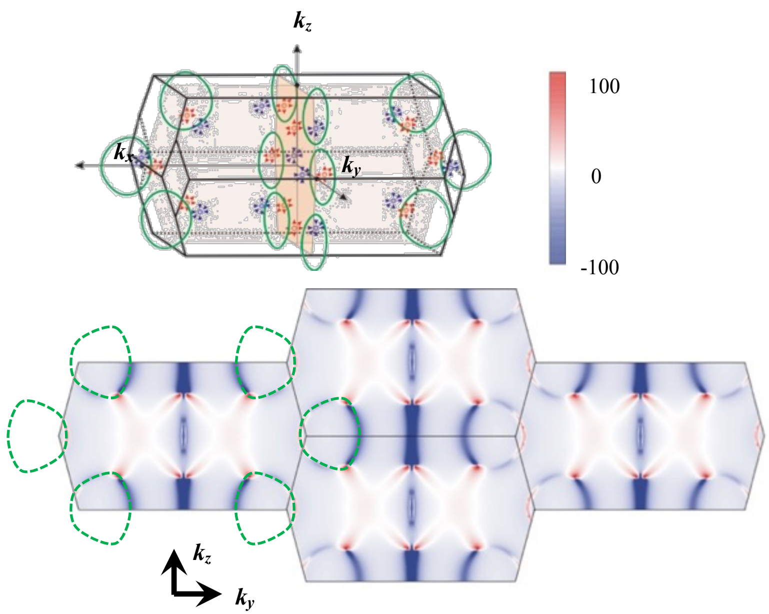


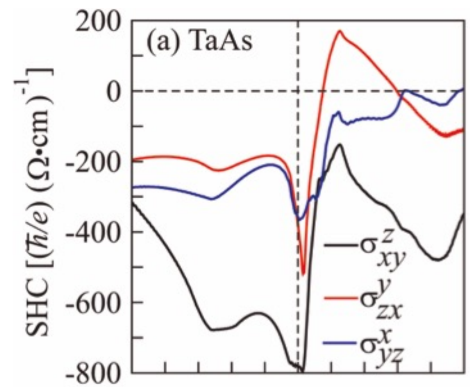
Axial-gravitational anomaly in NbP

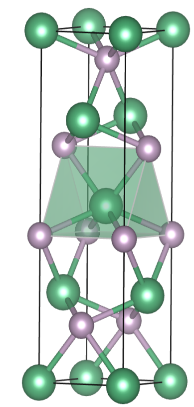
(MPI Dresden)
Shekhar et al. Nature Physics 11, 645 (2015)
Arnold, F *et al*, Nature Comm. 7, 11615 (2016).
Arnold,F *et al*, PRL 117, 146401, (2016).
Niemann, A. C. *et al. Sci. Rep.* 7, 43394 (2017).
Gooth J. *et al.* Nature 547, 324 (2017).



Spin Hall Conductivity







$$\boxed{Js_y^{\ z} = \sigma_{xy}^{\ z}\ J_x}$$

$$\sigma^k_{ij} = e\hbar \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \sum_n f_{n\vec{k}} \Omega^k_{n,ij}(\vec{k}),$$

$$\Omega^{s,k}_{n,ij}(\vec{k}) = -2Im \sum_{n' \neq n} \frac{< n\vec{k}|\hat{J}^k_i|n'\vec{k} >< n'\vec{k}|\hat{v}_j|n\vec{k} >}{(E_{n\vec{k}} - E_{n'\vec{k}})^2}$$

Anisotropic

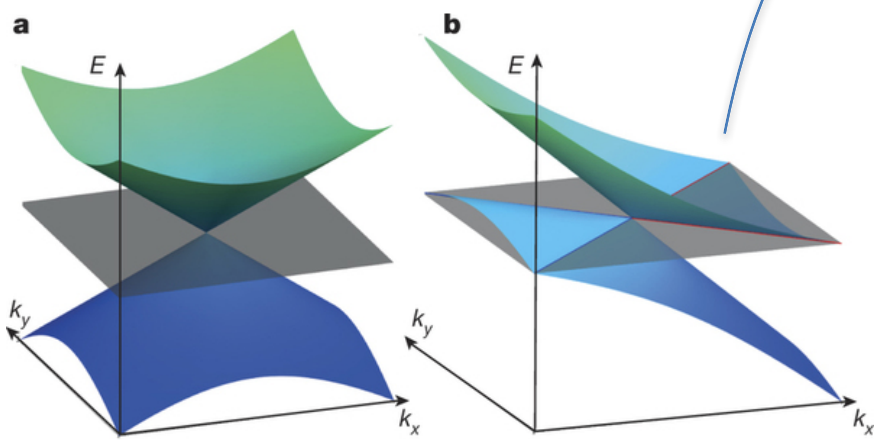
σ^z_{xy} ~ 800 (TaAs)

~ 2000 (Pt)

Spin Hall Angle

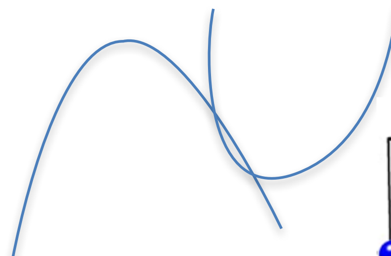
$\sigma^{Spin}/\sigma^{charge}$

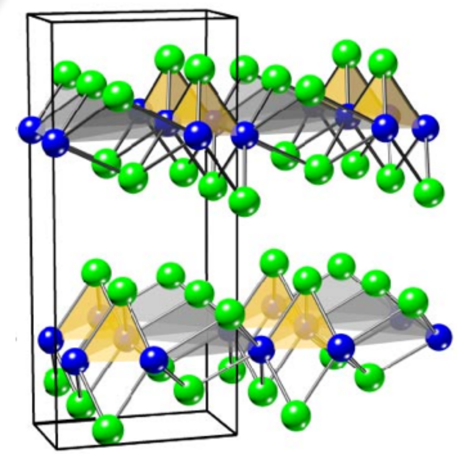
Two types of Weyl points



Type-I

Type-II





WTe_2, $MoTe_2$
(Td phase with inversion breaking)

<u>Stacking 2D TI layers into a WSM</u>

A. A. Soluyanov et al. Nature **527**, 495 (2015). (WTe2)

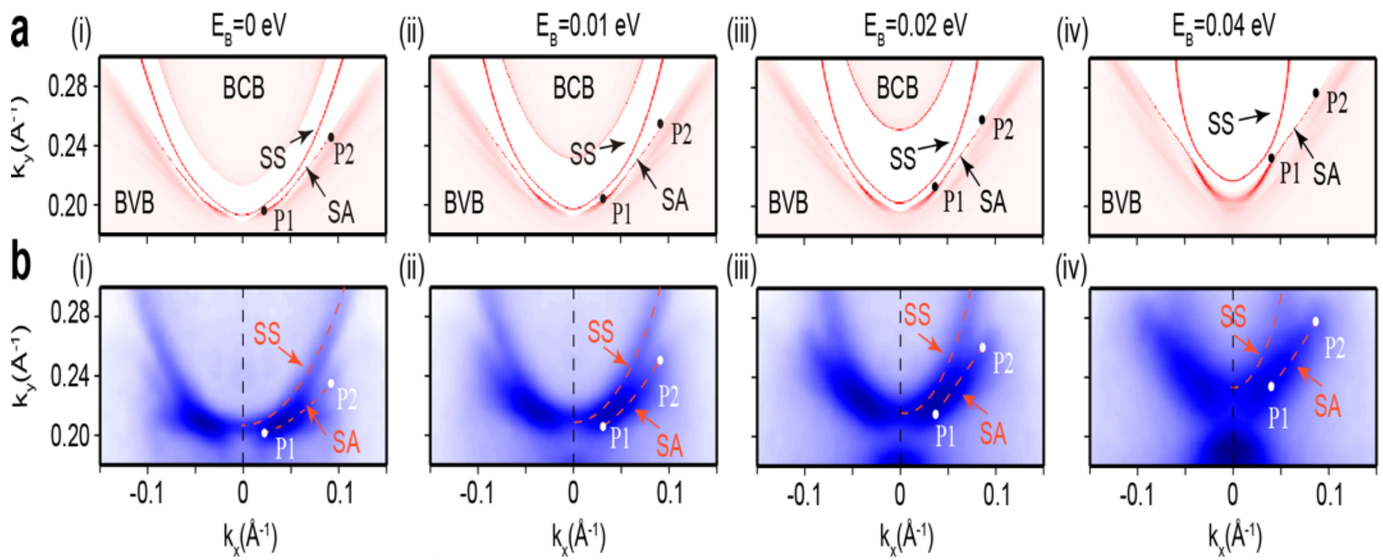
\- $MoTe_2$ -
Y. Sun, S.-C. Wu, M. N. Ali, C. Felser, and B. Yan, PRB **92**, 161107 (2015).

MoTe$_2$ ARPES

Fermi surface

Theory

ARPES

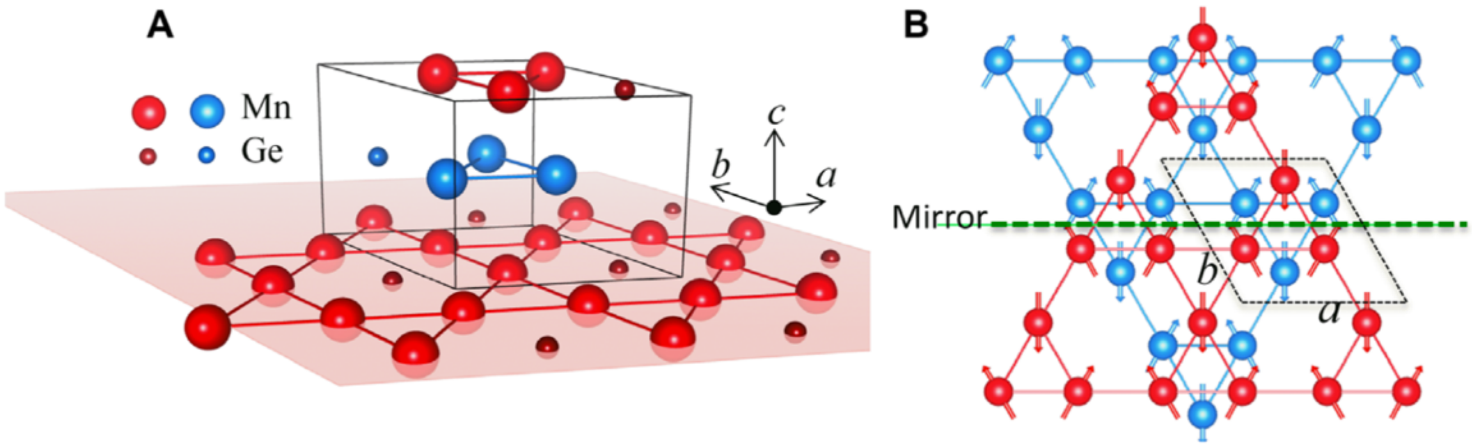


ARPES:

- Deng, K. et al. *Experimental observation of topological Fermi arcs in type-II Weyl semimetal MoTe2*. Nature Physics 12, 1105–1110 (2016).
- Huang, L. et al. *Spectroscopic evidence for a type II Weyl semimetallic state in MoTe2*. Nature Materials 15, 1155–1160 (2016).
- **Jiang, J. et al. *Signature of type-II Weyl semimetal phase in MoTe2*. Nature Commun. 8, 13973 (2017).**
- Tamai, A. et al. *Fermi Arcs and Their Topological Character in the Candidate Type-II Weyl Semimetal MoTe2*. Phys. Rev. X 6, 031021 (2016).
- Liang, A. et al. *Electronic Evidence for Type II Weyl Semimetal State in MoTe2*. arXiv:1604.01706 (2016).
- Sakano, M. et al. *Observation of spin-polarized bands and domain-dependent Fermi arcs in polar Weyl semimetal MoTe2*. Phys. Rev. B 95, 121101 (2017).

AFM WSMs from AHE materials

Room-temperature non-collinear AFM in the Kagome lattice

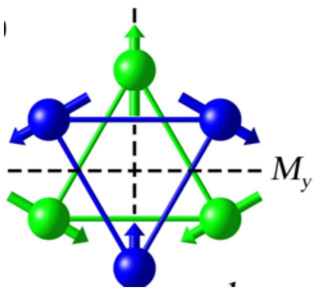


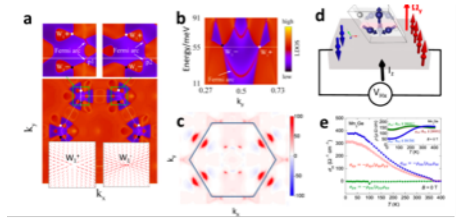
Observation of strong **AHE**:
Mn_3Sn (Tokyo) Nature 527, 212 (2015)
Mn_3Ge (MPI) Sci. Adv. 2, e1501870 (2016)

All spins align in-plane.

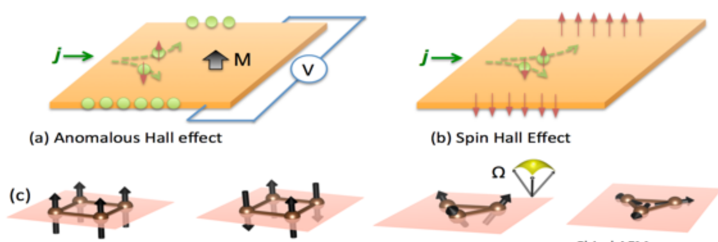
Observation of strong **SHE**
Mn_3Ir (MPI) Sci. Adv. **2**, e1600759 (2016)

AFM Weyl, AHE and SHE





Mn_3Sn	•	AFM WSMs
Mn_3Ge	•	Anomalous Hall and Nernst effects (AHE & ANE) at room temperature
	•	Intrinsic spin Hall effect due to spin texture (without SOC)



	Collinear FM	Collinear AFM	Chiral FM	Chiral AFM	TRS
AHE	$\rho_{xy} \propto M \lambda_{SOC}$	$\rho_{xy} = 0$	$\rho_{xy} \propto \boldsymbol{S_i} \cdot (\boldsymbol{S_j} \times \boldsymbol{S_k})$	$\rho_{xy} \propto \lambda_{SOC}$	0
SHE	λ_{SOC}	λ_{SOC}	$\cancel{\lambda_{SOC}}$?	$\cancel{\lambda_{SOC}}$?	λ_{SOC}

Nayak, A. K. *et al. Science Advances* **2,** e1501870–e1501870 (2016).
Zhang, W. *et al. Science Advances* **2,** e1600759–e1600759 (2016).
Yang, H. *et al. New Journal of Physics* **19,** 015008 (2017).
Zhang, Y. *et al. Physical Review B* **95,** 075128 (2017).
Železný, J., Zhang, Y., Felser, C. & Yan, B. arXiv:1702.00295
Šmejkal, L., Mokrousov, Y., Yan, B. & MacDonald, A. H. arXiv:1706.00670

Weyl materials

Linear response to a *dc* electric field field

SHE & AHE

- Both Weyl and ordinary bands contribute to AHC.
- Conventional materials work well.

Are there some properties for which a WSM is unique or better than ordinary materials?

Yes, possibly the nonlinear optical response.

Nonlinear optical response

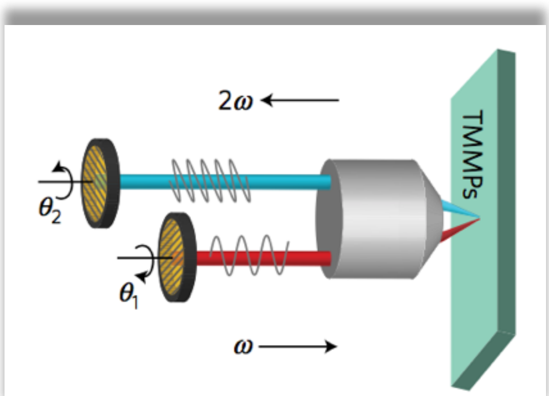
Second-order nonlinear response to the oscillating E-field of light

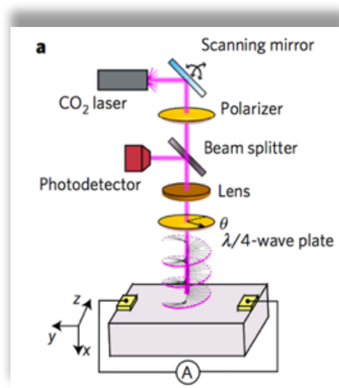
- Circular photogalvanic effect (CPGE)
- Second harmonic generation (SHE)

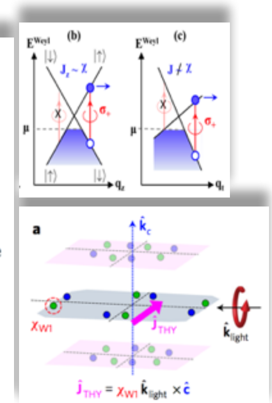
$$E_c(t) = Re\{\mathcal{E}_c e^{i\omega t}\}$$

$$j_a = \mathrm{Re}\{j_a^0 + j_a^{2\omega} e^{2i\omega t}\}$$

$$j_a^{(2\omega)} = \chi_{abc}\mathcal{E}_b\mathcal{E}_c \qquad j_a^{(0)} = \chi_{abc}\mathcal{E}_b\mathcal{E}_c^*$$



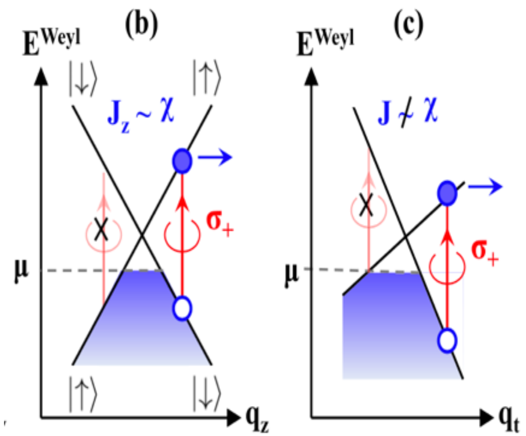




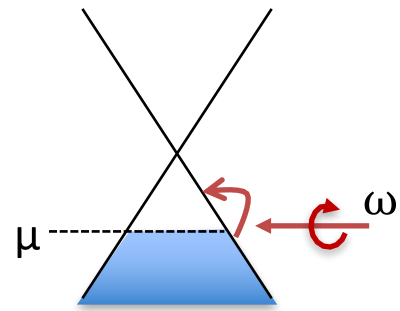
Experiment on WSM TaAs: Orenstein 17’, Gedik 17’, Wang 17’

Theory: Qi 15’, Pesin 15’, Burkov 15’, Ran 16’, Fu 15’, Moore 16’ 17’, Polini 17’, Nagaosa 16’, Tanaka 16’, Lee 17’…

Nonlinear optical response



Interband resonant transition



$$j_a^{(0)} = \chi_{abc}\mathcal{E}_b\mathcal{E}_c^*$$

<u>Intraband transition (low frequency)</u>

$$j_a = j_a^{(2\omega)}|_{\omega\to 0} = 2\chi_{abb}|\mathcal{E}_b|^2$$

At dc limit comes a nonlinear Hall effect.

[1] J. E. Moore and J. Orenstein, Phys. Rev. Lett. **105**, 026805 (2010).

[2] E. Deyo, L. E. Golub, E. L. Ivchenko, and B. Spivak, (2009), arxiv:0904.1917.

[3] I. Sodemann and L. Fu, Phys. Rev. Lett. **115**, 216806 (2015).

Semiclassical theory

Current

$$j_a = -e \int_k f(k) v_a$$

Anomalous velocity

$$v_a = \partial_a \epsilon(k) + \varepsilon_{\mathrm{abc}} \Omega_b \dot{k}_c, \qquad \dot{k}_c = -eE_c(t),$$

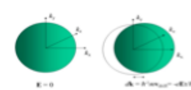
Light field

$$E_c(t) = \mathrm{Re}\{\mathcal{E}_c e^{i\omega t}\}$$

Solve the Boltzmann equation to the second order $-e\tau E_a \partial_a f + \tau \partial_t f = f_0 - f$

$$j_a = \mathrm{Re}\{j_a^0 + j_a^{2\omega} e^{2i\omega t}\} \qquad j_a^{(0)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c^* \qquad j_a^{(2\omega)} = \chi_{abc} \mathcal{E}_b \mathcal{E}_c$$

$$\chi_{\mathrm{abc}} = \varepsilon_{\mathrm{adc}} \frac{e^3 \tau}{2(1 + i\omega\tau)} \int_k (\partial_b f_0) \Omega_d$$



TRS

$$\Omega_c(k) = -\Omega_c(-k)$$

$$\sigma_{ab} = -\varepsilon_{abc} \frac{e^2}{\hbar} \int_k f_0 \Omega_c = 0$$

$$\int_k f_0 \Omega_c = 0 \qquad \int_k (f_0 + \partial_k f_0) \Omega_c = \int_k \partial_k f_0 \Omega_c \neq 0$$

[1] J. E. Moore and J. Orenstein, Phys. Rev. Lett. **105**, 026805 (2010).

[2] E. Deyo, L. E. Golub, E. L. Ivchenko, and B. Spivak, (2009), arxiv:0904.1917.

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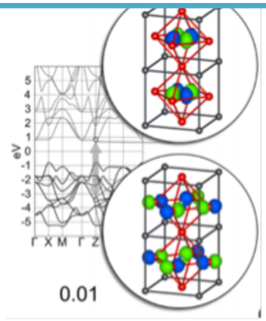
$$\chi_{\rm abc} = \varepsilon_{\rm adc} \frac{e^3 \tau}{2(1+i\omega\tau)} \int_k (\partial_b f_0) \Omega_d = -\varepsilon_{adc} \frac{e^3 \tau}{2(1+i\omega\tau)} \int_k f_0 \underline{(\partial_b \Omega_d)}$$

$\boxed{\text{Berry curvature dipole}}$ $$D_{ab} = \int_k f_0 (\partial_a \Omega_b).$$

- Intrinsic to the band structure
- Inversion symmetry breaking
- A Fermi surface property

I. Sodemann and L. Fu, Phys. Rev. Lett. **115**, 216806 (2015).

Ab initio calculations



Interband transitions are extensively studied for insulators, e.g. Rappe 12', Sipe and Shkrebtii 00'

Current work on intraband contributions in th Berry curvature dipole formalism

1. DFT (GGA) band structure and Bloch wave functions
   two representative familys: Tpe-I TaAs, type-II MoTe2
2. *Highly symmetric* Wannier functions for a single-particle Hamiltonian
3. Berry curvature **Ω**

$$\Omega_a^n(\mathbf{k}) = 2i \sum_{m \neq n} \frac{< n|\partial_{k_b}\hat{H}|m >< m|\partial_{k_c}\hat{H}|n >}{(\epsilon_n - \epsilon_m)^2}$$ *Xiao 10'*

4. Berry curvature dipole **D,** a tensor $$D_{bd} = \int_k f_0 \frac{\partial \Omega_d}{\partial k_b}$$ *Fu 15'*

Start with toy models

A single Weyl cone

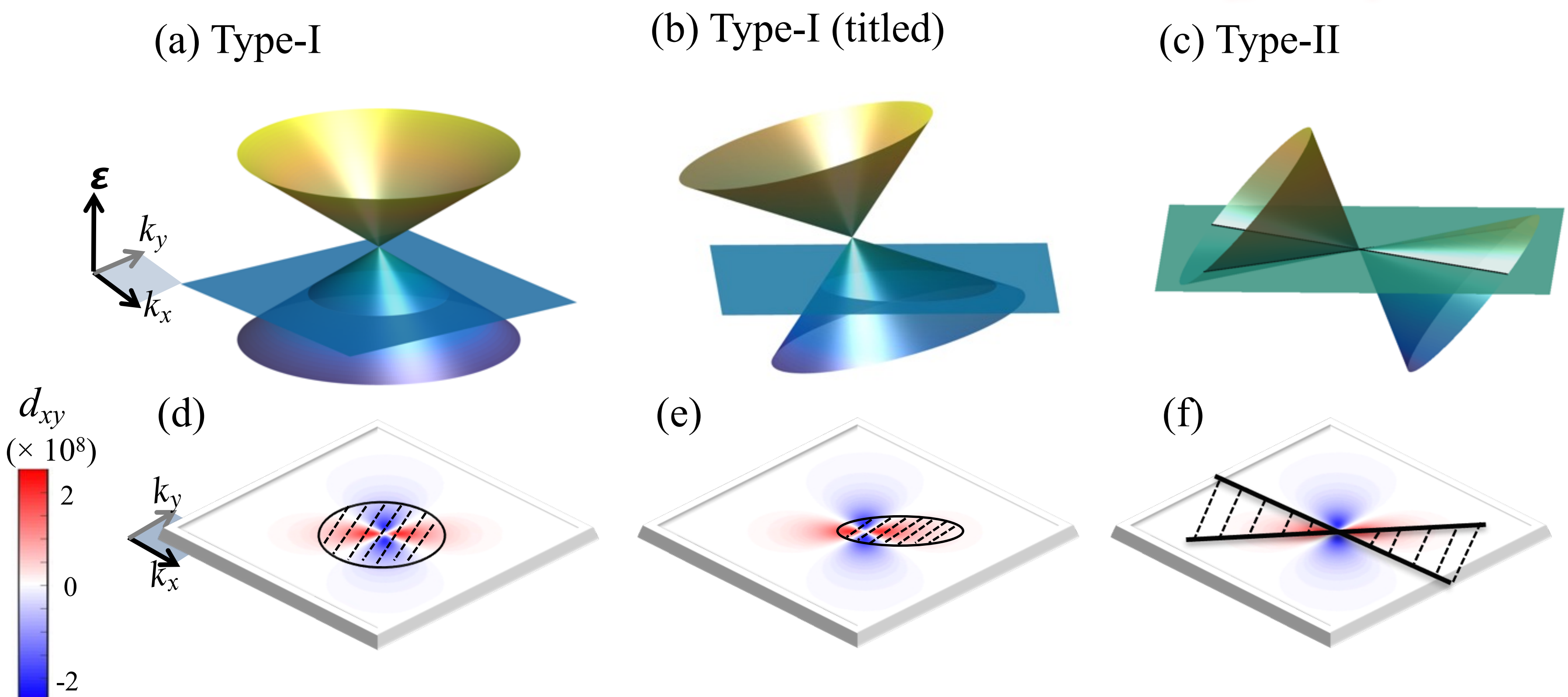
$$H_{Weyl}(\mathbf{q}) = \hbar v_t q_t \sigma_0 + \hbar v_F \mathbf{q} \cdot \sigma,$$

Berry curvature

$$\Omega(\mathbf{q}) = \frac{\mathbf{q}}{2q^3}$$

Berry curvature dipole

$$d_{xy} = \frac{\partial \Omega_y}{\partial q_x} = \frac{3q_x q_y}{2q^5}$$



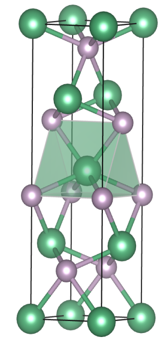
*Note that $d_{xy} = \partial\Omega_y/\partial k_x$ is **even** to Mx, My or TRS.*
So a pair of Weyl points contribute the same D_{xy}.

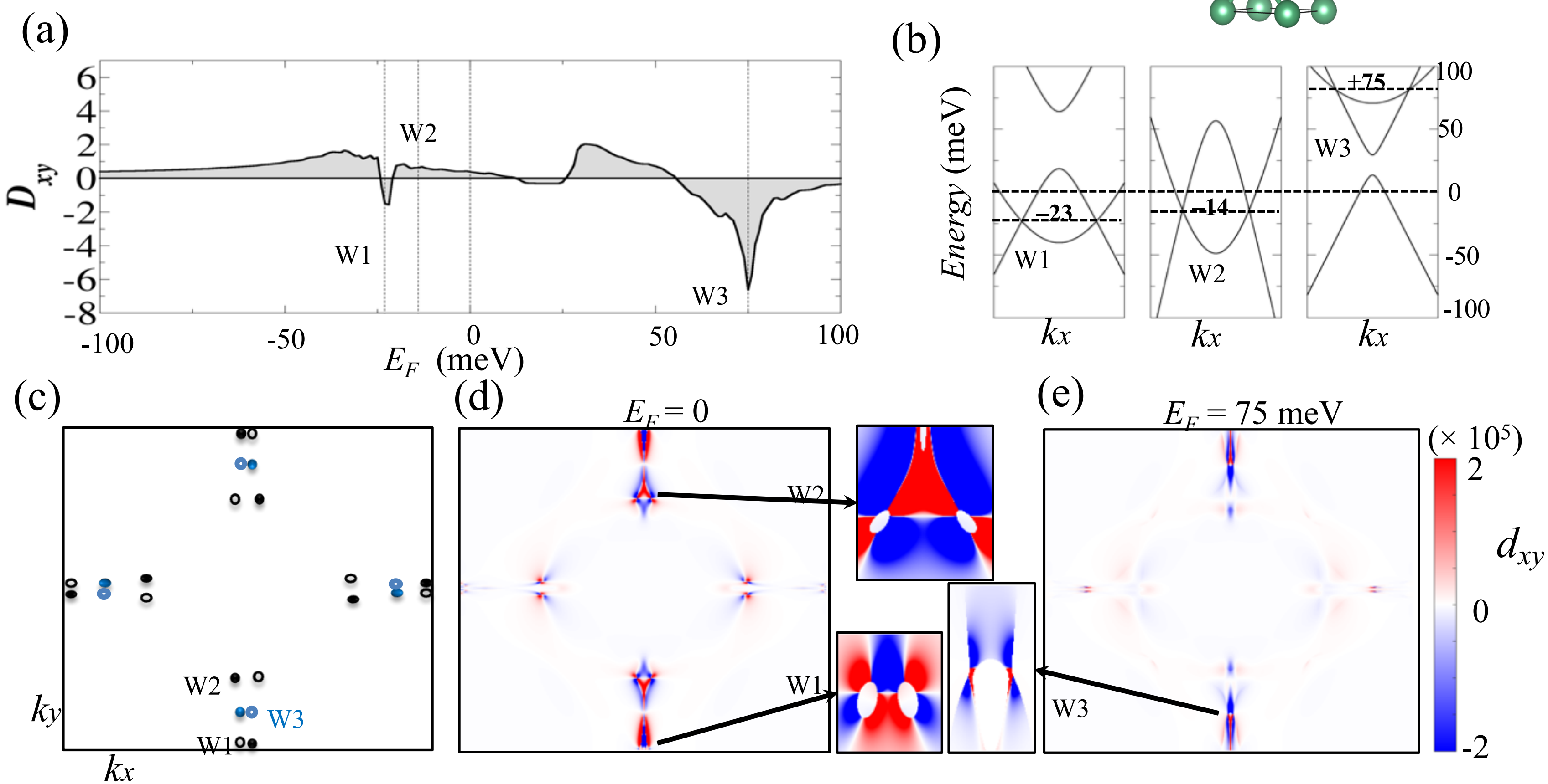
Berry curvature dipole for TaAs

- Point group C4v: M_x, M_y, C_4

  E.g. Mx: $k_x \rightarrow -k_x$, $\Omega_x \rightarrow \Omega_x$ *so* $d_{xx} \rightarrow -d_{xx}$ *then* $D_{xx} = 0$

  *Finally we have **only one** independent element* $D_{xy} = -D_{yx}$

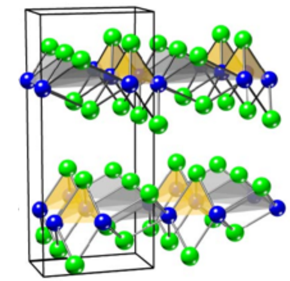


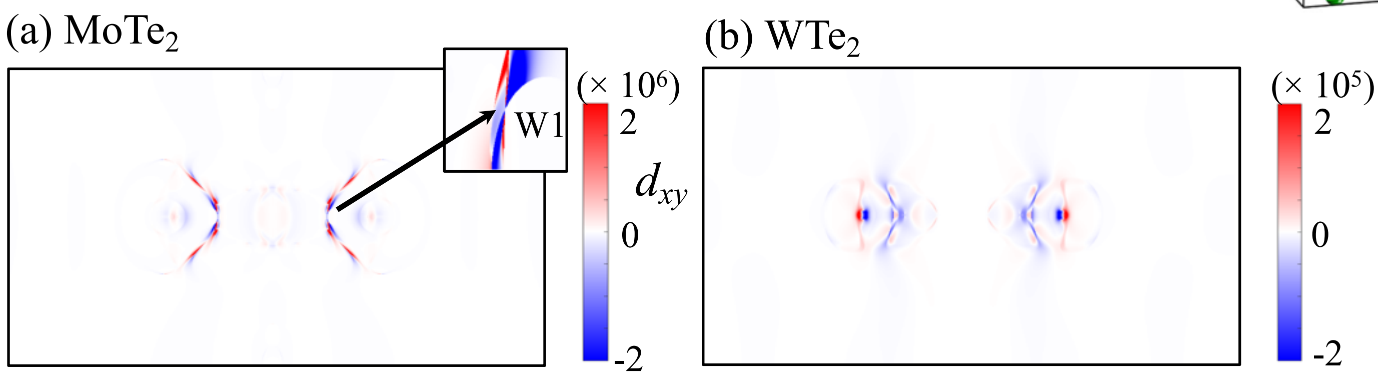


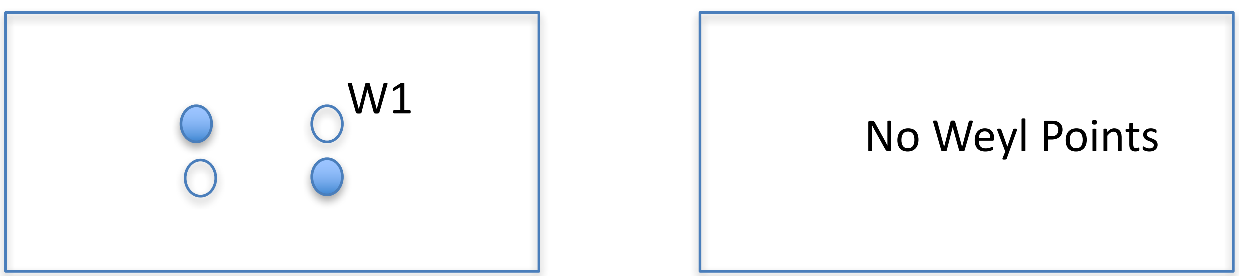
Berry curvature dipole for $MoTe_2$ and WTe_2

- Point group C2v

Finally we have two independent element D_{xy} and D_{yx}







Berry curvature dipole

Material	D_{xy}	Material	D_{xy}	D_{yx}
TaAs	0.39	$MoTe_2$	0.849	-0.703
TaP	0.029	WTe_2	0.048	-0.066
NbAs	-9.88			
NbP	20.06			

- WSM is better than non-WSM
- Type–II is generally better than type–I
- D_{xy} is not scaled by SOC, different from SHE
- A pair of Weyl points related by $M_{x,y}$ or TRS contribute the same D_{xy}

Y. Zhang, Y. Sun, B. Yan, *arXiv:1708.08589.*

Estimation for the nonlinear Hall effect

Material	D_{xy}	Material	D_{xy}	D_{yx}
TaAs	0.39	$MoTe_2$	0.849	-0.703
TaP	0.029	WTe_2	0.048	-0.066
NbAs	-9.88			
NbP	20.06			

$$\chi_{abc} = -\varepsilon_{adc} \frac{e^3 \tau}{2\hbar^2 (1 + i\omega\tau)} D_{bd}$$

D_{xy} corresponds to χ_{zxx} and χ_{xxz}

$d_{xy} = \partial\Omega_y/\partial k_x$
x: the current direction
y: berry curvature (B field)
z: Hall current

$$j_z = 2\chi_{zxx}\mathcal{E}_x^2 \qquad j_x = \sigma_{xx}\mathcal{E}_x$$

a Hall angle as $\gamma = j_z/j_x = 2(\chi_{zxx}/\sigma_{xx})\mathcal{E}_x$

AHE systems $\gamma \sim 10^{-3}$

$\tau \sim 10$ ps and $\sigma_{xx} \sim 10^6\ \Omega^{-1}\mathrm{m}^{-1}$

$\mathcal{E}_x \sim 10^2$ V/m

$\chi_{zxx} \sim 10^{-1} D_{xy}$

For TaAs, NbPAs, NbP, MoTe2

$\gamma \sim 10^{-5} - 10^{-4}$

Y. Zhang, Y. Sun, B. Yan, *arXiv:1708.08589.*

Fermi surface is tunable by gating, doping or strain.

Estimation for the nonlinear Hall effect

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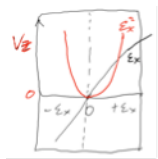
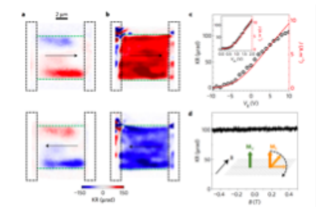


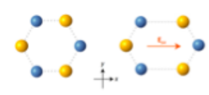
Signatures in earlier experiments



unstrained strained

Kerr rotation image of a single-layer MoS2 device

Valley magnetoelectricity in single-layer MoS2



Lee, J., Wang, Z., Xie, H., Mak, K. F. & Shan,
Nature Materials **16,** 887–891 (2017).

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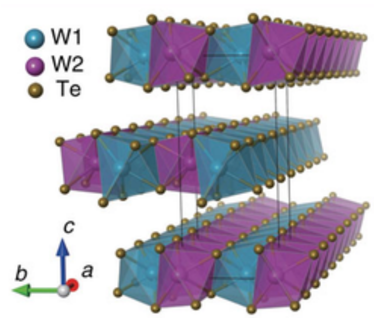
Magnetoelectric Effect in Polar Superconductors

Victor M. Edelstein

Institute of Solid State Physics, Russian Academy of Sciences, 142432 Chernogolovka Moscow Region, Russia

(Received 12 December 1994)

The question of how the lack of spatial reflection symmetry can affect properties of a superconductor is investigated. A novel magnetoelectric effect is predicted. The supercurrent in a metal of polar symmetry must be accompanied by the spin polarization of the carriers. The relevance to some known pyro- and antipyroelectric superconductors including a high-temperature system as well as the possibility of an experimental verification are briefly discussed.

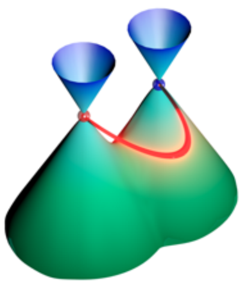


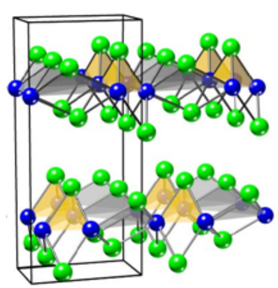
WTe2 ?
Inversion breaking
Weyl, QSH
Superconductor

NMR, Spin current

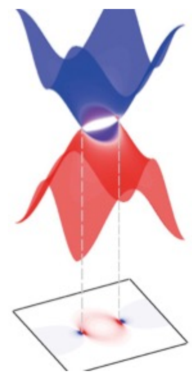
Summary

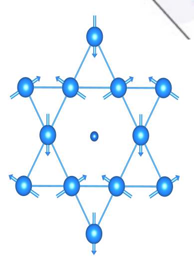
Topological materials





Berry curvature
Linear response

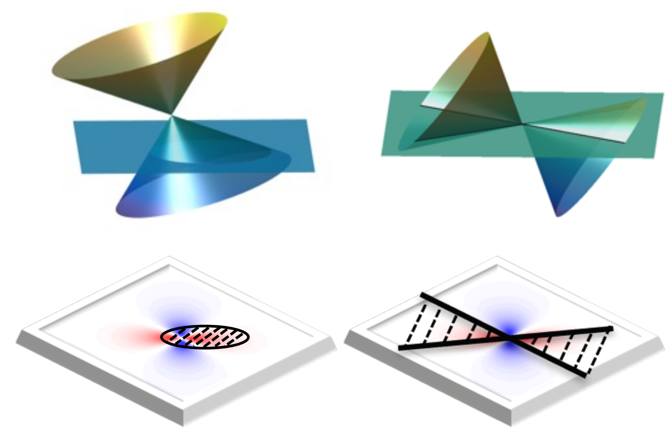




AFM Weyl
AHE, ANE
SHE w/o SOC

Mn_3Ge and Mn_3Sn

Berry curvature dipole
Nonlinear response



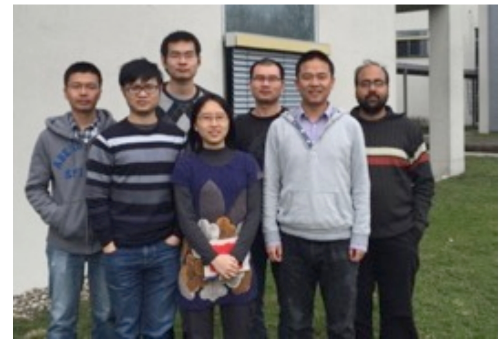
- Topological materials
- Experiments

- Berry phase induced electric and optical properties
- Develop ab initio tools

Acknowledgement

Collaborators
(MPI Dresden):

- Claudia Felser
- **Yan Sun , Yang Zhang， Yang Hao**



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- Liang Fu (MIT)
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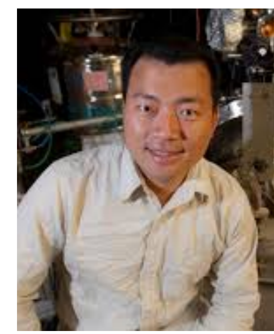
- Di Xiao (Carnegie Mellon U)
- Stuart Parkin (MPI Halle)



Thanks for your attention!