Topological transport in Weyl semimetal

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About myself :

"To be yourself in a world that is constantly trying to make you something else is the greatest accomplishment." —Ralph Waldo Emerson

Banasree Sadhukhan, PhD

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Education

PhD : Condensed matter Physics Presidency University 2018
Thesis title : "Study of electronic structure, optical and magnetic response of disordered solids"

M. Sc. : Physics University of Calcutta 2011

B. Sc. : Physics University of Calcutta 2009

Research Experience after PhD :

Researcher at KTH Royal institute of Technology, Stockholm, Sweden (September, 2022 - Present) (C)

Postdoctoral researcher at KTH Royal institute of Technology, Stockholm, Sweden (September, 2020 - August , 2022) (C)

Scientist at Institute for Solid State and Materials Research, IFW Dresden, Germany (March, 2019 - February, 2020) (B)

Postdoctoral researcher at Institute for Solid State and Materials Research, IFW Dresden, Germany (March, 2018 - February, 2019) (A)

Current research areas

(A) Energy harvesting modern technologies

(B) Quantum materials and Topological transport ★

(C) Light-matter interaction in Skyrmion

Introduction and motivation

Topology, Weyl semimetal, symmetry

Theory and computation behind transport

Results and discussions on current research

Linear transport

npj Quantum Materials **7**, 19 (2022) [Tunable chirality of noncentrosymmetric magnetic Weyl semimetals in rare-earth carbides]

Phys. Rev. B **107** (8), L081110 (2023) [Effect of chirality imbalances on Hall transport of $PrRhC_2$]

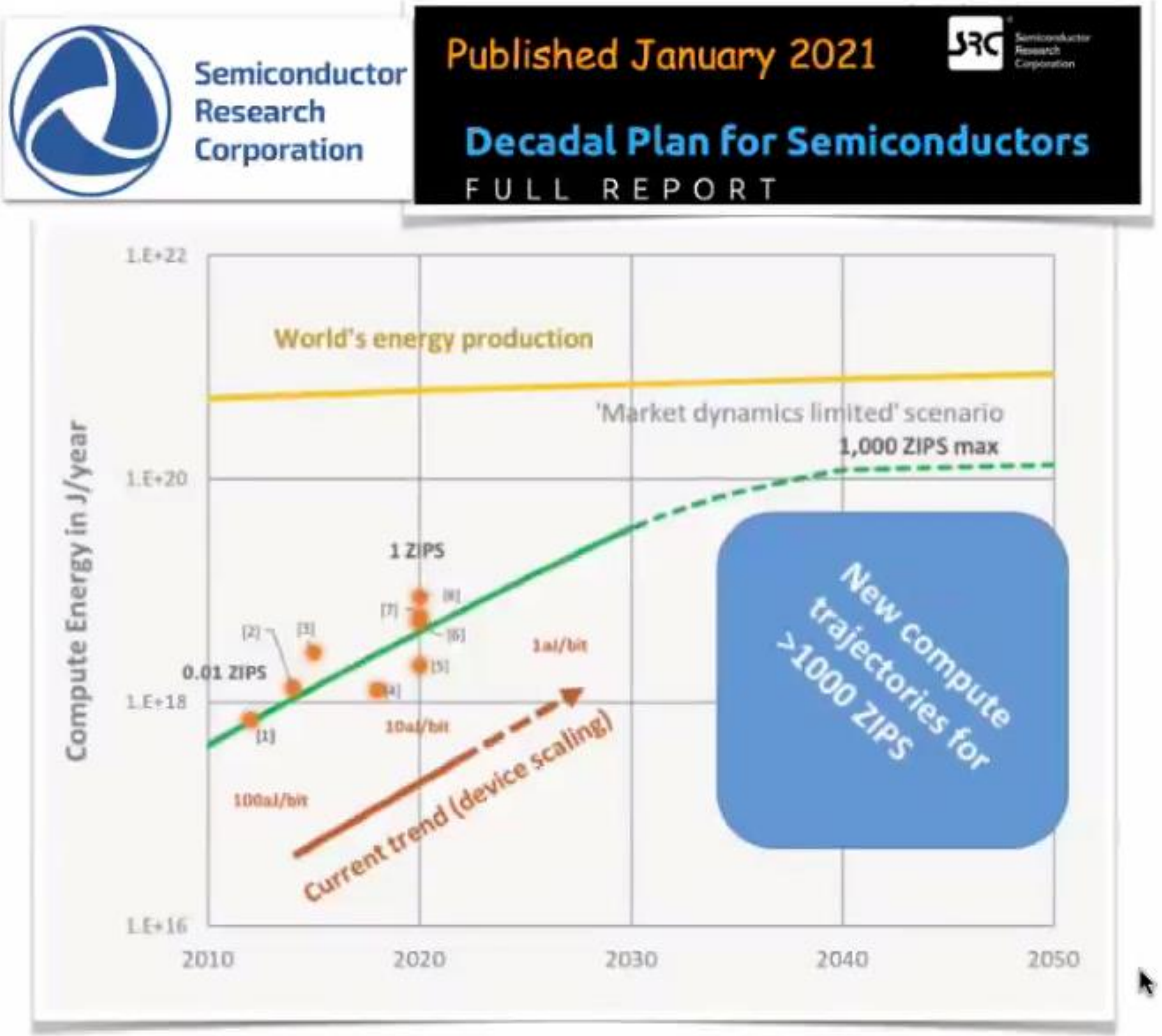
Non- Linear transport

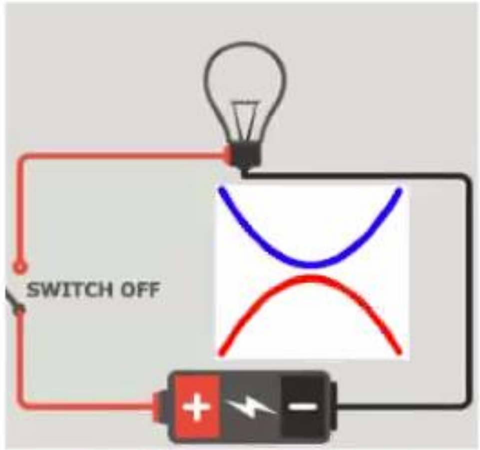
Phys. Rev. B **104**, 245122 (2021) [Electronic structure and unconventional nonlinear response in double Weyl semimetal $SrSi_2$]

Phys. Rev. B **103**, 144308 (2021) [Role of time reversal symmetry and tilting in circular photogalvanic responses]

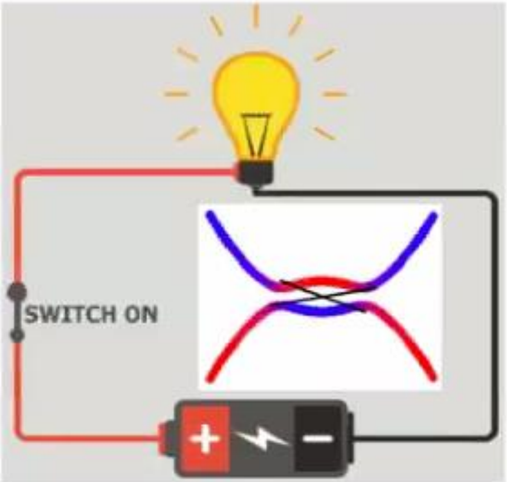
Conclusions

Topological Materials for Low-energy Electronics :





Ordinary Insulator



Topological Insulator

New mechanisms for electronic conduction without dissipation at room temperature

- Need new technology with capacity to switch at lower energy than silicon device

What is topology ?

★ Geometric properties (such as curvature) are local properties, but integral over local geometric properties give global topology

g = 0

Gauss-Bonnet theorem for a closed surface

$$\frac{1}{2\pi}\int_S K\,da = \chi = 2 - 2g$$

Gaussian curvature

Genus (g)

g = 1

★ Objects are described by topological invariants = Genus (g) of a surface = No of holes

Birth of topological materials :


David J. Thouless


F. Duncan M. Haldane


J. Michael Kosterlitz

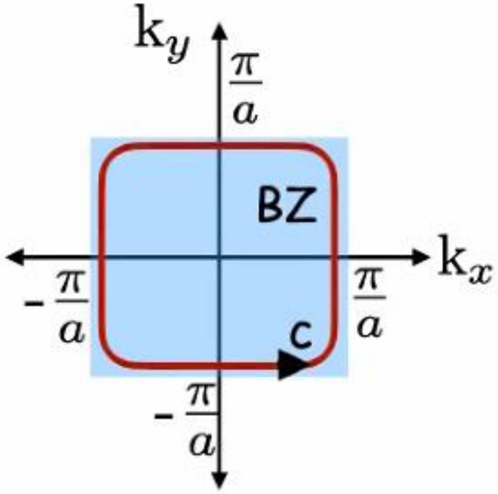
The Nobel Prize in 2016

Quantized Hall effect in 2D electron gas
(Klaus von Klitzing, Nobel Laureate 1985)

TKNN Theory (1982) :

The Chern Insulator and the birth of "topological materials"

Bloch's theorem : $\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}.\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$



Energy band can be characterized by a topological number

Berry phase : $e^{i\Phi_B(\Gamma)} = \exp\left(i \oint_\Gamma dk_a \mathcal{A}_n(\boldsymbol{k})\right)$

Berry curvature

$$F_n = \sum_{l \neq n} \nabla_{\mathbf{k}} \times \langle u_n(\mathbf{k}) | i\nabla_{\mathbf{k}} | u_l(\mathbf{k}) \rangle$$

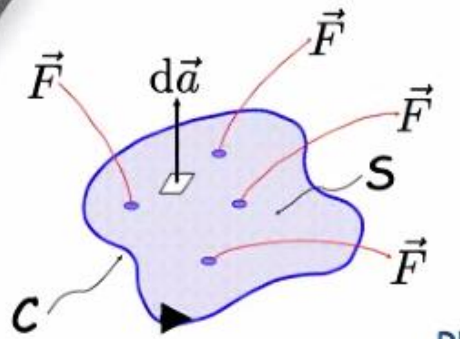
$\mathcal{A}_n(\boldsymbol{k})$

Topological invariant : Chern number

$$c_n = \frac{e^2}{\hbar} \sum_{\substack{\text{occupied}\\ \text{bands}}} \int_{BZ} \frac{d^2\mathbf{k}}{(2\pi)^2} F_n$$

$c_n = 0$
Normal insulator

$c_n \neq 0$
Topological Chern insulator

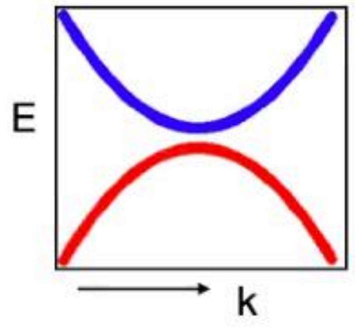


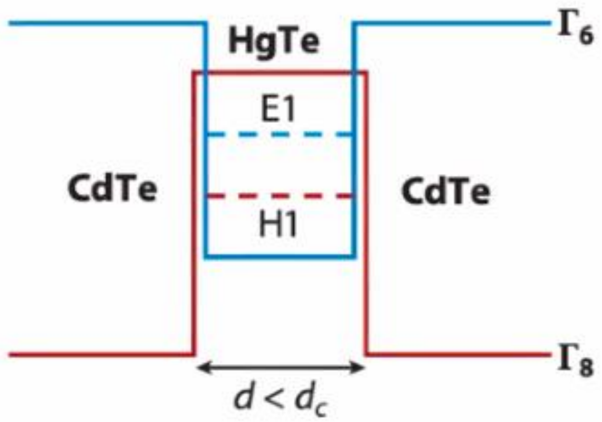
Phys. Rev. Lett. **49**, 405 (1982)

First realisation of topological material : CdTe/HgTe Quantum well

Science **314**, 1757 (2006) [Theory]; Science **318**, 766 (2007) [Experiment]

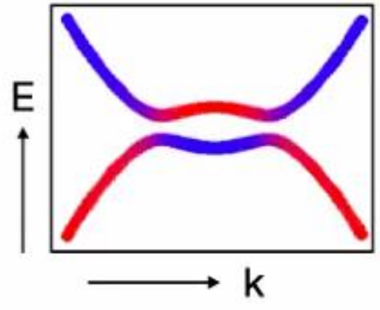
Normal insulator : CdTe

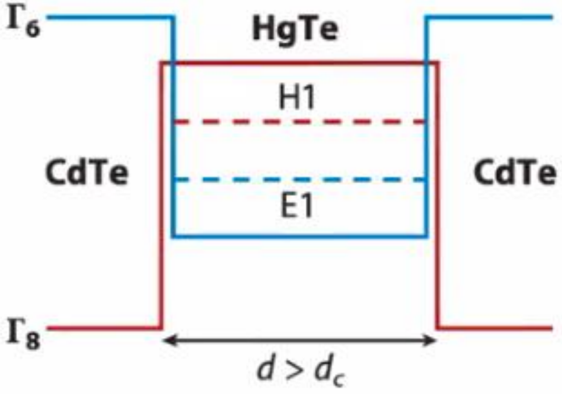




Trivial insulator :
$E_{\Gamma_6} > E_{\Gamma_8}$

Topological insulator : HgTe





Nontrivial insulator :
$E_{\Gamma_6} < E_{\Gamma_8}$

HgTe layer is thick and bands get inverted

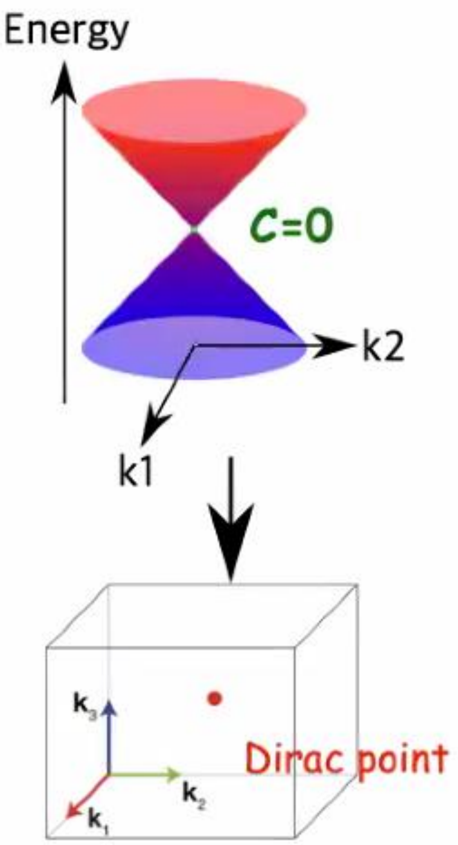
Annu. Rev. Condens. Matter Phys **2(1)**, 31 (2011)

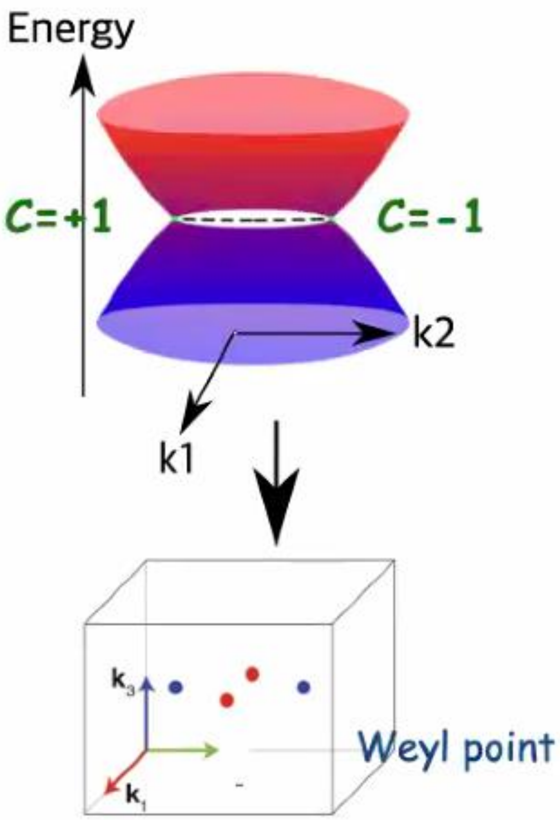
Various topological semimetals :

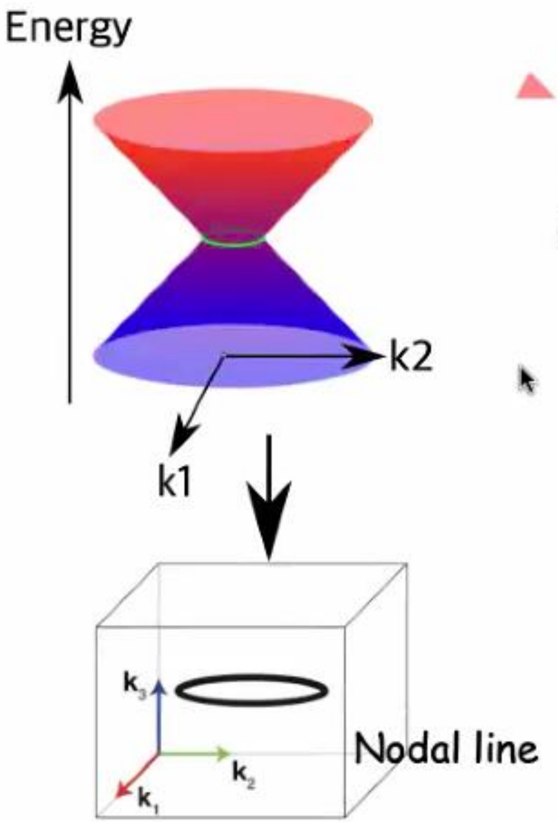
Chern no (Topological invariant) : $C_n = \frac{1}{2\pi}\int_a dS \cdot \Omega_{nk}$

Berry curvature of Bloch wave functions

Dirac semimetal	Weyl semimetal	Nodal line semimetal



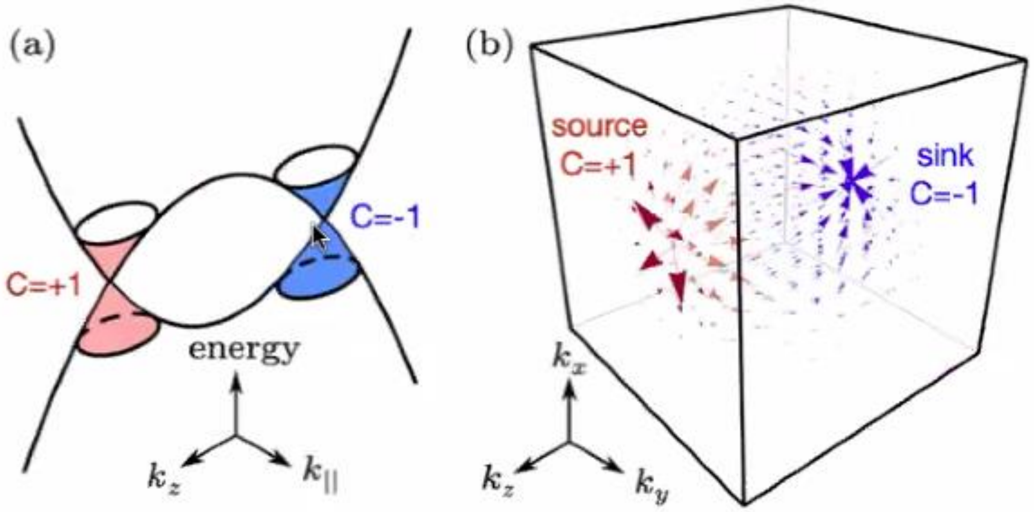




By breaking symmetries

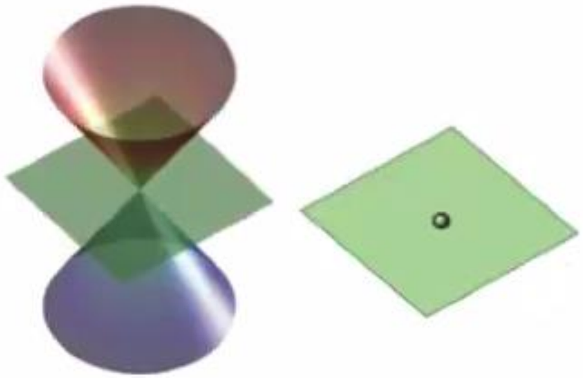
Annual Review of Materials Research 49(1), 153 (2019)

New realm of topological materials : WSMs



Weyl point : Monopole of Berry curvature

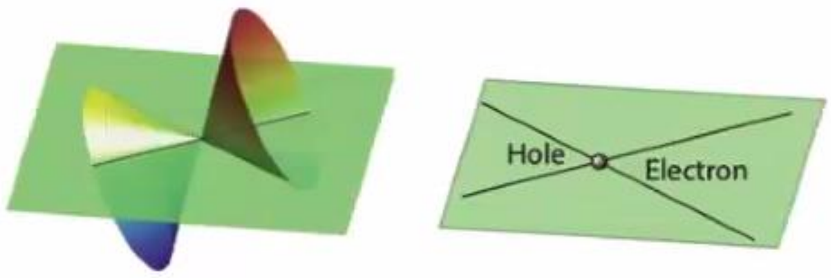
Low energy Weyl Hamiltonian : $H_{\text{Weyl}}(\mathbf{q}) = \hbar v_t q_t \sigma_0 + \hbar v_F \mathbf{q} \cdot \sigma$



$|v_t/v_f| < 1$

Point like Fermi surface

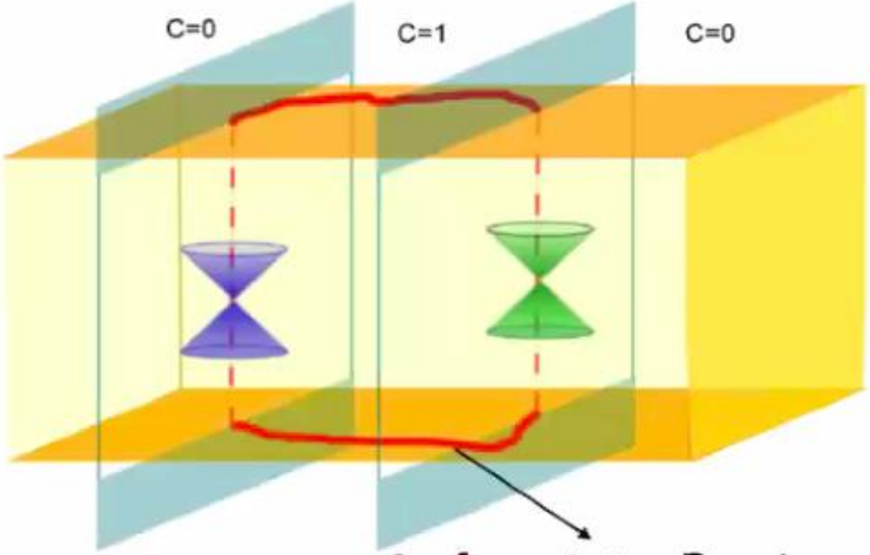
TaAs, Tap, NbAS, NbP



$|v_t/v_f| > 1$

Pocket like Fermi surface

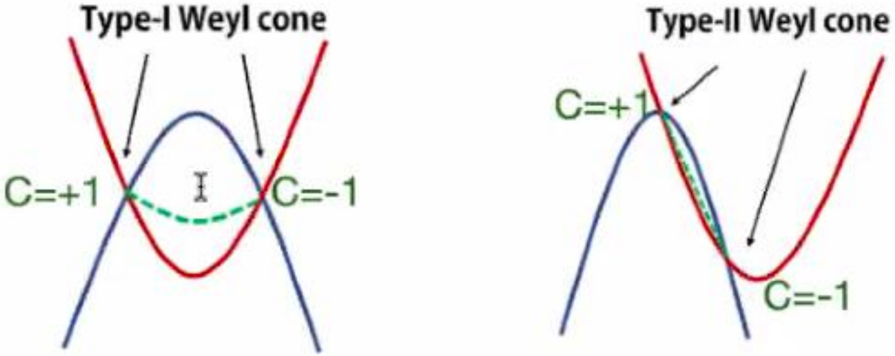
MoTe2, WTe2



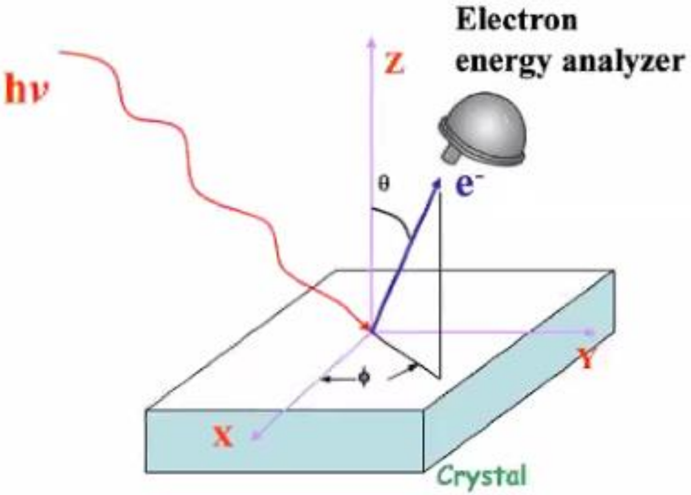
Surface state : Fermi arc

Annu. Rev. Condens. Matter Phys. 8, 337 (2017)

New realm of topological materials : WSMs

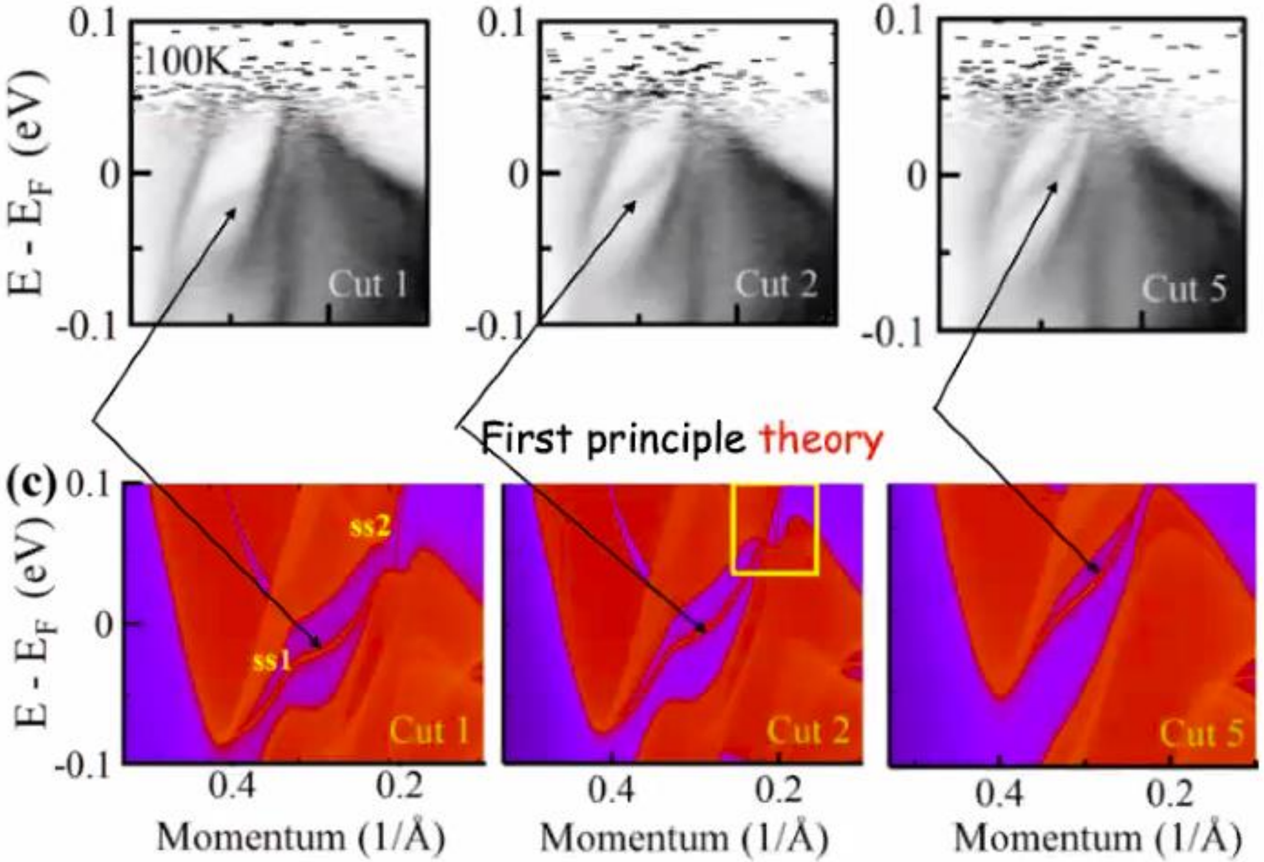


Experimental setup for ARPES



Type-II Weyl semimetal WTe2

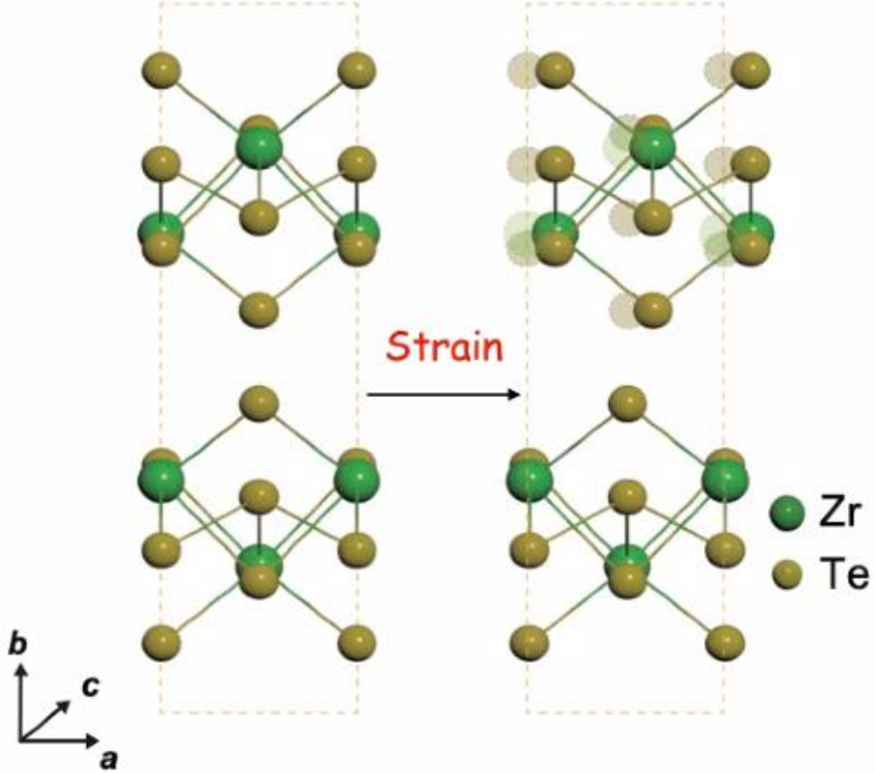
ARPES experiment



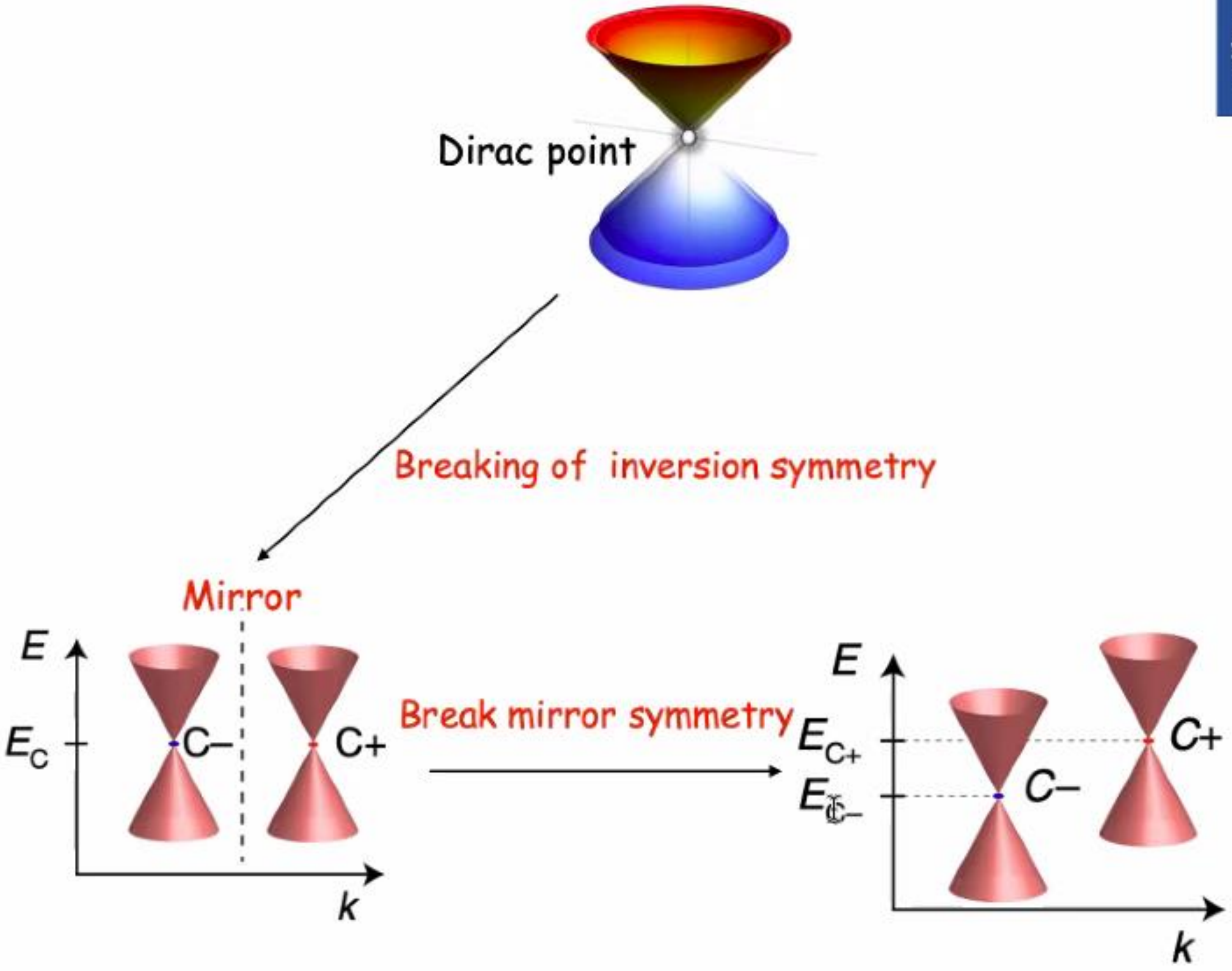
RMP 90, 015001 (2018), Nat Rev Phys 1, 609 (2019)

Different symmetries in WSMs :

Inversion symmetry $(x \rightarrow -x, y \rightarrow -y, z \rightarrow -z)$



Dirac semimetal : ZrTe5



Degenerated Weyl point

Weyl Semimetals like TaAs, MoTe2

Non-degenerated Weyl point

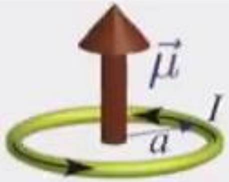
CoSi, RhSi, SrSi2

Nature Physics **15**, 759 (2019), PNAS **113** **(5)**, 1180 (2016)

Different symmetries in WSMs :

Time reversal symmetry →

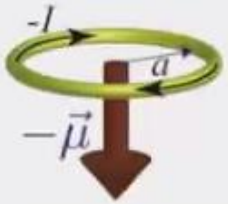
Classical Picture:



$$\vec{\mu} = \frac{\pi I a^2}{c}\hat{z}$$

And, applying the time-reversal operator:

$$\hat{\mathcal{T}} I = -I \longrightarrow \hat{\mathcal{T}}\vec{\mu} = -\vec{\mu}$$

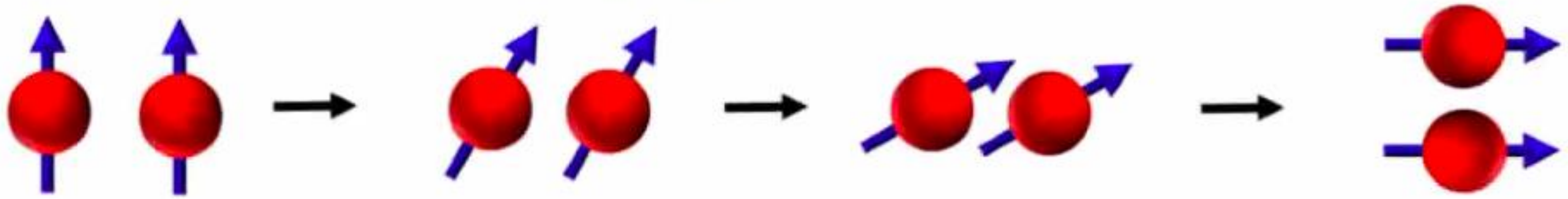


Which is the same as applying $\hat{\mathcal{T}} = i\sigma^y\hat{\mathcal{K}}$ to the spin.

Therefore, for a ferromagnet:

$$\hat{\mathcal{T}}\{\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\} = \downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow$$

Canting magnetization axis



Semi-classical framework of linear response :

The semiclassical equations of motion

$\sqrt{B} \ll \mu$

$$\dot{\mathbf{r}} = D(\mathbf{B}, \mathbf{\Omega_k})[\mathbf{v_k} + \underbrace{e(\mathbf{E} \times \mathbf{\Omega_k})}_{\text{AV}} + \underbrace{e(\mathbf{v_k} \cdot \mathbf{\Omega_k})\mathbf{B}}_{\text{CME}}],$$

$$\dot{\mathbf{k}} = D(\mathbf{B}, \mathbf{\Omega_k})[e\mathbf{E} + e(\mathbf{v_k} \times \mathbf{B}) + \underbrace{e^2(\mathbf{E} \cdot \mathbf{B})\mathbf{\Omega_k}}_{\text{CA}}]$$

- Charge current $\mathbf{J} = \int \frac{d^3k}{(2\pi)^3} D\dot{\mathbf{r}} f_{\mathbf{k},\mathbf{r},t}$

$$\mathbf{J} = \mathbf{J}_{\mathrm{D}} + \mathbf{J}_{\mathrm{AH}} + \mathbf{J}_{\mathrm{CA/CME}}$$

Drift current

Anomalous Hall current

Chiral current

For CA : (B . E)

For CME : E = 0

$$\mathbf{J}_{\mathrm{D}} \approx \int \frac{d^3k}{(2\pi)^3} \mathbf{v_k} f_{\mathbf{k},\mathbf{r},t}$$

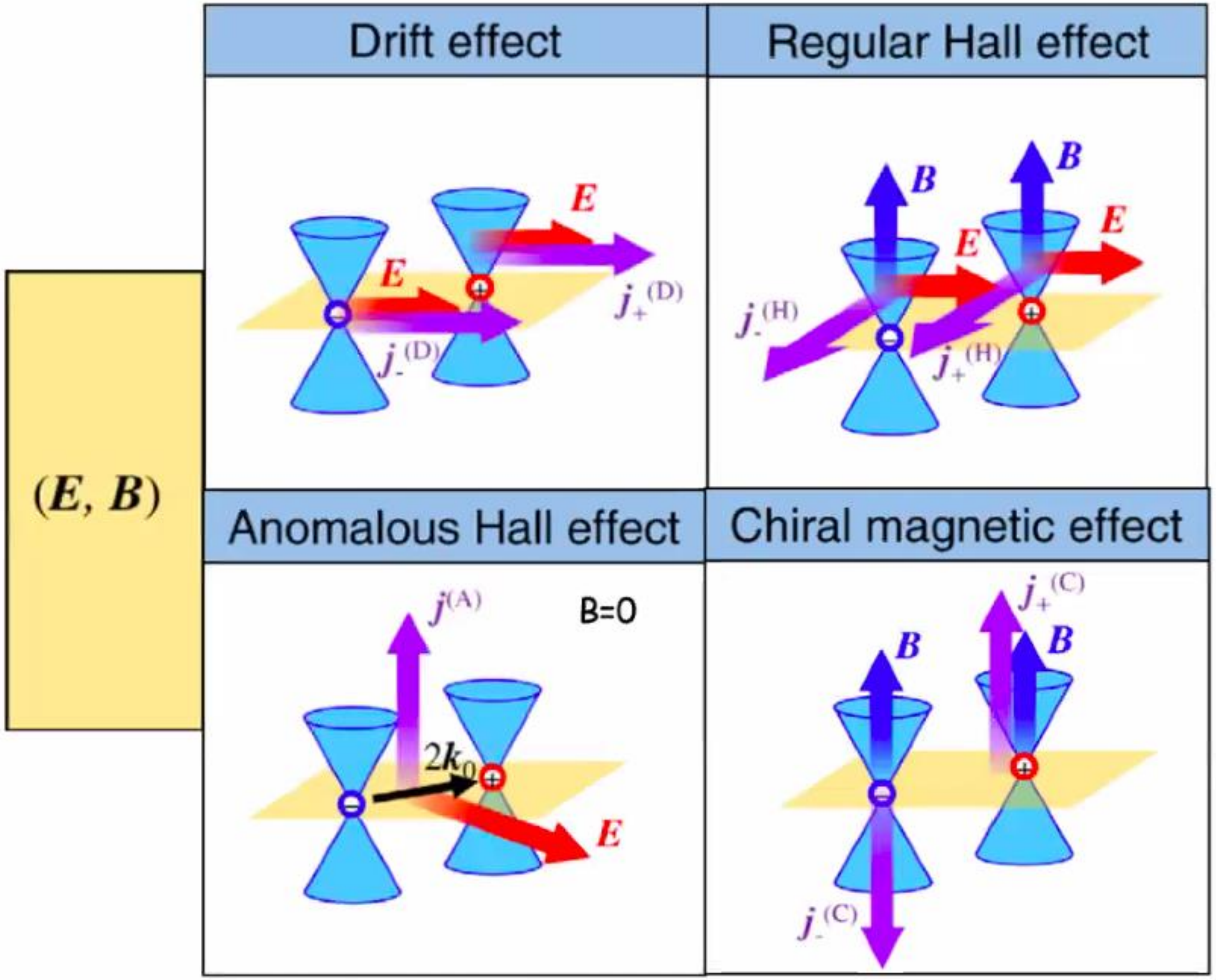
$$\mathbf{J}_{\mathrm{AH}} \approx \mathbf{E} \times \int \frac{d^3k}{(2\pi)^3} \mathbf{\Omega_k} f_{\mathbf{k},\mathbf{r},t}$$

Berry curvature

$$\mathbf{J}_{\mathrm{CA/CME}} \approx \mathbf{B} \int \frac{d^3k}{(2\pi)^3} (\mathbf{v_k} \cdot \mathbf{\Omega_k}) f_{\mathbf{k},\mathbf{r},t}$$

Chiral contribution

Ann. Phys.(Berlin) 532, 1900287 (2020), PRB 88 104412 (2013)



Drift current

$$\mathbf{J}_{\mathrm{D}} \approx \int \frac{d^3k}{(2\pi)^3} \mathbf{v}_{\mathbf{k}} f_{\mathbf{k},\mathbf{r},t}$$

Anomalous Hall current

$$\mathbf{J}_{\mathrm{AH}} \approx \mathbf{E} \times \int \frac{d^3k}{(2\pi)^3} \mathbf{\Omega}_{\mathbf{k}} f_{\mathbf{k},\mathbf{r},t}$$

Chiral current

$$\mathbf{J}_{\mathrm{CA/CME}} \approx \mathbf{B} \int \frac{d^3k}{(2\pi)^3} (\mathbf{v}_{\mathbf{k}} \cdot \mathbf{\Omega}_{\mathbf{k}}) f_{\mathbf{k},\mathbf{r},t}$$

"Chiral magnetic effect" works if Weyl points appear at different energy levels.

Ann. Phys.(Berlin) 532, 1900287 (2020), PRB 88 104412 (2013)

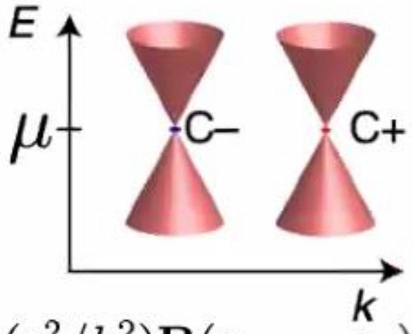
- **Magneto-conductivity :** $J_i = \alpha_{ij} B_j \qquad \alpha = -\frac{e^2}{\hbar} \sum_n \int d^3\mathbf{k}/(2\pi)^3 f_{\mathbf{k}n} \left(\mathbf{v}_{\mathbf{k}n} \cdot \Omega_{\mathbf{k}n}\right)$

Fermi surface integral and integrating by parts for the term $f_{\mathbf{k}n} \left(\mathbf{v}_{\mathbf{k}n} \cdot \Omega_{\mathbf{k}n}\right)$ and putting $\frac{\delta f^0}{\delta \mathbf{k}} = -\hat{\mathbf{v}}_{\mathbf{f}} \delta^3(\mathbf{k} - \mathbf{k}_f)$ with $\hat{\mathbf{v}}_{\mathbf{f}}$ the FS normal at $\mathbf{k}_{\mathbf{f}}$, and introduce the Chern number $C_{na} = (1/2\pi) \int_{S_{na}} dS(\hat{\mathbf{v}}_F \cdot \mathbf{\Omega}_{\mathbf{k}n})$ of the ath Fermi sheet S_{na} in band n

- **Magneto-conductivity for CME :** $\alpha^{\mathrm{CME}} = -(e^2/h^2) \sum_{n,a} \mu_{na} C_{na} \qquad$ with $J_{CME} = \alpha_{CME} B$

For $\mathbf{E} = \mathbf{0}$, chiral magnetic effect (CME) : $J_{CME} = -\frac{e^2}{\hbar^2} \sum_{m\alpha} \mu_{m\alpha} C_{m\alpha}$

$\mu_R = \mu_L = \mu$

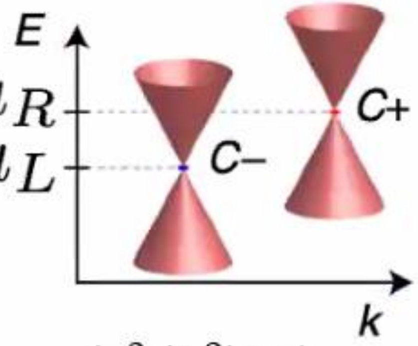


$J_{CME} = (e^2/h^2)\mathbf{B}(\mu_{\mathbf{R}} - \mu_{\mathbf{L}}) = \mathbf{0}$

Chiral chemical potential = $\mu_R - \mu_L$

μ_R

μ_L



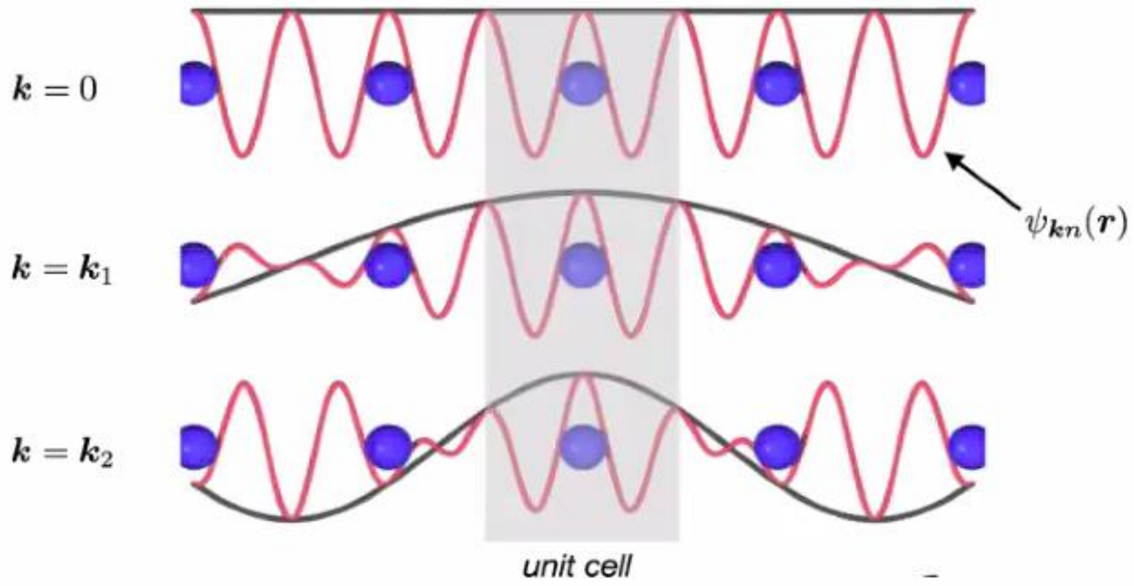
$J_{CME} = (e^2/h^2)\mathbf{B}(\mu_{\mathbf{R}} - \mu_{\mathbf{L}}) \neq \mathbf{0}$

For non-zero chiral chemical potential

PRL **109**, 181602 (2012), PRB **88**, 104412 (2013), PRL **116**, 077201 (2016), Eur. Phys. J. B (2018) 91: 83, PRB **92**, 085138 (2015)

Computational framework and Wannier functions :

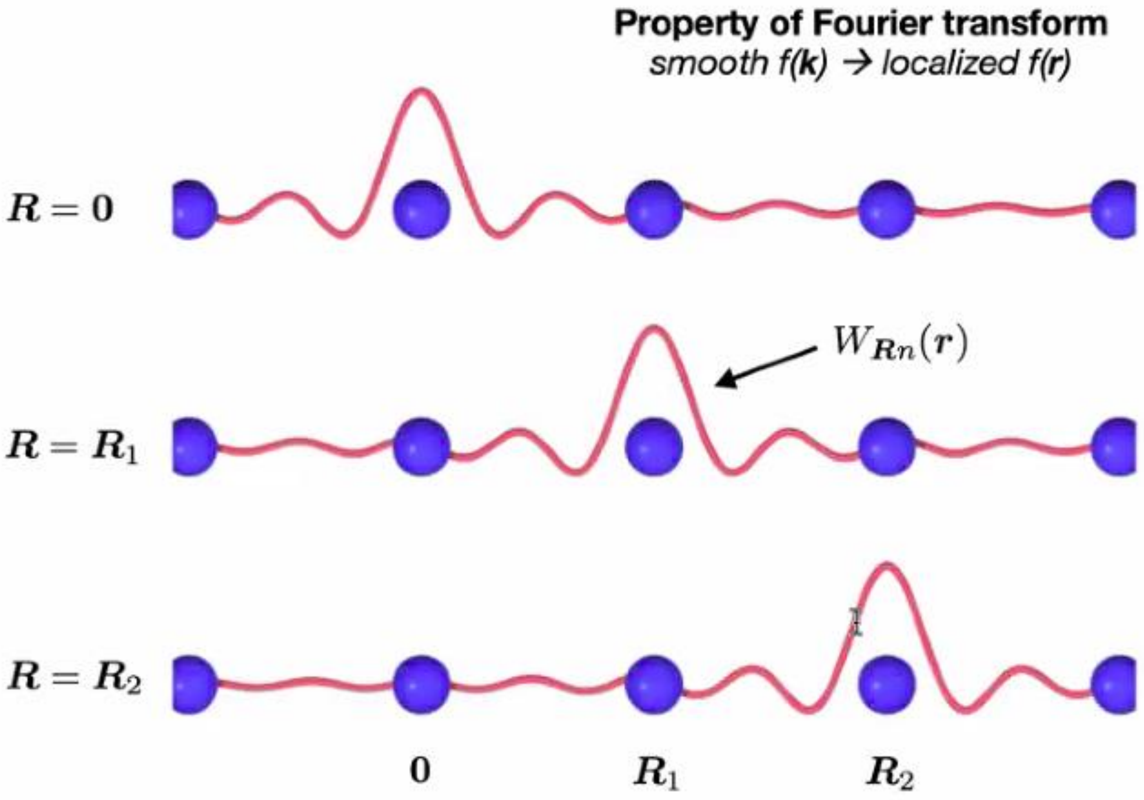
Bloch wave functions : $\psi_{\boldsymbol{k}n}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}n}(\boldsymbol{r})$



- Bloch functions are extended and delocalized

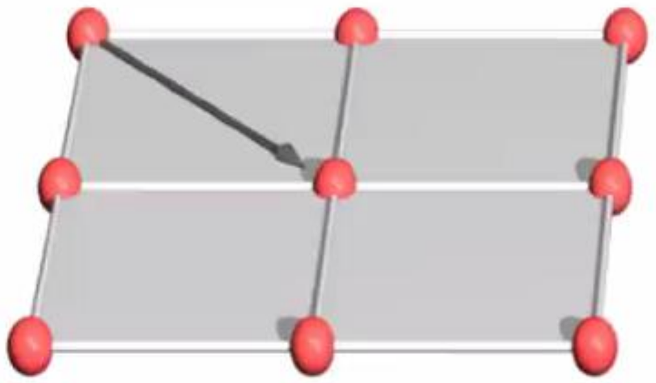
- Localized wave functions in real space offer more microscopic insights into the underlying physics.

Wannier function : $W_{\boldsymbol{R}n}(\boldsymbol{r}) = \frac{1}{N}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}} \psi_{\boldsymbol{k}n}(\boldsymbol{r})$



Computational framework and Wannier Interpolation :

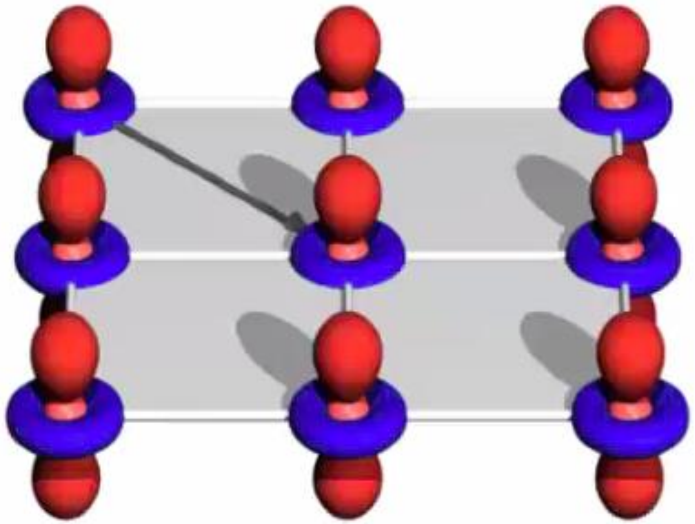
$H(\boldsymbol{k})$



DFT on coarse mesh
*(e.g., 8^3 **k**-points)*

DFT packages : VASP, FPLO, WIEN2K, Quantum Expresso

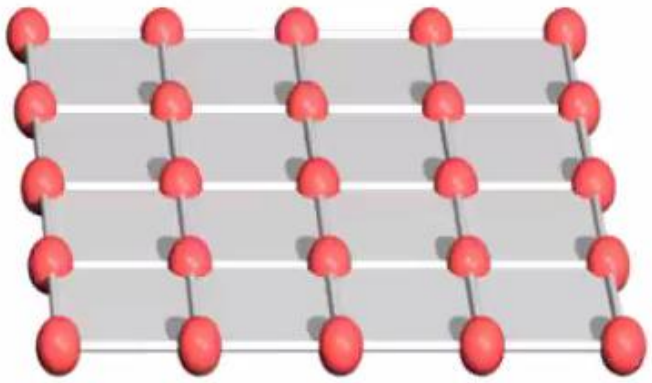
$H(\boldsymbol{R})$



maximally localized
Wannier functions

$$H = \sum_{\boldsymbol{R}\boldsymbol{R}'} \sum_{nn'} t_{nn'}(\boldsymbol{R}, \boldsymbol{R}') |W_{\boldsymbol{R}n}\rangle \langle W_{\boldsymbol{R}'n'}|$$

$H(\boldsymbol{q})$



(Developed transport code)

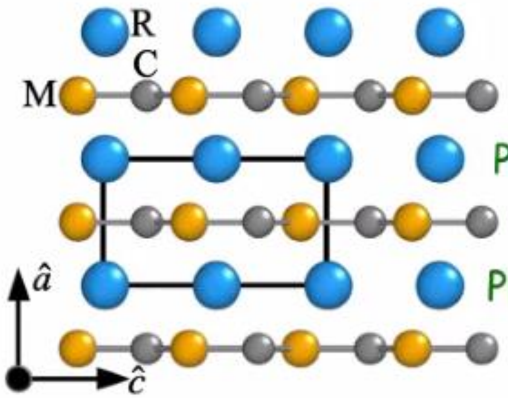
much finer sampling
*(e.g., 200^3 **q**-points)*

Berry curvature, Transport

New family of WSM : Rare earth carbides

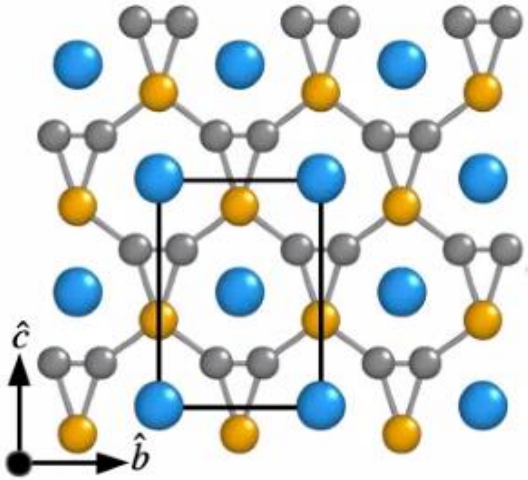
I : inversion symmetry   T : time reversal symmetry

Amm2 space group (SG no 38)

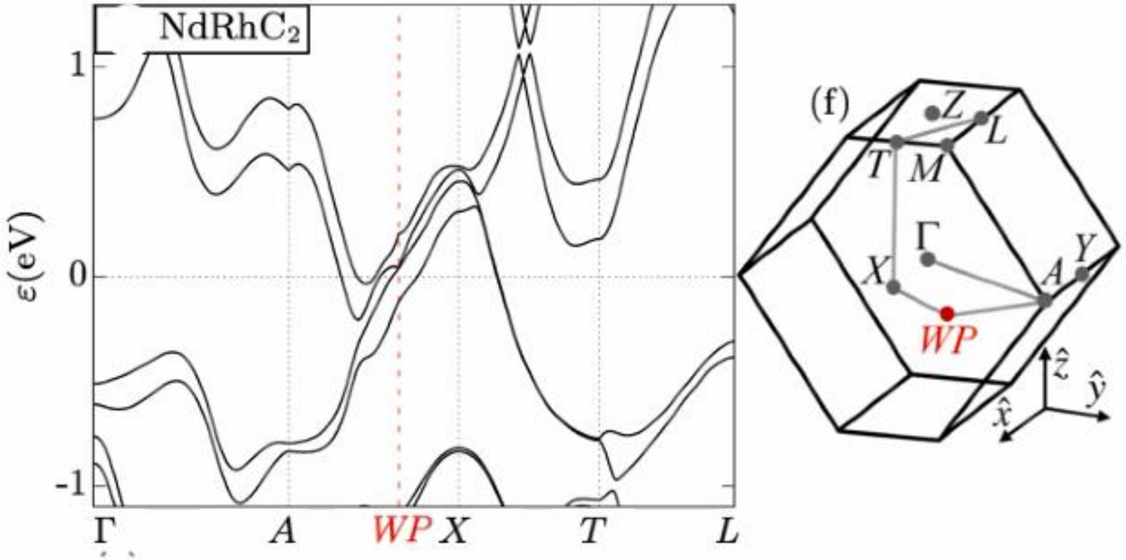


Class I	Class II	Class III	Class IV
T - symmetric I - broken	T - broken I - symmetric	T - broken I - broken	Insulators
$YCoC_2$, $LuCoC_2$	$GdRuC_2$	$PrRhC_2$, $NdRhC_2$ $GdCoC_2$, $GdNiC_2$	$LaRhC_2$

RMC (R= Rare earth and M= transition materials)



PrRhC2/NdRhC2



Why pickup materials where both I and T symmetries are broken?

R. Ray,, B. Sadhukhan et al. npj Quantum Materials 7, 19 (2022)

Interplay between topology and magnetism : tuning degeneracy of WNs

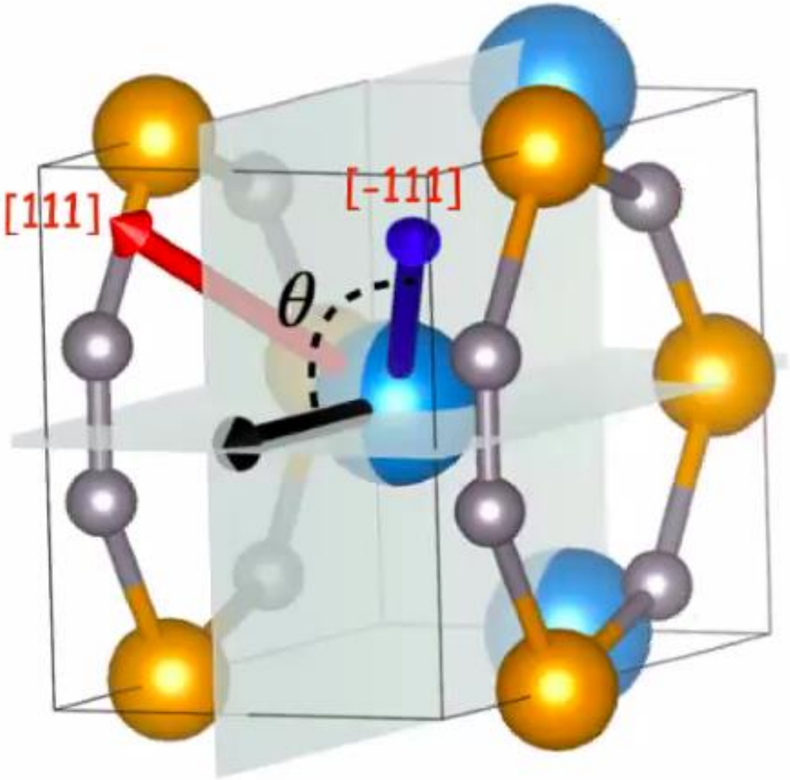
Crystal symmetry : {E, m(x), m(y), C2(z)}

T is time reversal symmetry

m(x) : mirror along x

m(y) : mirror along y

C2(z) : rotation along z



Magnetization axis	Symmetry	Degeneracy of Weyl nodes
Principle axis say, [001]	{ E, m(x)T, m(y)T, C2(z) }	4
Face diagonal say, [011]	{ E, m(x)T }	2
Body diagonal say, [111]	{E}	1

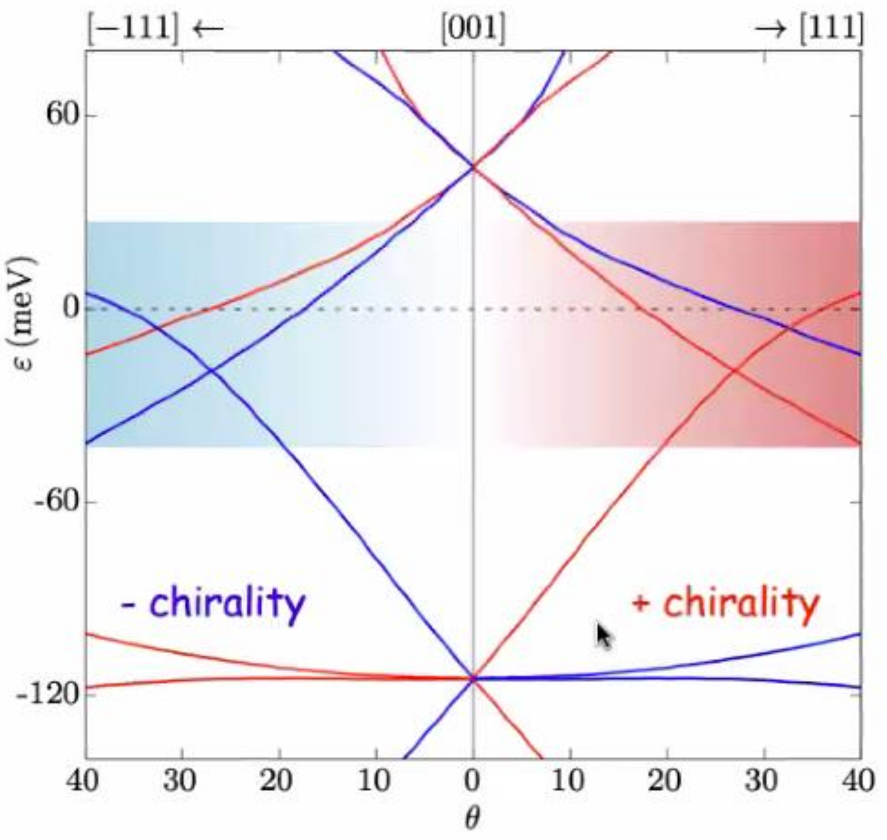
Breaks all symmetries

All Weyl nodes are non-degenerate

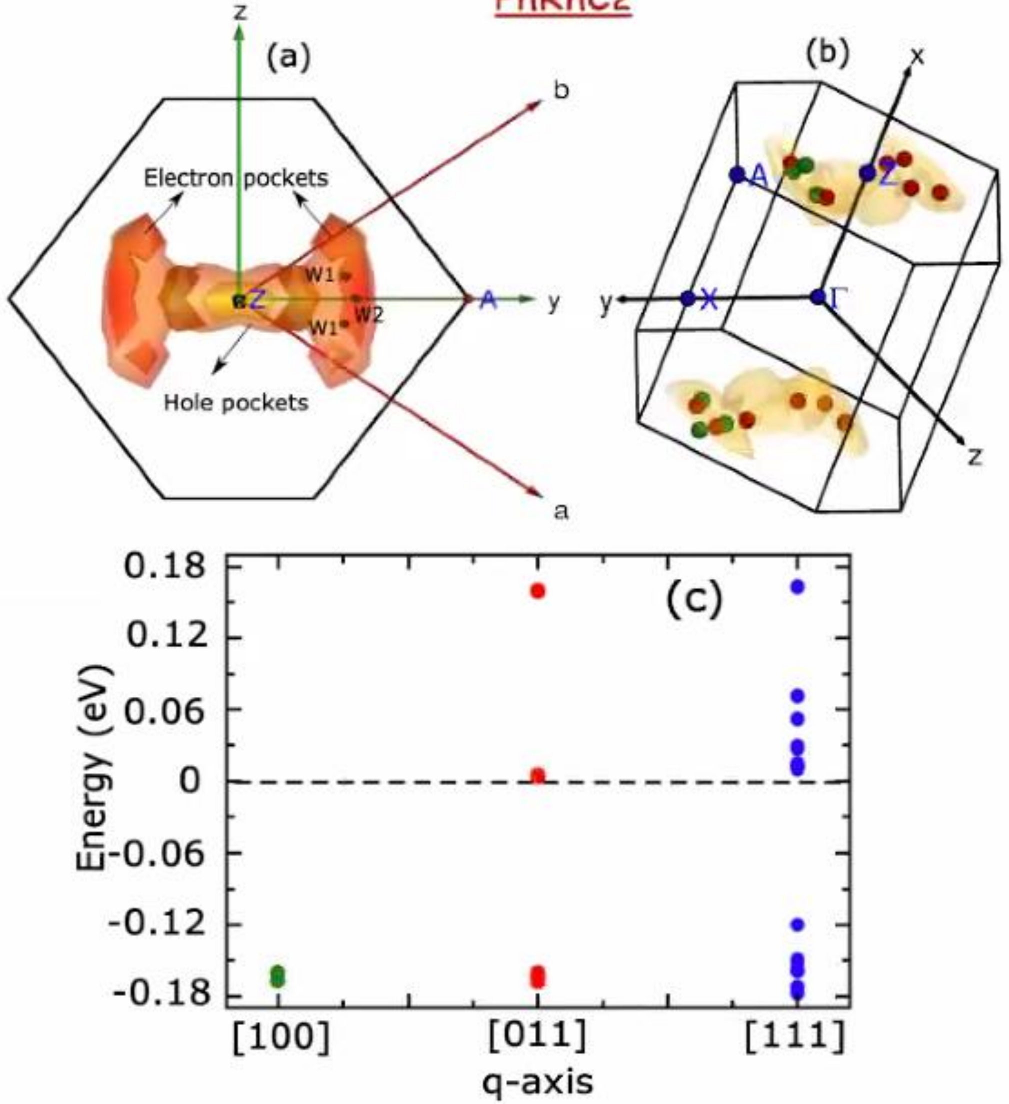
R. Ray, B. Sadhukhan et al. npj Quantum Materials 7, 19 (2022)

Chirality pumping at Fermi surface :

NdRhC2



PhRhC2



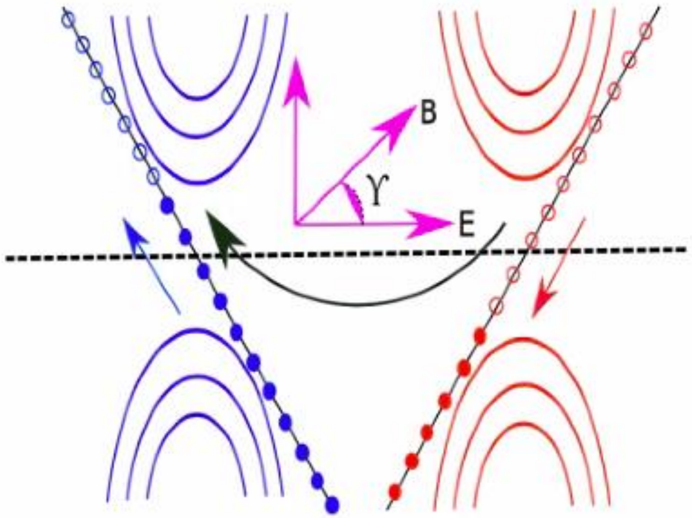
K. Ray, B. Sadhukhan et al. npj Quantum Materials 7, 19 (2022)

B. Sadhukhan et al. Phys. Rev. B **107** (8), L081110 (2023)

Chiral anomaly and planar Hall response :

Planar Hall transport mediated by chiral anomaly

What is chiral anomaly?

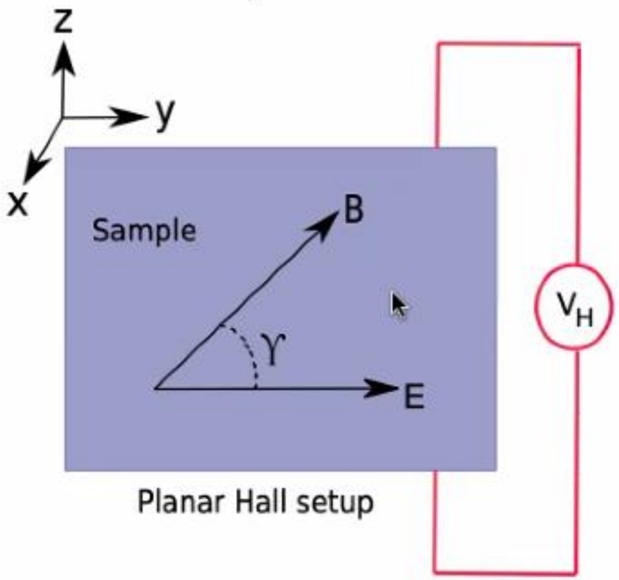


Chiral anomaly (E.B)

Continuity equation: $\frac{\partial n_i}{\partial t} + \nabla \cdot \mathbf{J}_i = \frac{C_i}{4\pi^2}\mathbf{B}\cdot\mathbf{E}$

Phys. Rev. lett. **109**, 181602 (2012)

Phys. Rev. lett. **119**, 176804 (2017)



$\boxed{T \ll \sqrt{B} \ll \mu}$ $\quad \mathbf{B} = B\cos\gamma\hat{y} + B\sin\gamma\hat{z},\ \mathbf{E} = E\hat{y}$

$$\sigma_{zy} \simeq e^2 \int \frac{d^3k}{(2\pi)^3} D\tau \left(-\frac{\partial f_0}{\partial \epsilon}\right) [(v_z + \frac{eB\sin\gamma}{\hbar}(\mathbf{\Omega_k}\cdot\mathbf{v_k})) (v_y + \frac{eB\cos\gamma}{\hbar}(\mathbf{\Omega_k}\cdot\mathbf{v_k}))]$$

Planar Hall conductivity

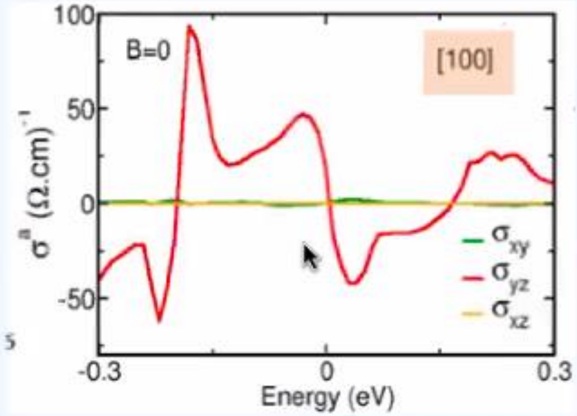
$$\sigma_{zy} \propto sin\gamma cos\gamma$$

Longitudinal magneto conductivity

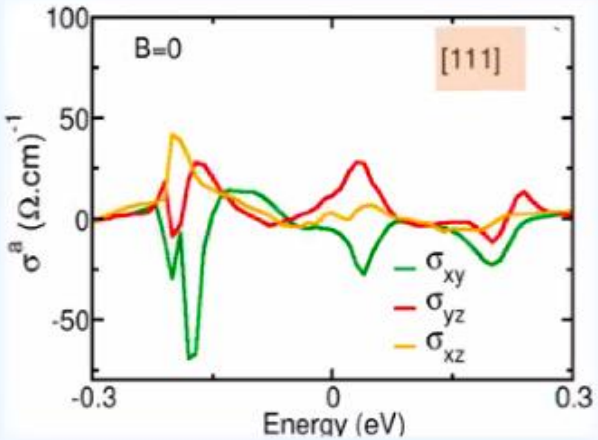
$$\sigma_{yy} \propto cos^2\gamma$$

Enhancement of planar Hall effect in PrRhC2 :

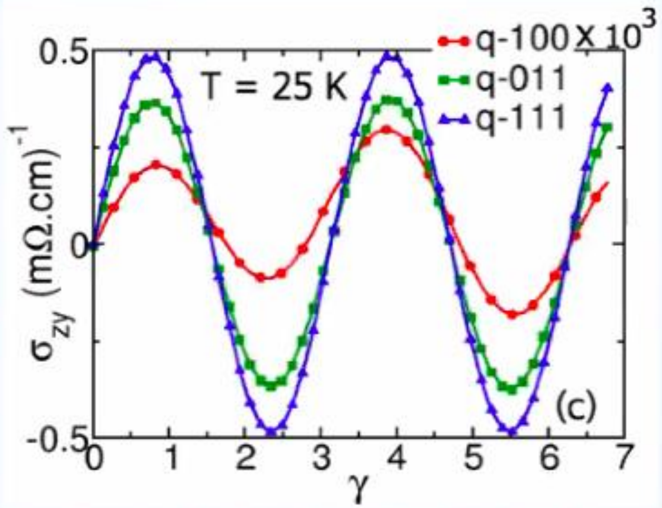
Anomalous Hall effect (B=0)

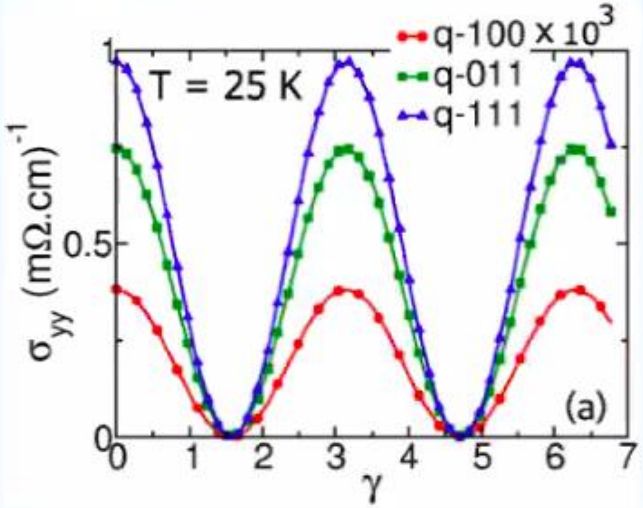


Higher to lower symmetry



Planar Hall effect (B ≠ 0)





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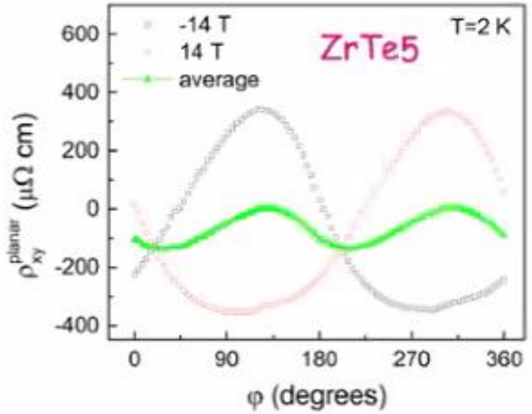
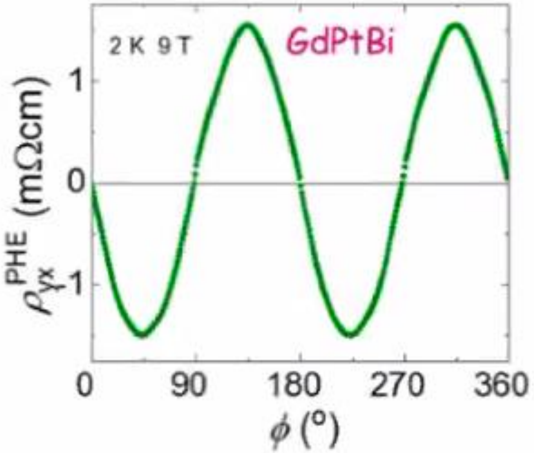
Experimental findings from other groups

Phys. Rev. B **98**, 121108(R) (2018)

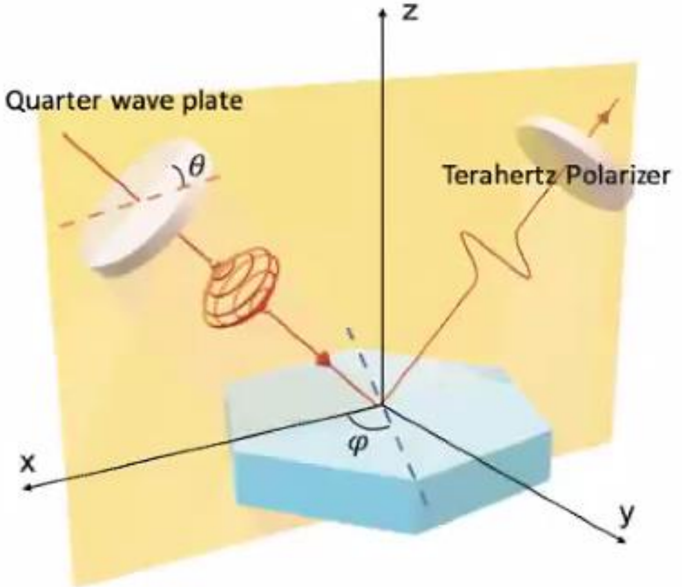


Phys. Rev. B **98**, 041103(R) (2018)



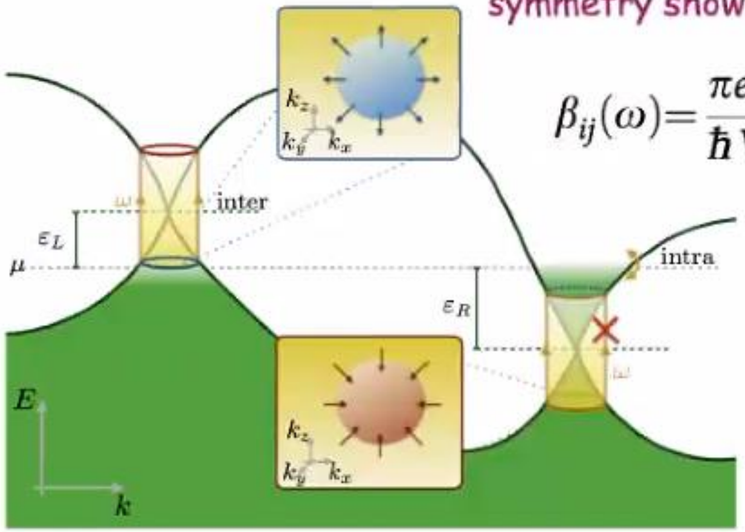
Some Highlights on "Circular Photovoltaic effect" :

Chiral WSMs without having symmetry and inversion symmetry show quantized CPGE response



$$\frac{dJ_a}{dt} = \beta_{ab}(\omega)[\mathbf{E}(\omega) \times \mathbf{E}^*(\omega)]_b$$

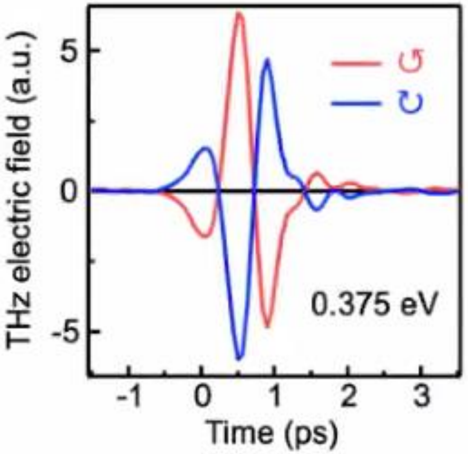
CPG tensor

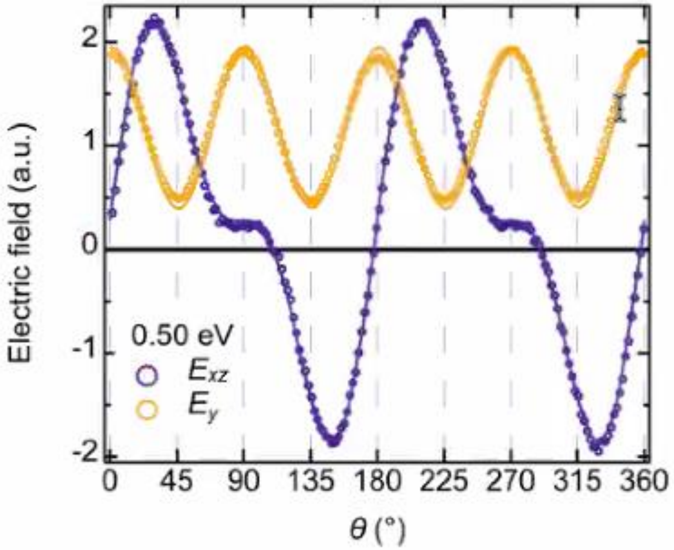


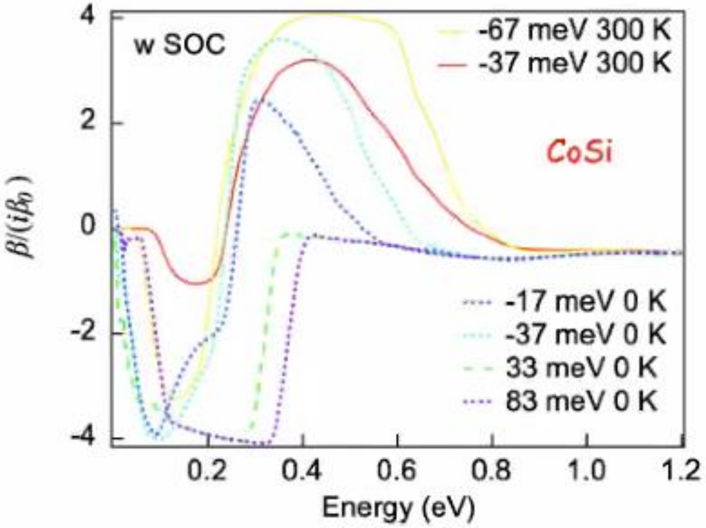
$$\beta_{ij}(\omega) = \frac{\pi e^3}{\hbar V} \epsilon_{jkl} \sum_{\mathbf{k},n,m} f^{\mathbf{k}}_{nm} \Delta^i_{\mathbf{k},nm} r^k_{\mathbf{k},nm} r^l_{\mathbf{k},mn} \delta(\hbar\omega - E_{\mathbf{k},mn})$$

$$\boxed{\mathrm{Tr}[\beta(\omega)] = i\pi \frac{e^3}{h^2} C_L \equiv i\beta_0}$$

- Nat. Commun. **8**, 15995 (2017)



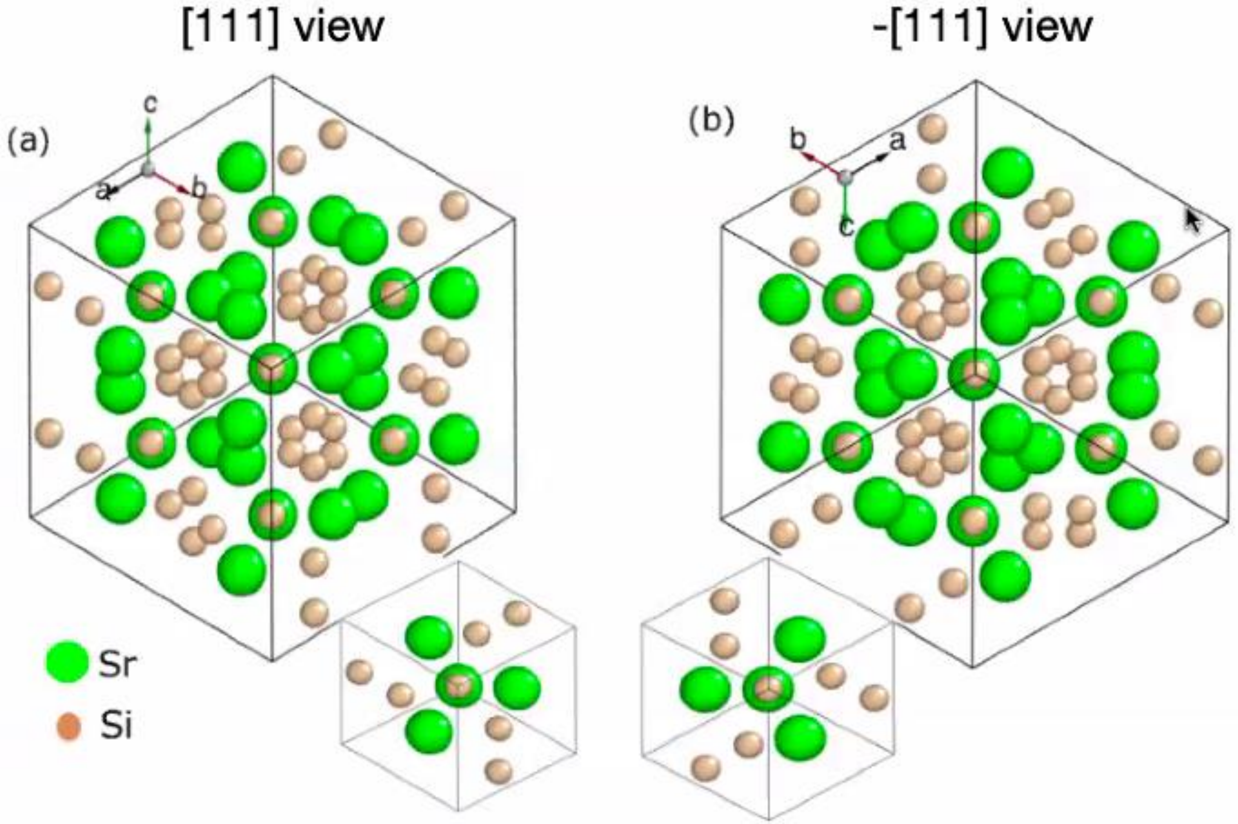


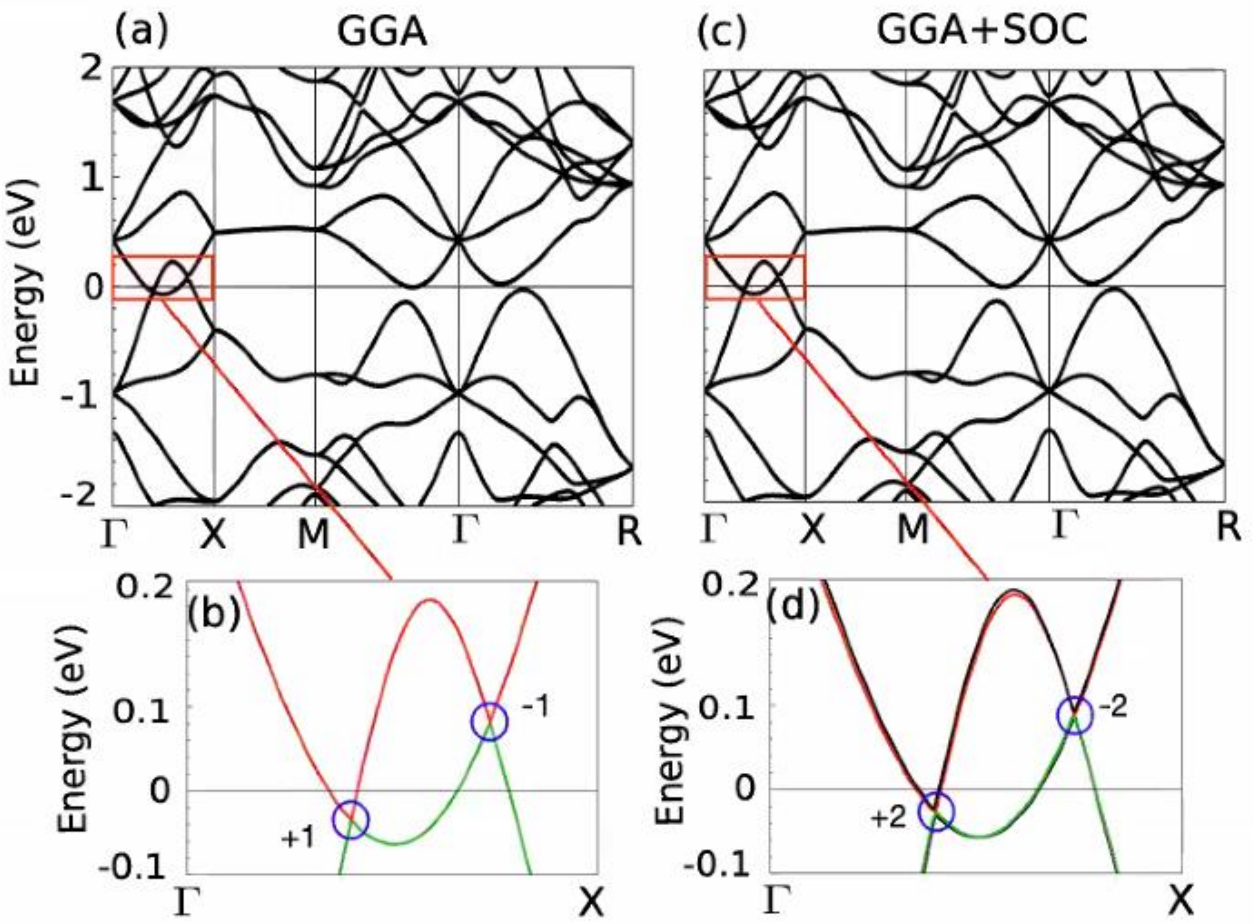


Some experimental findings from other group

(Nature Communications **12**, 154 (2021))

Space group P4332 (212) with the lattice constant 6.563 Å





-[111] view is mirror+flipped view of [111]. Structural chirality generates a distinct handedness which affect topological properties

Chiral WSM SrSi2 = Breaking of (Inversion+mirror) symmetries

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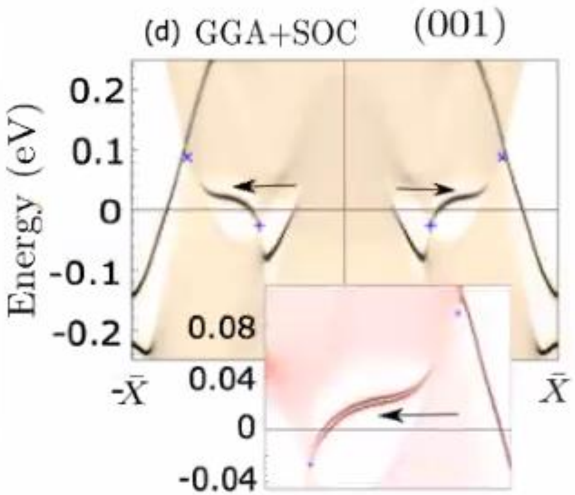
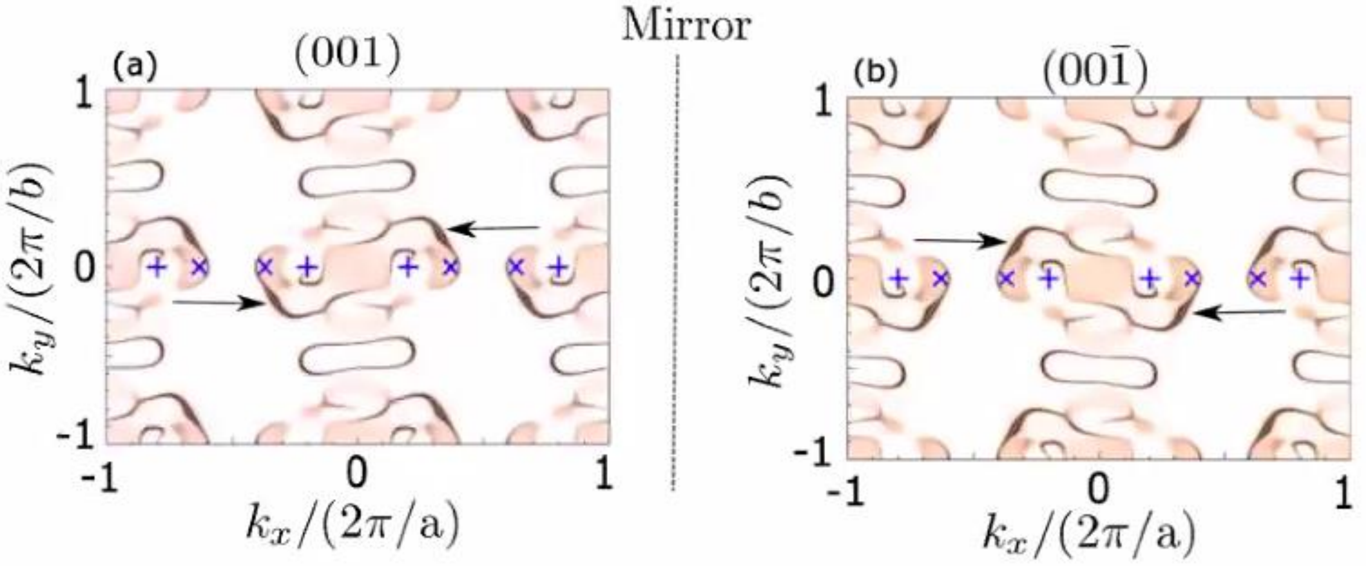
TABLE I. Positions, Chern numbers, and energies of the WNs with SOC ($W_{1,2}$) and without SOC ($V_{1,2}$).

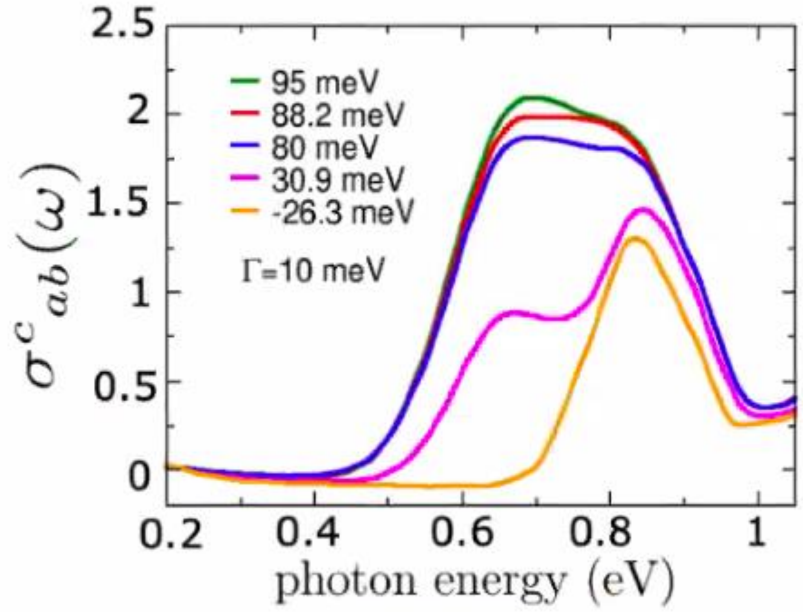
WP	Position $[(k_x, k_y, k_z)]$ in $(\frac{2\pi}{a}, \frac{2\pi}{b}, \frac{2\pi}{c})$	C	E (meV)
V_1	$(\pm 0.2001, 0, 0)$	+1	−34.4
V_2	$(\pm 0.3691, 0, 0)$	−1	82.3
W_1	$(\pm 0.2003, 0, 0)$	+2	−26.3
W_2	$(\pm 0.3696, 0, 0)$	−2	88.2



$$\sigma^c_{ab}(\omega) = \frac{e^3}{\omega^2}\mathrm{Re}\left\{\phi_{ab}\sum_{\Omega=\pm\omega}\sum_{l,m,n}\int_{BZ}\frac{d^3k}{(2\pi)^3}(f_l^{\vec{k}} - f_n^{\vec{k}}) \times \frac{\langle n_{\vec{k}}|\hat{v}_a|l_{\vec{k}}\rangle\langle l_{\vec{k}}|\hat{v}_b|m_{\vec{k}}\rangle\langle m_{\vec{k}}|\hat{v}_c|n_{\vec{k}}\rangle}{(E_{\vec{k}n} - E_{\vec{k}m} - i\Gamma)(E_{\vec{k}n} - E_{\vec{k}l} - \hbar\Omega - i\Gamma)}\right\}$$

$$\boxed{\approx iC\beta_0\tau}$$



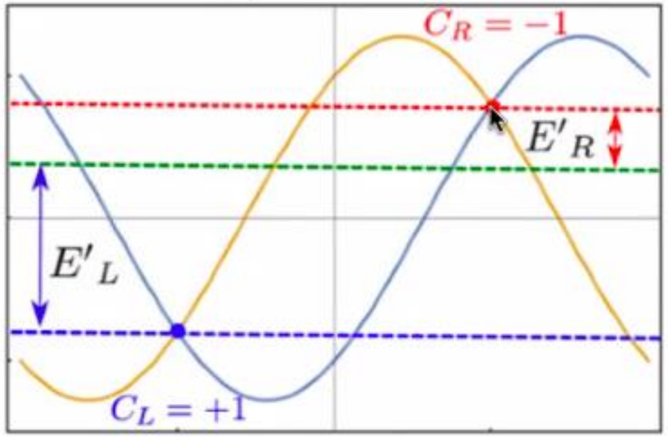


B. Sadhukhan et al. Phys. Rev. B **104**, 245122 (2021)

Effect of time reversal symmetry on CPGE quantization :

Chiral WSM

Why CPGE get quantized at one of WN, not other WN for $SrSi_2$?



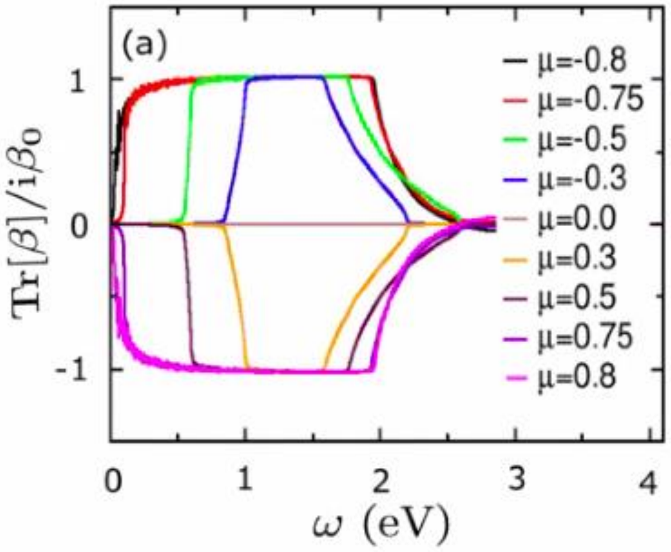
Calculated CPGE response at two opposite WNs

$$\frac{dJ_i}{dt} = \beta_{ij}(\omega)[\mathbf{E}(\omega) \times \mathbf{E}^*(\omega)]_j$$

$$\beta_{ij}(\omega) = \frac{\pi e^3}{\hbar V} \epsilon_{jkl} \sum_{\boldsymbol{k},n,m} \Delta f_{\boldsymbol{k},nm} \Delta v^i_{\boldsymbol{k},nm} r^k_{\boldsymbol{k},nm} r^l_{\boldsymbol{k},mn} \times \delta(\hbar\omega - E_{\boldsymbol{k},mn}),$$

$$\begin{aligned} \mathrm{Tr}[\beta(\omega)] &= \frac{i\pi e^3}{\hbar^2 V} \sum_{\boldsymbol{k}} \Delta f_{\boldsymbol{k},12} \partial_{k_i} E_{\boldsymbol{k},12} \Omega_{i,\boldsymbol{k}} \delta(\hbar\omega - E_{\boldsymbol{k},12}) \\ &= \frac{i\pi e^3}{\hbar^2 V} \sum_{\boldsymbol{k}} \Delta f_{\boldsymbol{k},12} \Delta v_{i,12} \Omega_{i,\boldsymbol{k}} \delta(\hbar\omega - E_{\boldsymbol{k},12}). \end{aligned}$$

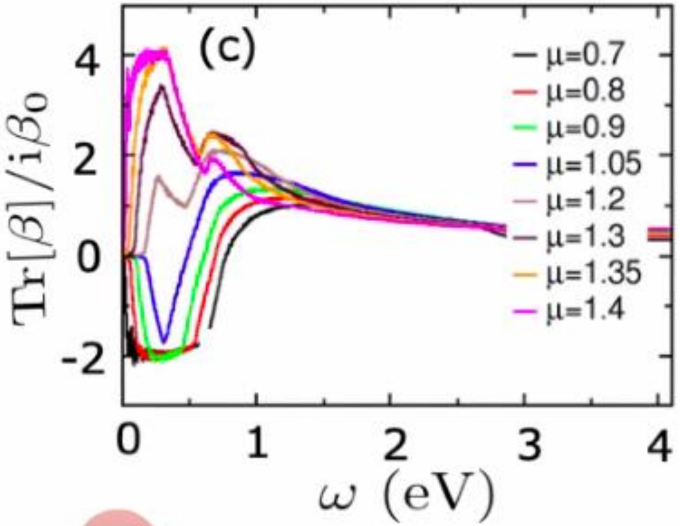
Time reversal symmetry broken



Key message :

CPGE quantization = anti symmetric behaviour at opposite WNs

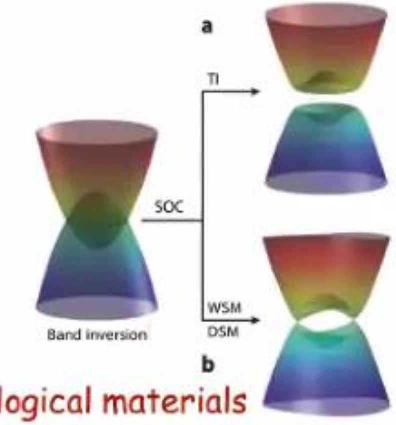
Time reversal symmetry invariant



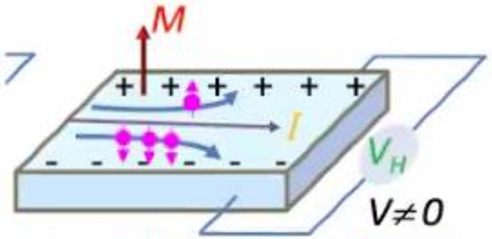
CPGE quantization ≠ anti symmetric behaviour at opposite WNs

B. Sadhukhan et al. Phys. Rev. B **103**, 144308 (2021)

My Research domain :



Topological materials

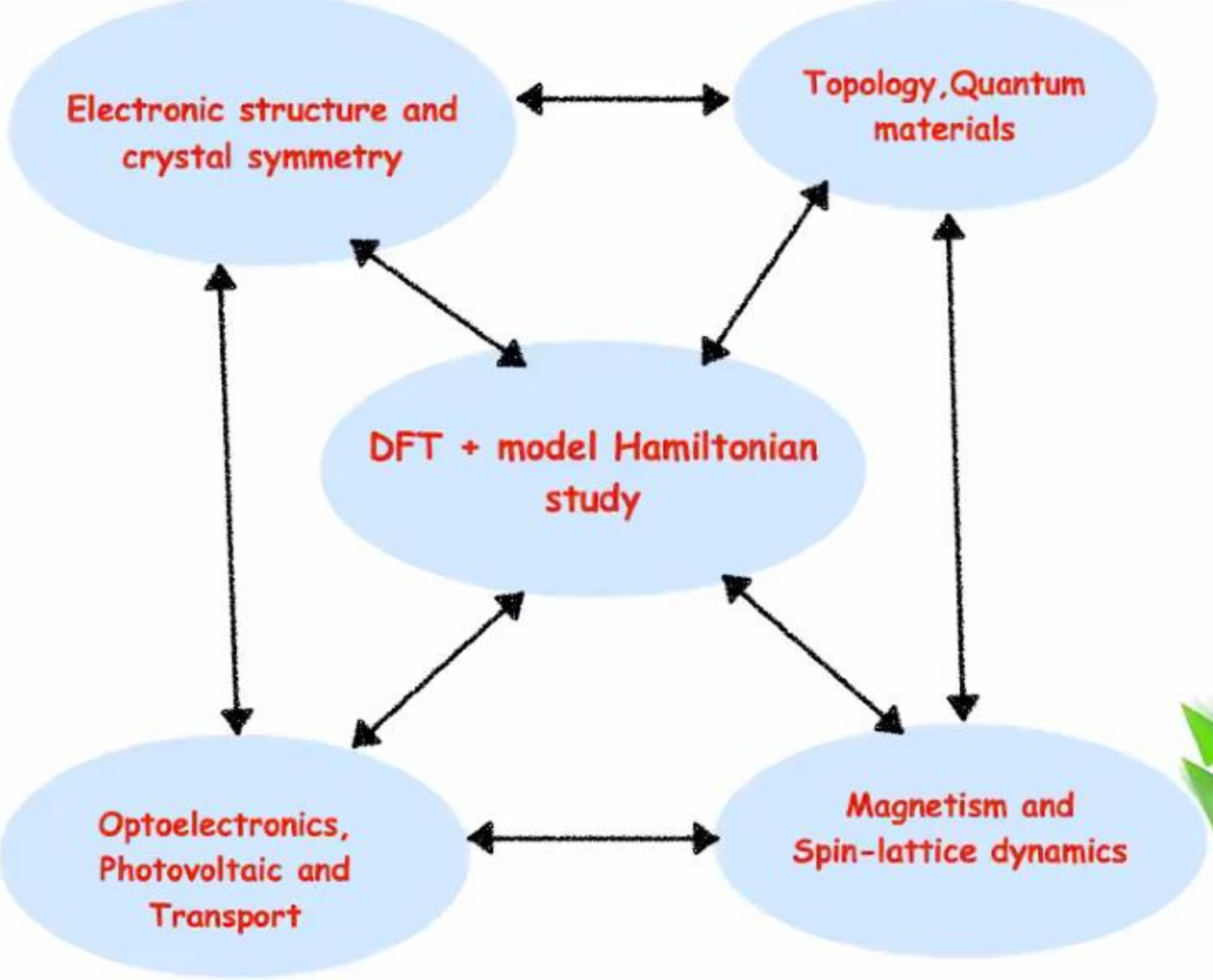


Experimental connection (AHE)

Photovoltaic

B. Sadhukhan et al. Phys. Rev. Mat **4**, 064602 (2020)

B. Sadhukhan et al. J. Appl. Phys. **129**, 084106 (2021)

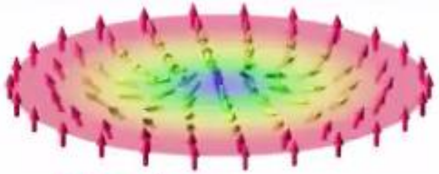


Energy source | Energy harvesting

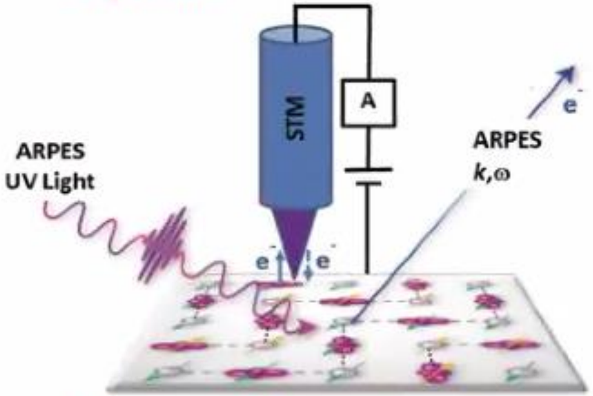
Light | Photovoltaic

Quantum materials, topology

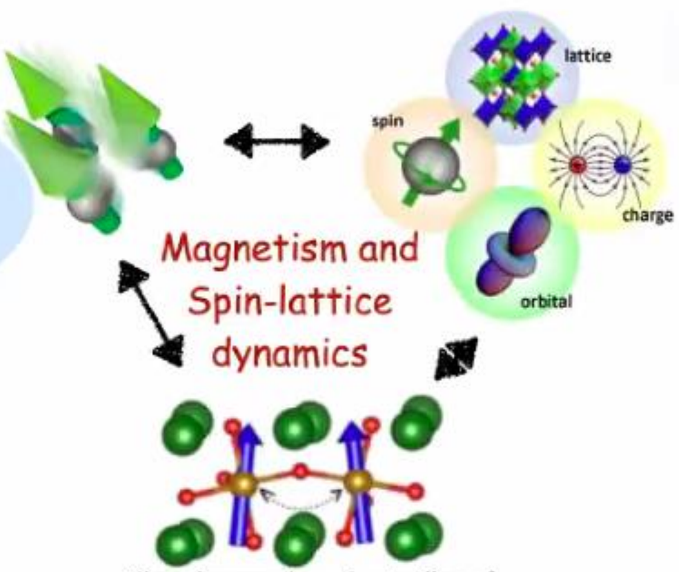
Heat | Thermoelectric



Skyrmion



Experimental connection (ongoing)



The microscopic understanding of how spin and lattice degree of freedom interact

B. Sadhukhan et al., Phys. Rev. B **105**, 104418 (2022)

Research contributions on three different fields :

Total publications : 16 (PhD tenure : 6, Postdoctoral tenure : 10)

Quantum materials and topological transport

(1) "Effect of chirality imbalance on Hall transport of PrRhC2" B. Sadhukhan, T. Nag, Physical Review B **107** (8), L081110 (2023)

(2) "Tunable chirality of noncentrosymmetric magnetic Weyl semimetals in rare-earth carbides" R. Ray, B. Sadhukhan, M. Richter, J.I. Facio, J. van den Brink, npj Quantum Materials **7**, 19 **(2022)**

(3) "Electronic structure and unconventional nonlinear response in double Weyl semimetal SrSi2" B. Sadhukhan, T. Nag Phys. Rev. B **104**, 245122 **(2021)**

(4) "Role of time reversal symmetry and tilting in circular photogalvanic responses" B. Sadhukhan, T. Nag Phys. Rev. B **103**, 144308 **(2021)**

Bulk Photovoltaic and sustainable energy

(1) "A new topological quantum material ZnGeSb2 with pressure-driven tunable properties in chalcopyrite series" S. Sadhukhan, B. Sadhukhan, S. Kanungo, Phys. Rev. B **106 (12)**, 125112 **(2022)**

(2) "Bulk photovoltaic effect in $BaTiO_3$-based ferroelectric oxides: An **experimental** and theoretical study" S. Pal, S. Muthukrishnan, B. Sadhukhan, S. NV, D. Murali, P. Murugavel J. Appl. Phys. **129**, 084106 **(2021)**

(3) "First-principles calculation of shift current in chalcopyrite semiconductor ZnSnP2" B. Sadhukhan, Y. Zhang, R. Ray, J. van den Brink Phys. Rev. Mat **4**, 064602 **(2020)**

(4) "Electronic, magnetic, optical and thermoelectric properties of Ca 2 Cr 1− x Ni x OsO 6 double perovskites" B. Sadhukhan et al. RSC Advances **10 (27)**, 16179-16186 **(2020)**.

Light-matter interaction in topological materials

(1) "Effect of spin-lattice couplings on a Skyrmion multilayers Pd/Fe/Ir(111)" B. Sadhukhan, A. Bergman, J. Hellsvik, A. Delin (Manuscript under preparation)

(2) "Topological magnon in kagome spin spiral of YMn6Sn6" B. Sadhukhan, A. Bergman, P. Thunström, M. Pereiro, O. Eriksson, A. Delin (Manuscript under preparation)

(3) "Spin-lattice couplings in two-dimensional CrI3 from first-principles computations" B. Sadhukhan, A. Bergman, Y. O. Kvashnin, J. Hellsvik, A. Delin Phys. Rev. B **105**, 104418 **(2022)**

(4) Developing "**UppASD package**" code for atomistic spin-lattice simulation (https://gitlab.com/UppASD/UppASD)

Future research plan

Topology in electronic structure and transport

Systems : Topological insulators, Weyl semimetals, multifold Fermions, Nodal line semimetals, Twisted bilayer systems

Topological properties and transport :
Anomalous Hall effect,
Planar Hall effect,
Circular photogalvanic effect,
Shift current response and anomalous photovoltaic effect,
Berry curvature dipole
Anomalous Nernst effect

Sustainable transport via modern technologies

Different probes :
Pressure, Strain, doping,
Electric and magnetic fields and many more

Collaboration with Experimental and Theoretical team

Light-matter interactions in Quantum magnets

Systems : Topological magnon, Skyrmions, Spin spiral

Non-trivial transport :
Magnon Hall effect, Skyrmions Hall effect

Acknowledgements :

Thankful to all my supervisors, collaborators,
parents and family

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NORDITA

MIT Physics

RWTH AACHEN UNIVERSITY

IFW Leibniz Institute for Solid State and Materials Research Dresden

SISSA

INDIAN INSTITUTE OF TECHNOLOGY MADRAS

Thank you for your attention !!