Shift photocurrent: Wannier interpolation & dipole selection rules

Julen Ibañez-Azpiroz

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Bulk photovoltaic effect

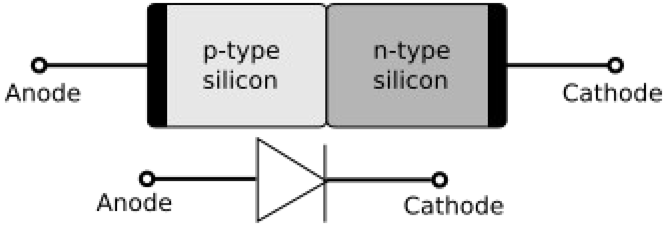
- Nonlinear light-absorption process of **non-centrosymmetric** crystals

- Large photovoltage (above band-gap)

- Studied in the 70-80's, renewed interest today

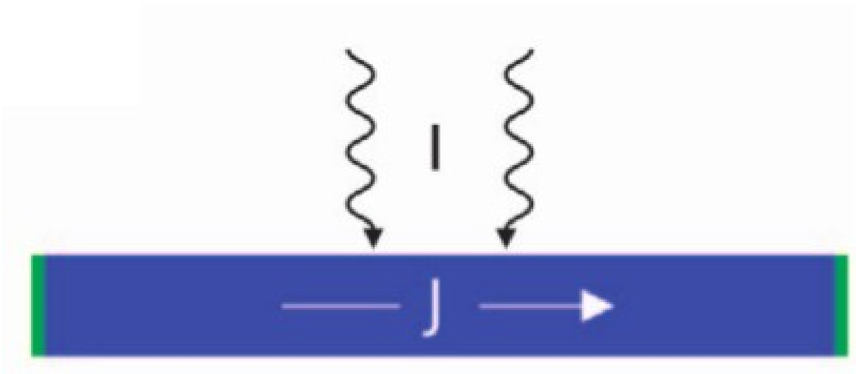
  Book: Sturman & Fridkin (1992)

Usual photovoltaics
need of an interface between two different materials



Wikipedia

Bulk photovoltaics
one homogeneous material with broken inversion symmetry



Tan etal, NPJ Comp. Mat. (2016)

Early measurements

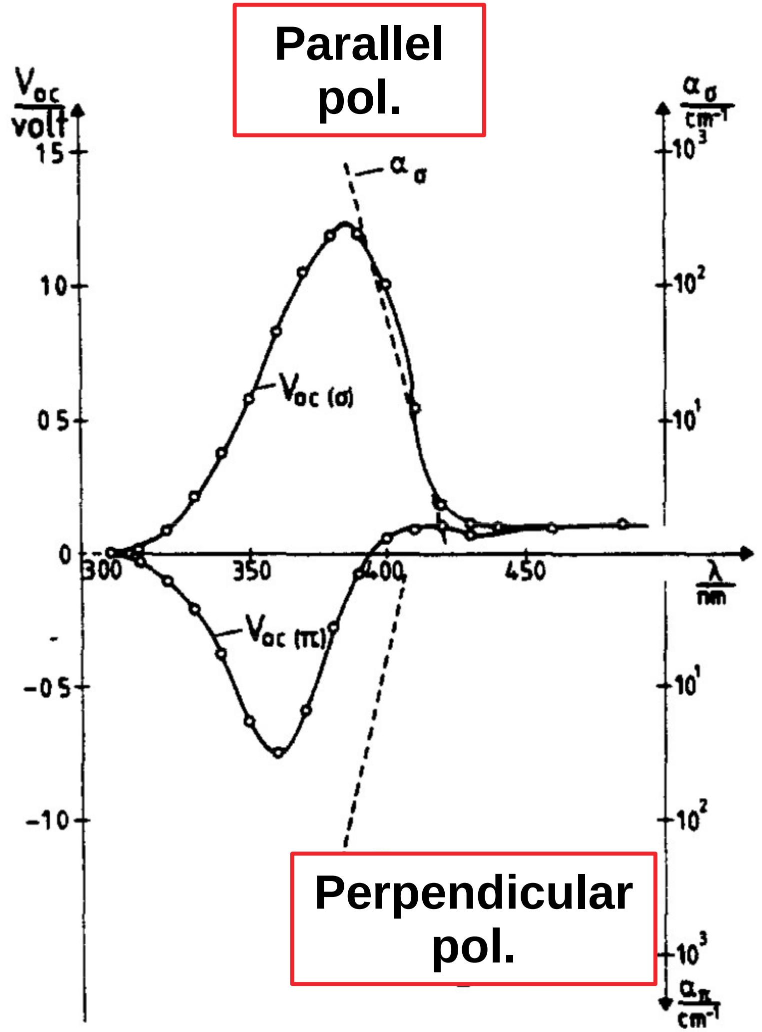
BULK PHOTOVOLTAIC EFFECT IN $BaTiO_3$

W T.H Koch, R Munser, W Ruppel and P Wurfel

Institut fur angewandte Physik, Universitat Karlsruhe, Karlsruhe, Germany

(*Received* 12 *May* 1975 *by M Cardona*)

In melt-grown $BaTiO_3$ single crystals steady-state photocurrents proportional to the light intensity have been observed parallel to the crystallographic *c*-axis The open-circuit photovoltage exceeds the value of the band gap Light polarized parallel and perpendicular to the *c*-axis respectively produces photovoltages with opposite sign This photovoltaic effect is restricted to the ferroelectric phase



Recent interest: connection to topology

PRL **116,** 237402 (2016) PHYSICAL REVIEW LETTERS week ending 10 JUNE 2016

Enhancement of the Bulk Photovoltaic Effect in Topological Insulators

Liang Z. Tan and Andrew M. Rappe
The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA
(Received 14 August 2015; published 8 June 2016)

RESEARCH ARTICLE

OPTICS

Topological nature of nonlinear optical effects in solids

Takahiro Morimoto[1]* and Naoto Nagaosa[2,3]

Science Advances 2016

Recent interest: 2D materials

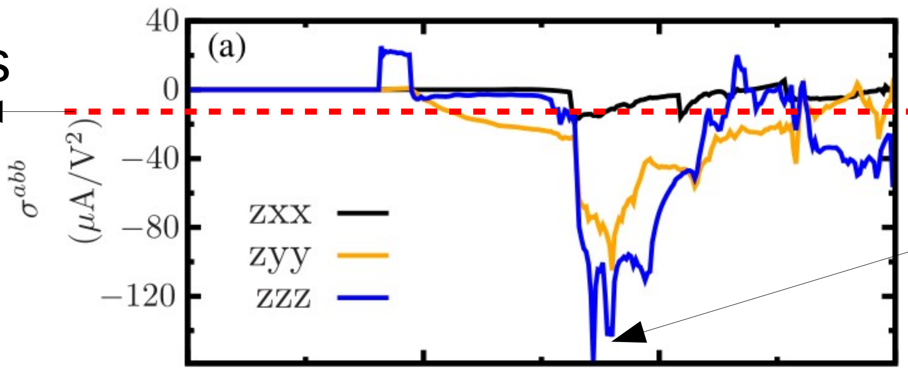
PRL 119, 067402 (2017) PHYSICAL REVIEW LETTERS week ending 11 AUGUST 2017

Large Bulk Photovoltaic Effect and Spontaneous Polarization of Single-Layer Monochalcogenides

Tonatiuh Rangel,[1,2] Benjamin M. Fregoso,[2,3] Bernardo S. Mendoza,[4] Takahiro Morimoto,[2] Joel E. Moore,[2] and Jeffrey B. Neaton[1,2,5]

Typical bulk values

$\sim 10\ \mu\mathrm{AV}^{-2}$



Order of magnitude enhancement of conductivity in 2D

nature COMMUNICATIONS

ARTICLE

Received 10 Aug 2015 | Accepted 6 Dec 2016 | Published 25 Jan 2017 DOI: 10.1038/ncomms14176 OPEN

Design principles for shift current photovoltaics

Ashley M. Cook[1,2,*], Benjamin M. Fregoso[1,*], Fernando de Juan[1], Sinisa Coh[1,†] & Joel E. Moore[1,3]

Recent interest: 2D materials

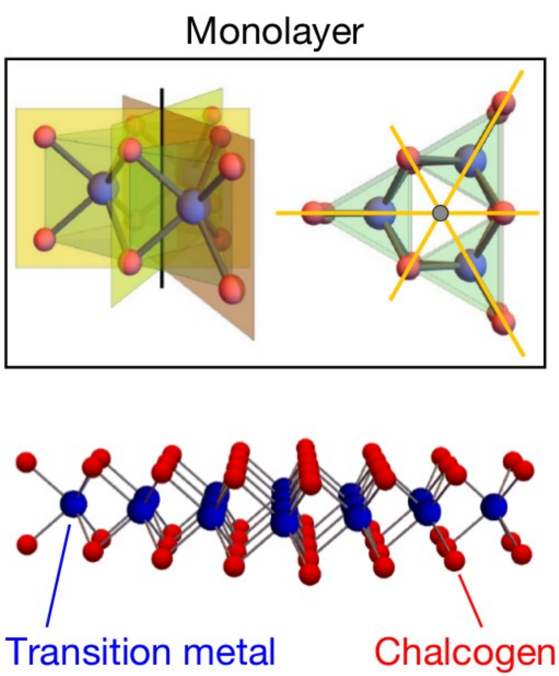
LETTER

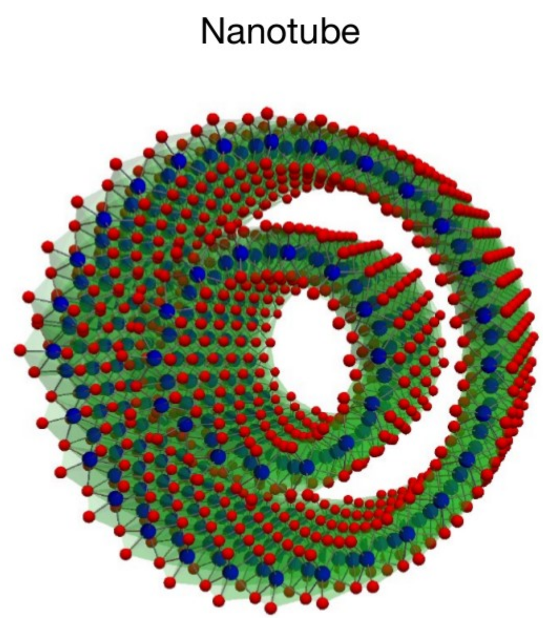
Zhang et. al. Nature (2019)

https://doi.org/10.1038/s41586-019-1303-3

Enhanced intrinsic photovoltaic effect in tungsten disulfide nanotubes

Y. J. Zhang[1,2]*, T. Ideue[3], M. Onga[3], F. Qin[3], R. Suzuki[3], A. Zak[4], R. Tenne[5], J. H. Smet[2] & Y. Iwasa[3,6]





Recent interest: 2D materials

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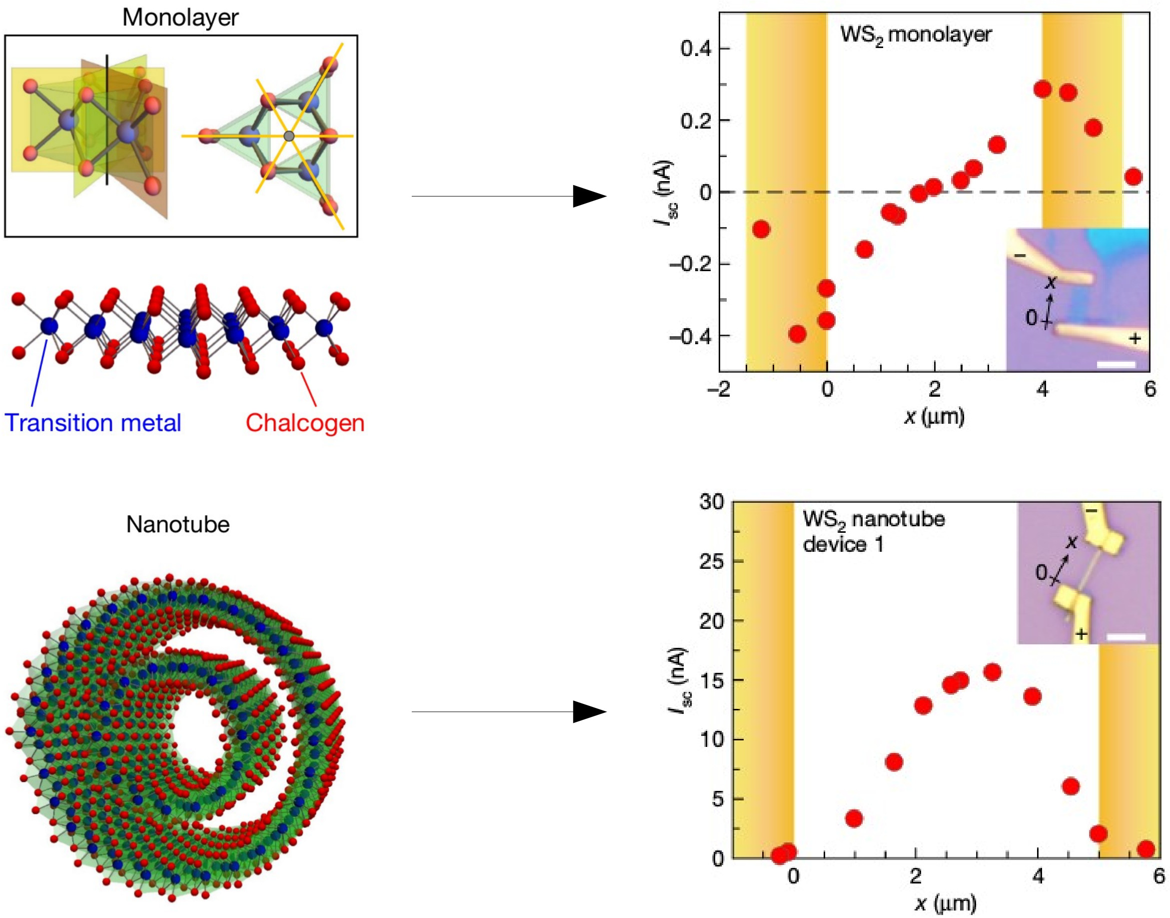
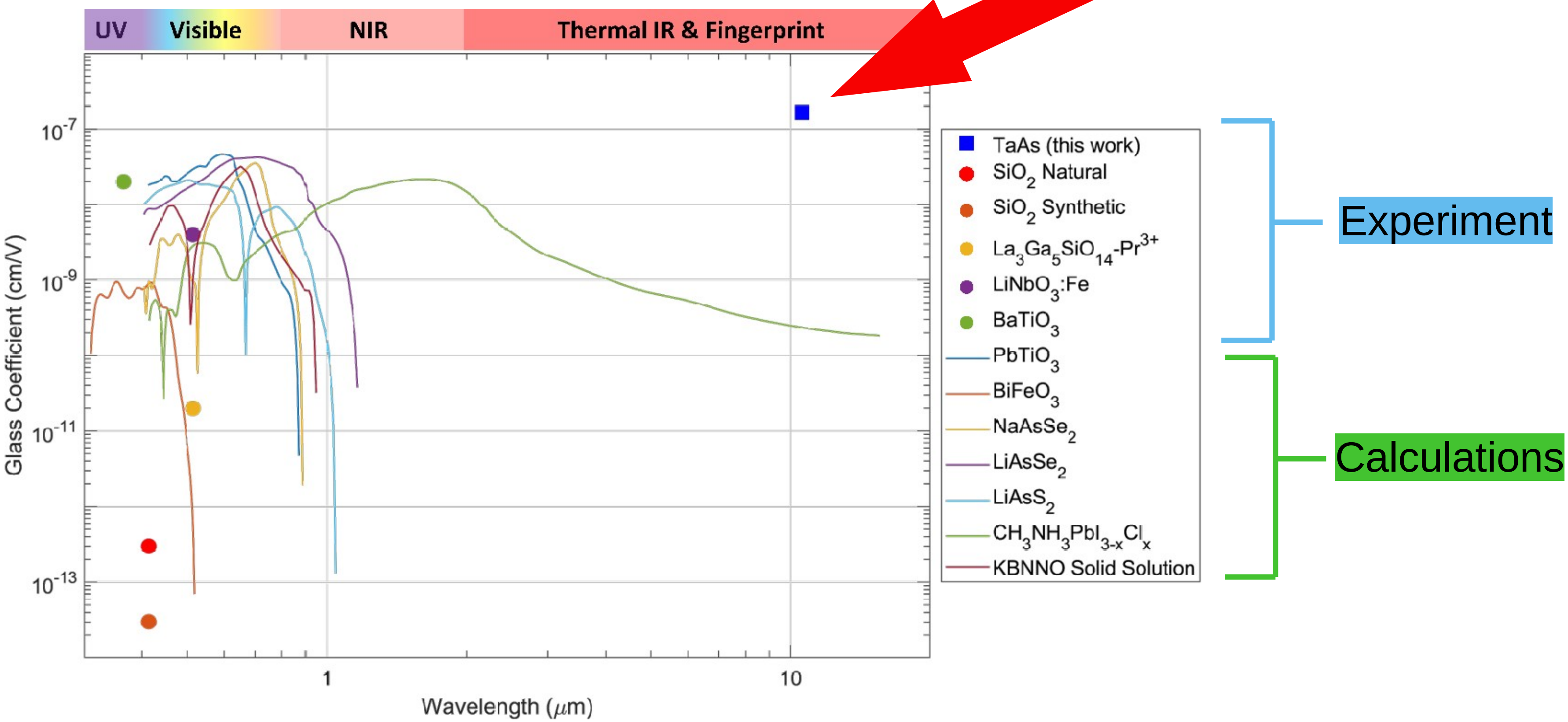


Recent interest: topology and Weyl semimetals

nature materials
ARTICLES
https://doi.org/10.1038/s41563-019-0297-4

Colossal mid-infrared bulk photovoltaic effect in a type-I Weyl semimetal

Gavin B. Osterhoudt[1], Laura K. Diebel[1], Mason J. Gray[1], Xu Yang[1], John Stanco[1], Xiangwei Huang[2], Bing Shen[3], Ni Ni[3], Philip J. W. Moll[2,4], Ying Ran[1] and Kenneth S. Burch[1*]



And many more

nature photonics
ARTICLES
PUBLISHED ONLINE: 8 AUGUST 2016 | DOI: 10.1038/NPHOTON.2016.143

Power conversion efficiency exceeding the Shockley–Queisser limit in a ferroelectric insulator

Jonathan E. Spanier[1,2,3*†], Vladimir M. Fridkin[2,4†], Andrew M. Rappe[5], Andrew R. Akbashev[1], Alessia Polemi[1], Yubo Qi[5], Zongquan Gu[3], Steve M. Young[6], Christopher J. Hawley[1], Dominic Imbrenda[3], Geoffrey Xiao[1], Andrew L. Bennett-Jackson[1] and Craig L. Johnson[1]

nature COMMUNICATIONS
ARTICLE
https://doi.org/10.1038/s41467-019-11832-3 OPEN

Switchable magnetic bulk photovoltaic effect in the two-dimensional magnet CrI_3

Yang Zhang[1,2,3], Tobias Holder[4], Hiroaki Ishizuka[5], Fernando de Juan[6,7], Naoto Nagaosa[8,9], Claudia Felser[1] & Binghai Yan[4]

Science

Flexo-photovoltaic effect

Ming-Min Yang,* Dong Jik Kim,* Marin Alexe†

Department of Physics, University of Warwick, Coventry, CV4 7AL, UK.

Outline

First-principles scheme:

- *Wannier interpolation of the shift photocurrent*

Applications:

- *Dipole selection rules in graphitic BC_2N*
- *Variety of nonlinear responses in Weyl semimetal $TaIrTe_4$*

Shift current response

- **Second order DC** response to external electric field

$$J^a(0) = \sigma^{abc}(\omega)E^b(\omega)E^c(-\omega)$$

- Shift photoconductivity
  Sipe and Shkrebtii PRB 2000

$$\sigma^{abc}(\omega) = \frac{\pi|e^3|}{4\hbar^2}\int d\mathbf{k}\sum_{nm}(f_n - f_m)r^c_{mn}r^b_{nm;a}\delta(\omega_{mn}-\omega) + b \leftrightarrow c$$

- Transition matrix elements
  - Dipole : $r^b_{mn} = i\langle u_{\mathbf{k}m}|\partial_{k_b}u_{\mathbf{k}n}\rangle$
  - Covariant derivative: $r^c_{mn;a} = \underline{\partial_{k_a}r^c_{mn}} - i(A^a_{mm} - A^a_{nn})r^c_{mn}$

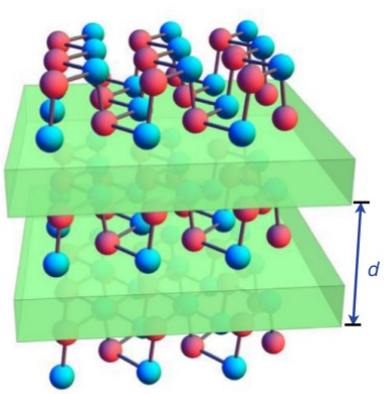
Troublesome quantity due to **k**-space phase indeterminacy of Bloch states

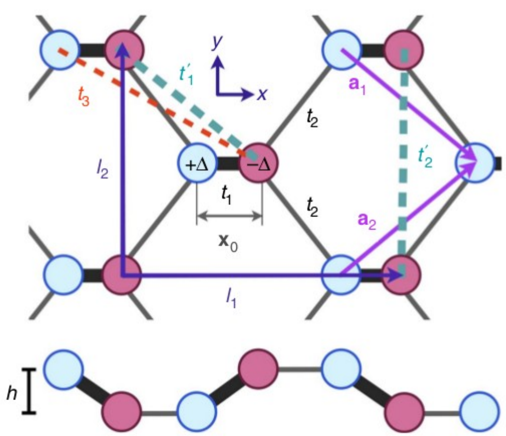
Sum-rule expression

$$\partial_{k_a} r^b_{mn} \propto \sum_l \left(\frac{r^a_{nl} r^b_{lm}}{\omega_{nl}} + \frac{r^b_{nl} r^a_{lm}}{\omega_{lm}} \right)$$

Aversa and Sipe, PRB 1995
Sipe and Shkrebtii, PRB 2000

Unbounded sum over virtual states:
truncation error





Amenable to tight-binding formulation
Cook et. al., Nat. Comm. 2017

Strategies for calculating the covariant derivative

Discretized expression

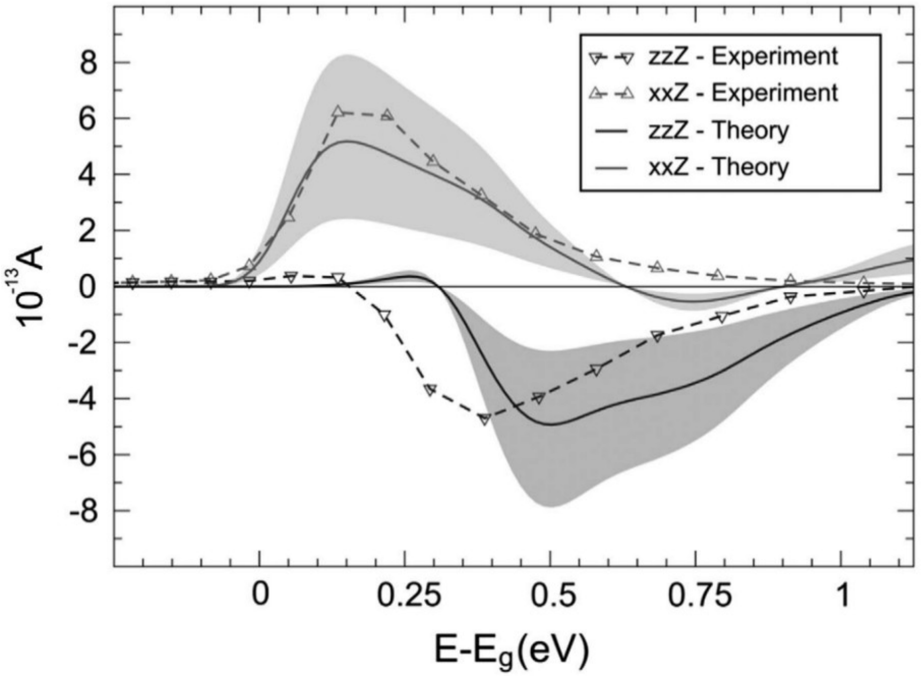
King-Smith and Vanderbilt, PRB 1993
Young and Rappe, PRL 2012

$$\langle u_{\mathbf{k}m}|\partial_{k_b} u_{\mathbf{k}n}\rangle = \lim_{\Delta k_b \to 0} \frac{1}{\Delta k_b} \mathrm{Log}\langle u_{\mathbf{k}m}|u_{\mathbf{k}+\Delta k_b \mathbf{q},n}\rangle$$

See also: Young, Zheng and Rappe, PRL 2012, Tan and Rappe, PRL 2016; Tan, Rappe et. al., NPJ 2016; Wang, Rappe et. al., Nat. Comm. 2016

Suitable for regular k-space grids commonly used in DFT calculations

Can become computationally heavy, need of many k-points calculated from first principles



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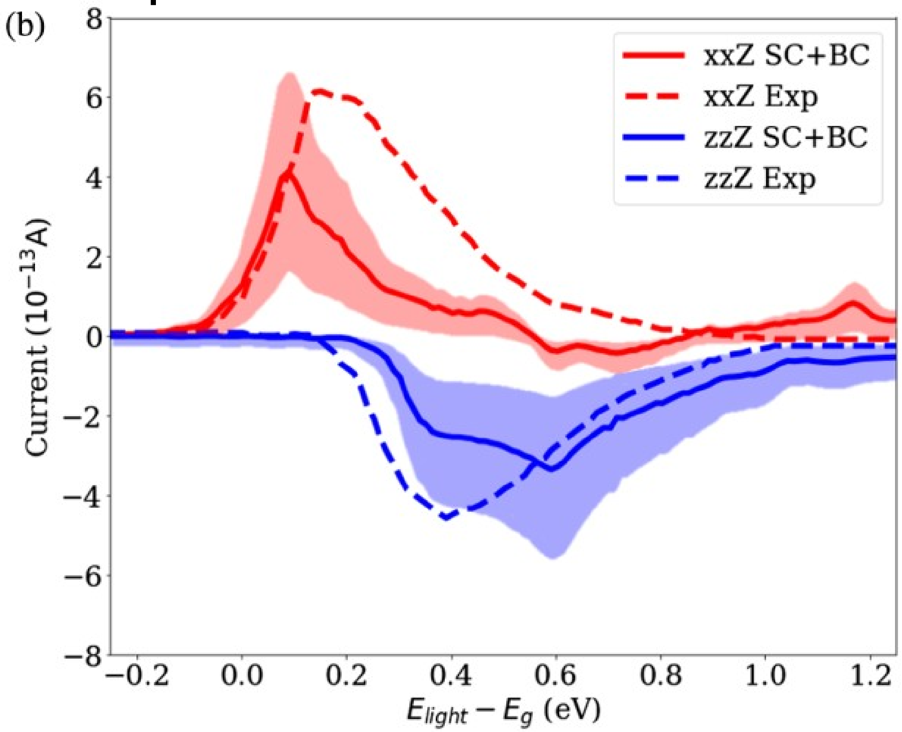
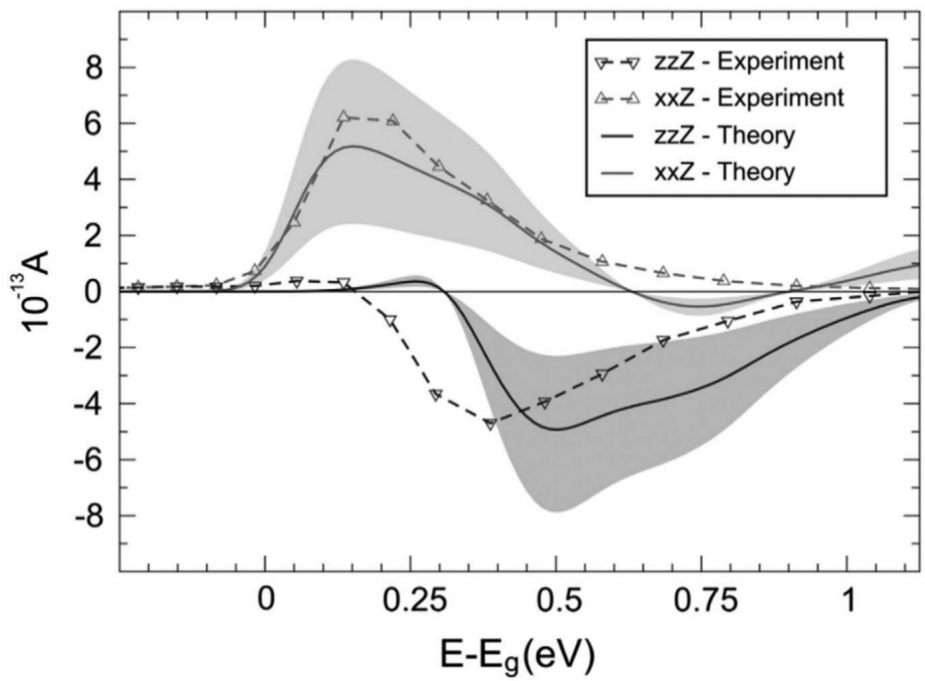
See also: Young, Zheng and Rappe, PRL 2012, Tan and Rappe, PRL 2016; Tan, Rappe et. al., NPJ 2016; Wang, Rappe et. al., Nat. Comm. 2016

(Shift + phonon-assisted ballistic current)

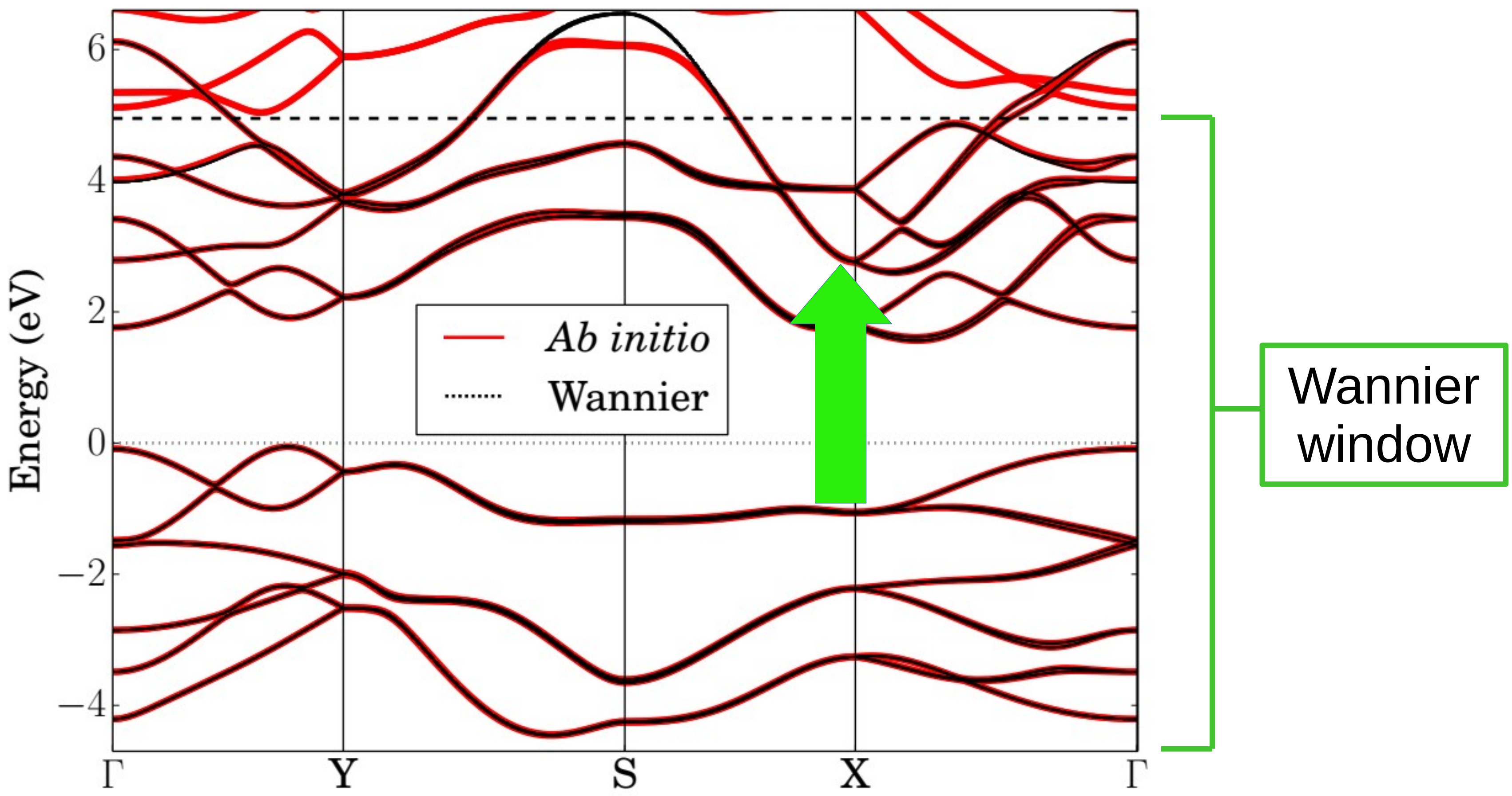




Dai, Schankler, Gao, Tan and Rappe
PRL, 126, 177403 (2021)

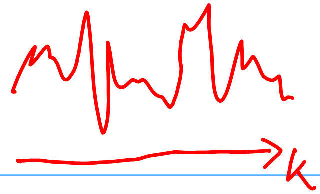
Wannier interpolation

Strategy: k dot p perturbation theory within subspace of Wannierized bands

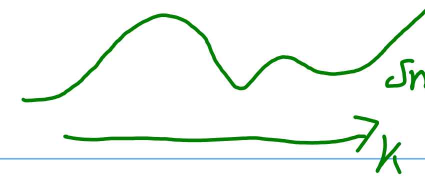


Wang, Yates, Souza and Vanderbilt PRB 74, 195118 (2006)

Yates, Yates, Vanderbilt and Souza PRB 75, 195121 (2007) not smooth



$$|u_n^H\rangle = \sum_m S_{nm}(k)\,|u_m^W\rangle$$



smooth

→ Matrix elements of Hamiltonian ("normal" operator)

$$H^H_{nm} = \langle u_n^H|\hat{H}|u_m^H\rangle = \sum_{\ell p} S^\dagger_{\ell n}\underbrace{\langle u_\ell^W|\hat{H}|u_p^W\rangle}_{H^W_{\ell p}} S_{pm} \Rightarrow$$

$$\boxed{H^H = S^\dagger H^W S}$$

Wannier functions (FT $\bar{k} \longrightarrow \bar{R}$): $|u_n^W\rangle = \sum_{\bar{R}} e^{-i\bar{k}(\bar{r}-\bar{R})}\,|\underline{\underline{\bar{R}\,n}}\rangle$

$$H^W_{\ell p} = \sum_{R R'} e^{i\bar{k}(\bar{R}-\bar{R}')}\langle \bar{R}\ell|\hat{H}|\bar{R}'p\rangle = \sum_R e^{i\bar{k}\cdot\bar{R}}\boxed{\langle \bar{0}\ell|\hat{H}|\bar{R}p\rangle}$$

↕ same matrix element

Taking derivatives very easy:

$$\partial_a H^W_{\ell p} = \sum_R i\,\underline{\underline{R_a}}\, e^{i\bar{k}\cdot\bar{R}}\boxed{\langle \bar{0}\ell|\hat{H}|\bar{R}p\rangle}$$

→ Matrix elements of Berry connection (special)

$$A^{H}_{a,nm} = i \langle u^{H}_{n} | \partial_a u^{H}_{m} \rangle$$

Extra Term! $\propto H^{H}_{a,nm} / (\mathcal{E}_n - \mathcal{E}_m)$

$$A^{H}_{a} = S^{\dagger} A^{W}_{a} S + i \underbrace{S^{\dagger} \partial_a S}$$

$$A^{W}_{a,nm} = \langle u^{w}_{n} | \partial_a u^{w}_{m} \rangle = \sum_{\bar{R}} e^{i \bar{k} \cdot \bar{R}} \boxed{\langle \bar{0} n | \hat{r}_a | \bar{R} m \rangle}$$

→ Matrix elements for shift current

$$(\partial_a A^{W}_{b})_{nm} = \sum_{\bar{R}} i R_a e^{i \bar{k} \bar{R}} \boxed{\langle \bar{0} n | \hat{r}_b | \bar{R} m \rangle}$$

Wannier interpolation

PHYSICAL REVIEW B **97**, 245143 (2018)

***Ab initio* calculation of the shift photocurrent by Wannier interpolation**

Julen Ibañez-Azpiroz,[1] Stepan S. Tsirkin,[1] and Ivo Souza[1,2]

See also Wang, Liu, Kang, Gu, Xu and Duan PRB 96, 115147 (2017)

$$|\mathbf{R}n\rangle = \int d\mathbf{k} \sum_m U_{nm}(\mathbf{k}) e^{i(\mathbf{r}-\mathbf{R})\cdot\mathbf{k}} |u_{m\mathbf{k}}\rangle$$

$$r^c_{mn;a} = \partial_{k_a} r^c_{mn} - i(A^a_{mm} - A^a_{nn}) r^c_{mn}$$

Final expression for the shift current contains many terms, but all are calculated from **two matrix elements**:

Hamiltonian **Position**

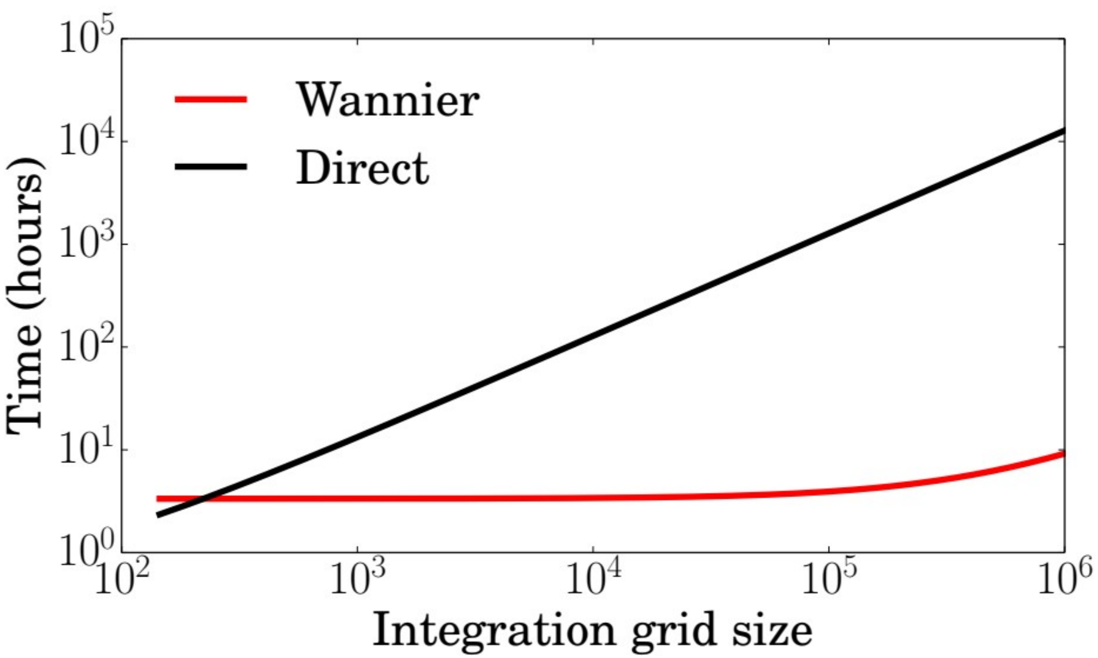
$$\langle \mathbf{0}n|\hat{H}|\mathbf{R}m\rangle \quad \& \quad \langle \mathbf{0}n|\hat{\mathbf{r}}|\mathbf{R}m\rangle$$

Main advantages

- Exact treatment of the sum-over-states contribution: **no truncation error**

- **Efficient calculation** thanks to Wannier interpolation: **beyond 10^6 k-points** feasible, reduce computational time heavily

- Implemented into Wannier90 v.3 on and WannierBerri



WANNIER90

G. Pizzi et. al., J. Phys. Cond. Matt. 32, 165902 (2020)

WANNIER BERRI

S. S. Tsirkin, npj CM 7, 33 (2021)

Wannier interpolation + Many-body effects

PHYSICAL REVIEW B **107**, 205101 (2023)

Including many-body effects into the Wannier-interpolated quadratic photoresponse tensor

Peio Garcia-Goiricelaya,[1,*] Jyoti Krishna,[1] and Julen Ibañez-Azpiroz[1,2]
[1]*Centro de Física de Materiales, Universidad del País Vasco UPV/EHU, 20018 San Sebastián, Spain*
[2]*Ikerbasque Foundation, 48013 Bilbao, Spain*

$$\sigma_2^{abc}(1,2,3) = \iiint \sum_{\text{def}} \varepsilon^{-1,da}(1,4)\sigma_2^{\text{KS},def}(4,5,6)\varepsilon^{-1,eb}(5,2)\varepsilon^{-1,fc}(6,3)d4d5d6$$
$$+ \iiint \sum_{\text{def}} \sigma_1^{ad}(1,4)K_{\text{xc},2}^{\text{def}}(4,5,6)\sigma_1^{eb}(5,2)\sigma_1^{fc}(6,3)d4d5d6.$$

Outline

First-principles scheme:

- *Wannier interpolation of the shift photocurrent*

Applications:

➡ • *Dipole selection rules in graphitic BC_2N*

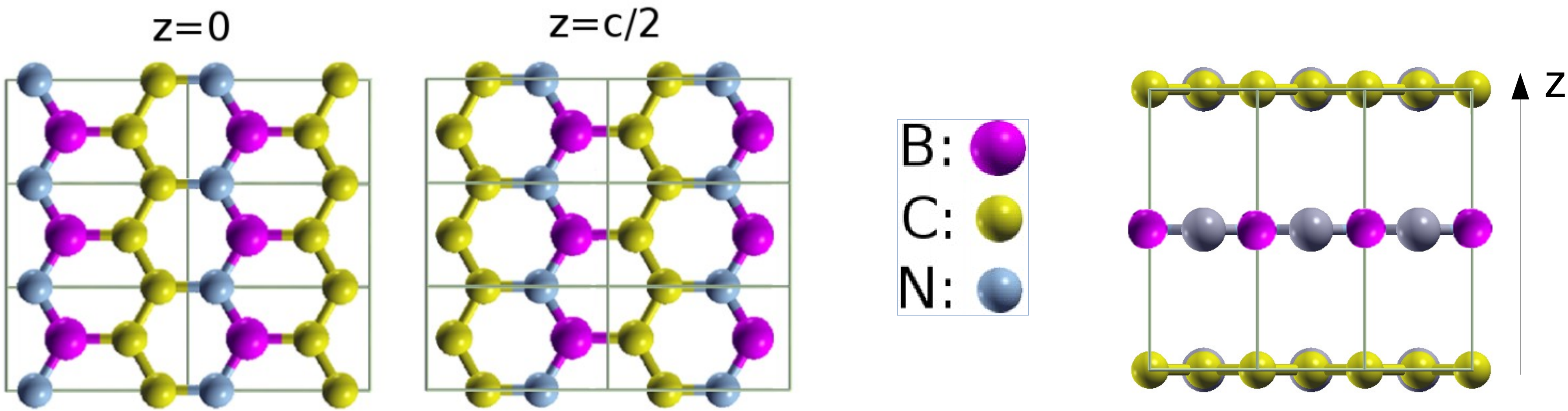
- *Variety of nonlinear responses in Weyl semimetal $TaIrTe_4$*

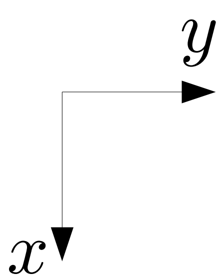
Search for non-trivial response: graphitic BC_2N

Space group 25 Pmm2,
A2 polytype*:* **no inversion symmetry**
Pan, Sun & Chen, PRB 2006

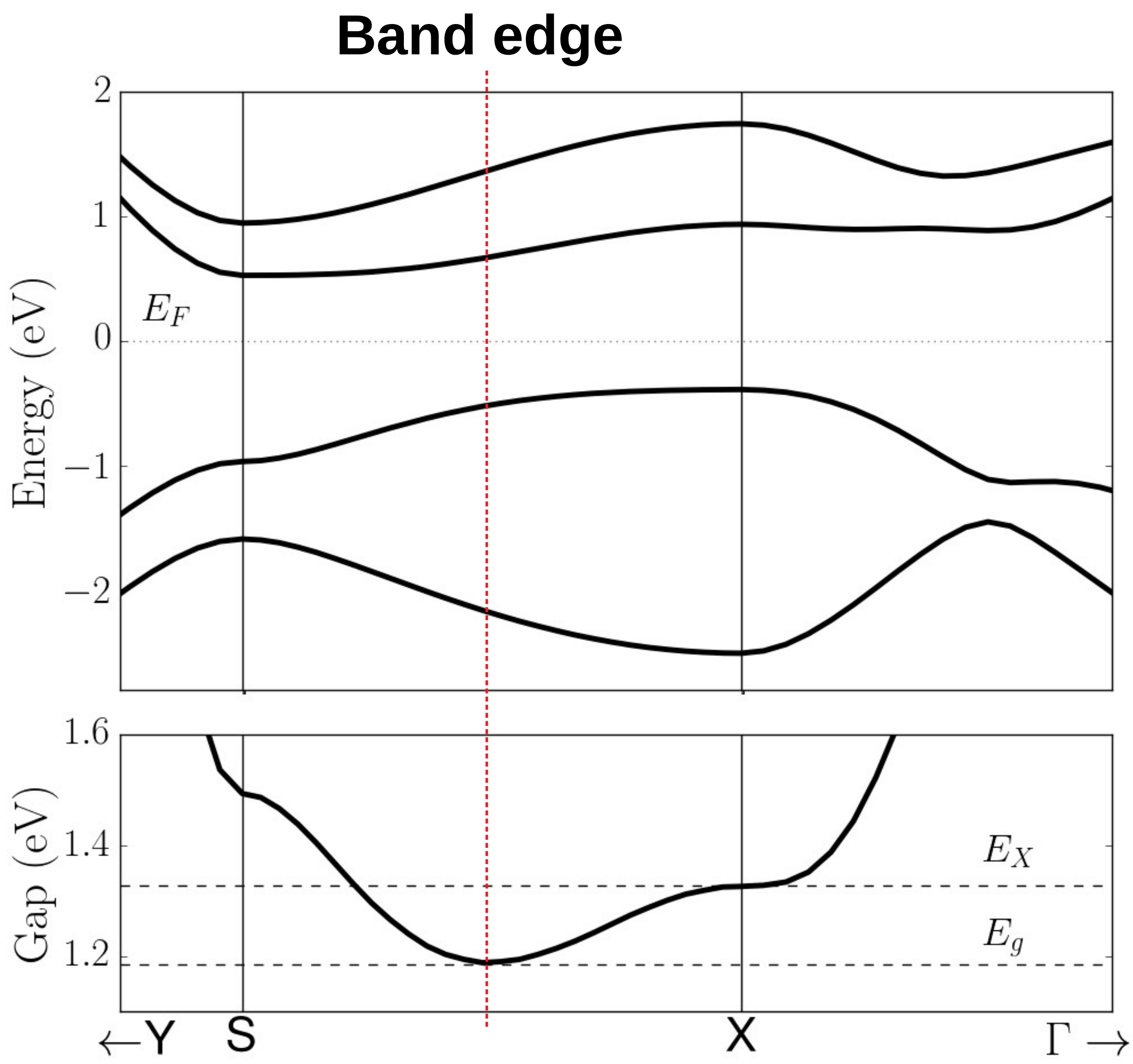
Top view of adjacent layers

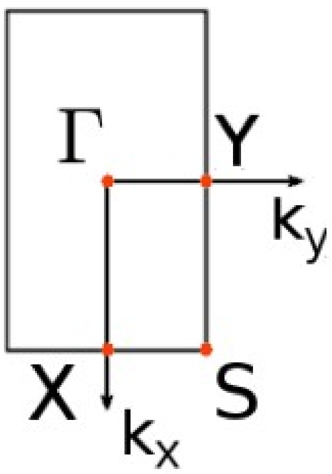
Side view





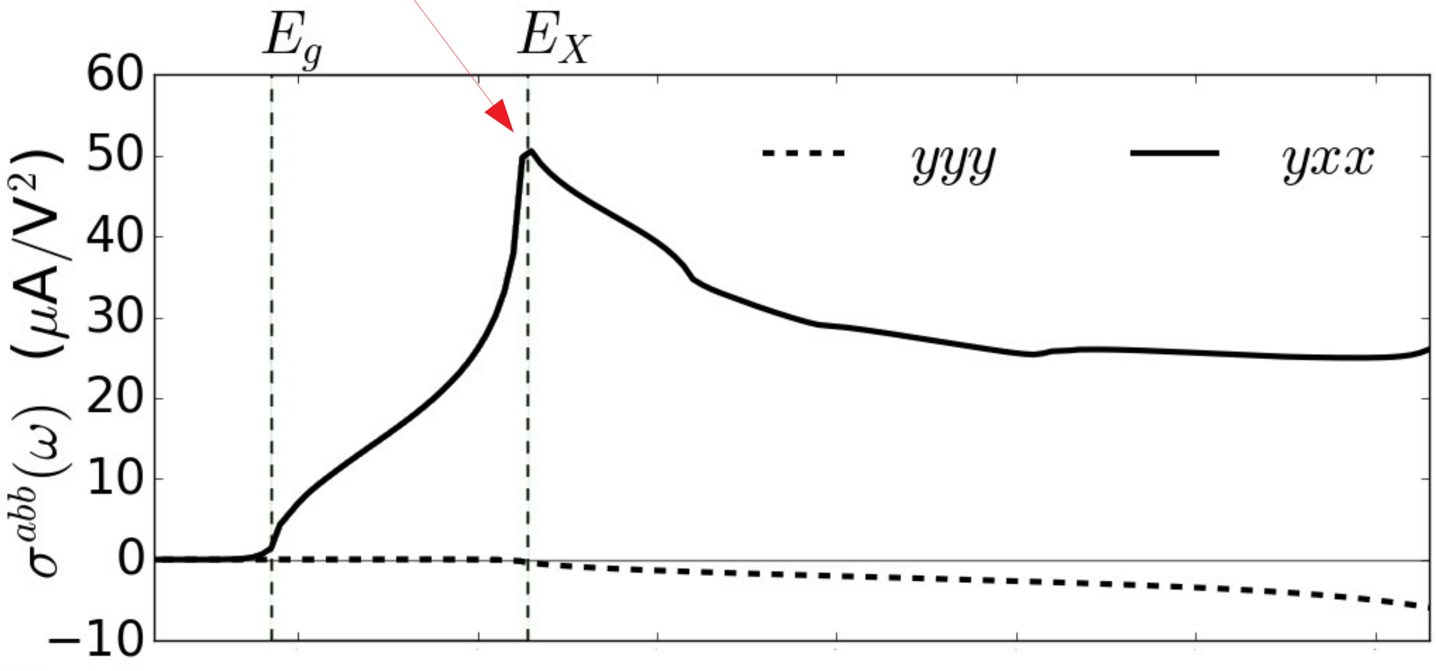
Weakly coupled layers
↓
Quasi-2D properties
↓
Large shift current response expected


Band edge
2
1
0
−1
−2
Energy (eV)
E_F
1.6
1.4
1.2
Gap (eV)
E_X
E_g
←Y
S
X
Γ →


Γ
Y
k_y
X
S
k_x

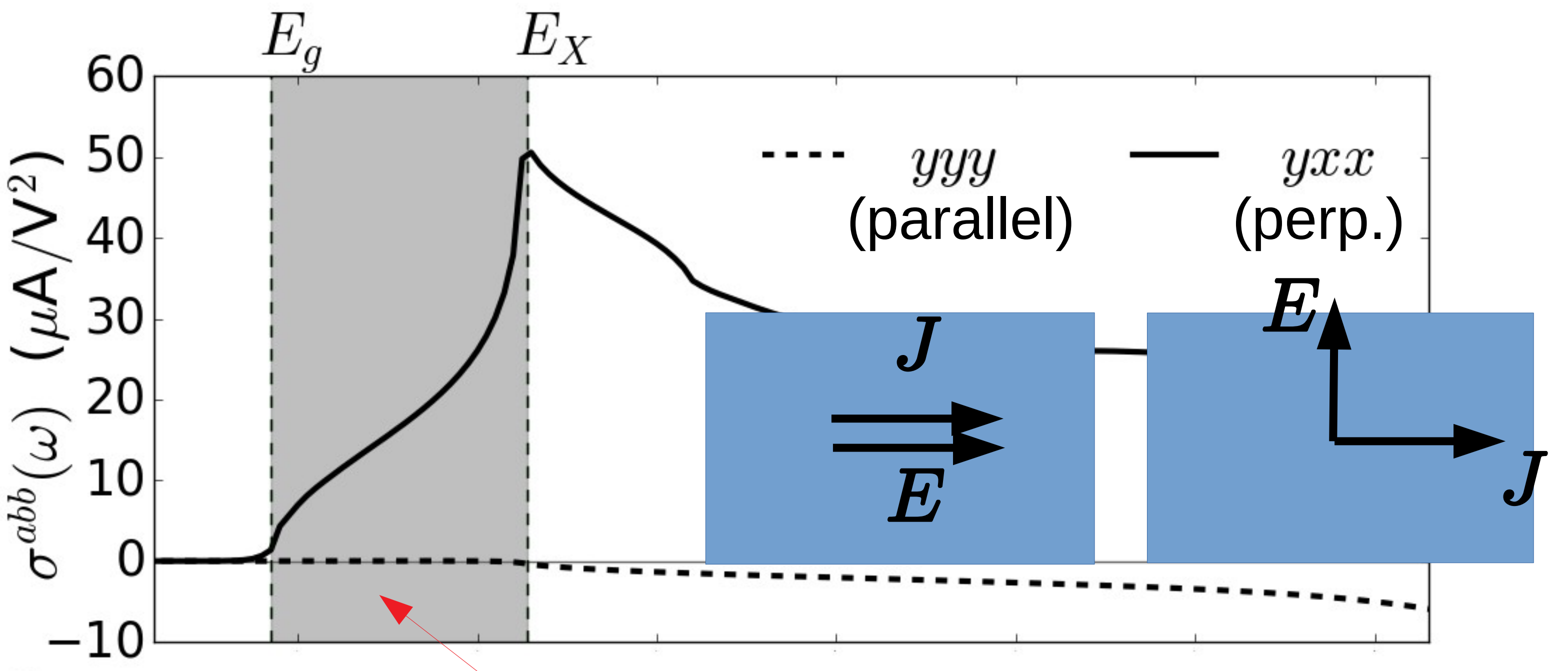
Shift-current spectrum

- **Large magnitude for a semiconductor**
- **Peaks in the suitable energy range**



(10^6 k-points needed to converge integrals)

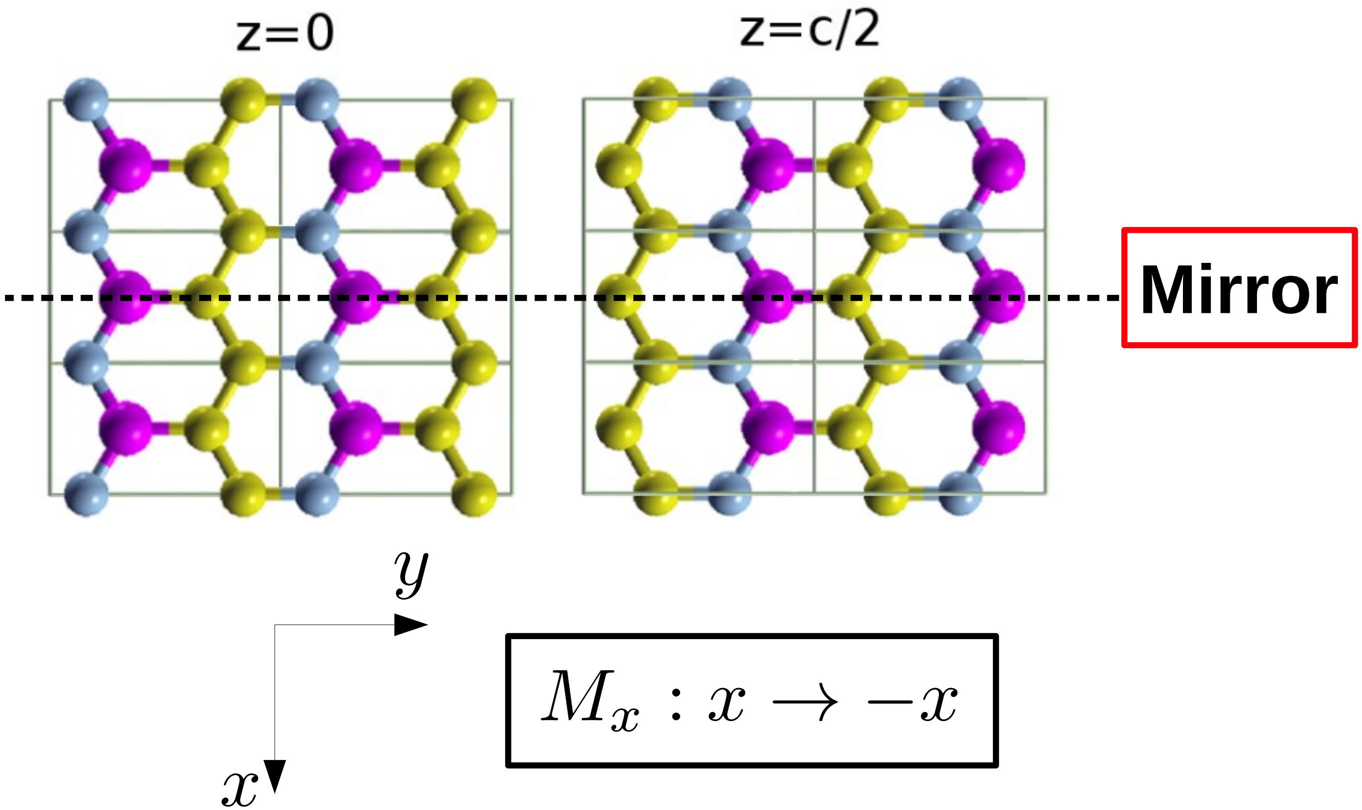
Shift-current spectrum



Band-edge region: current only flows perpendicular to field

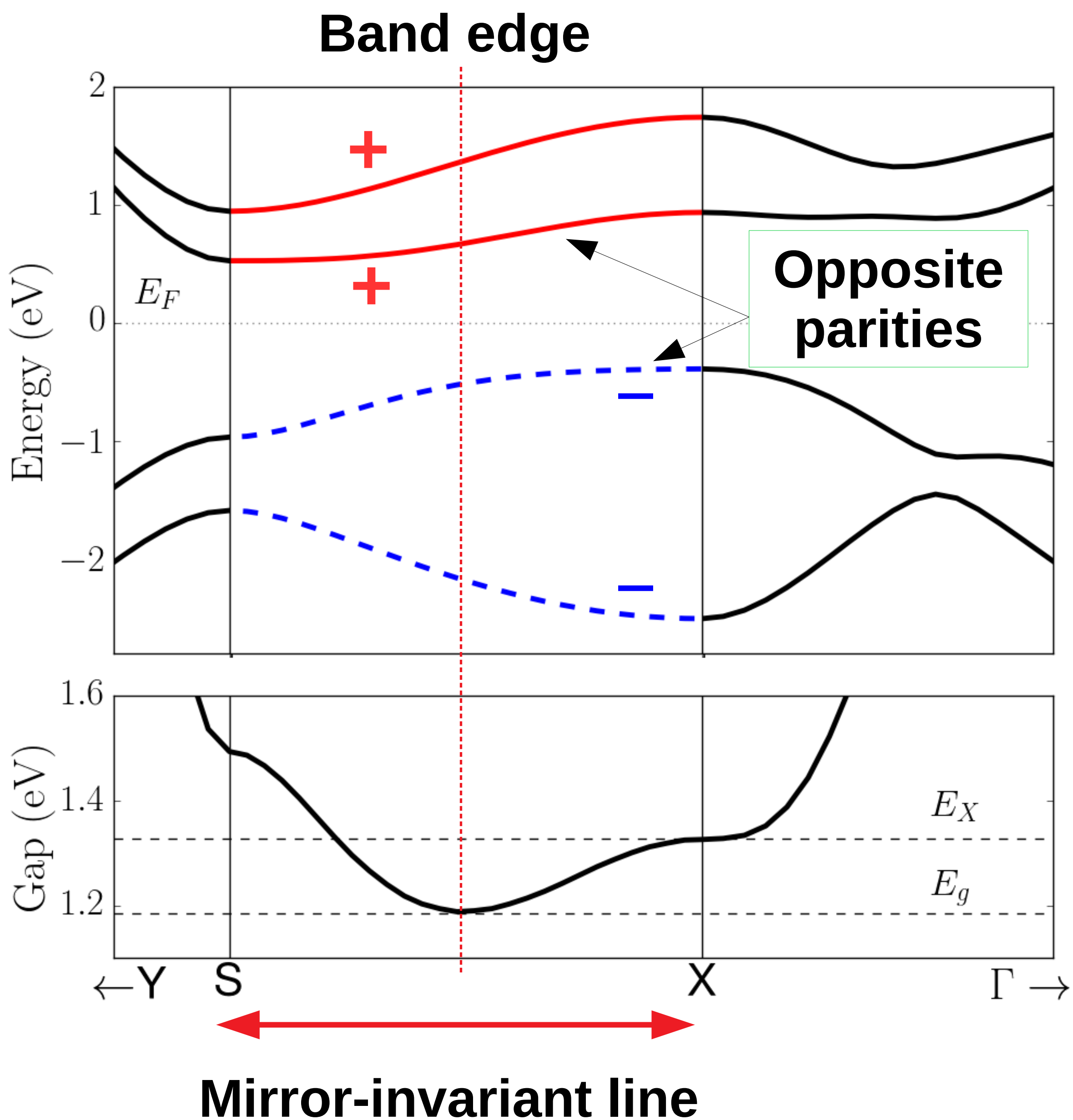
… why?

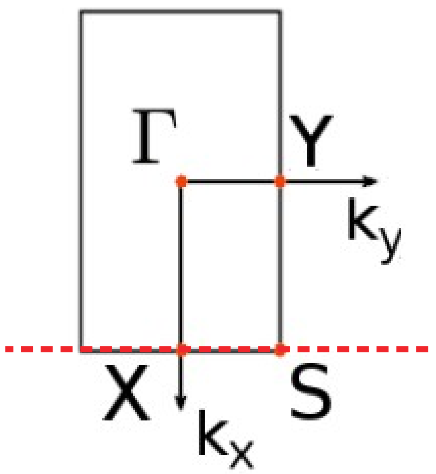
Back to the structure



$$M_x : x \rightarrow -x$$

Band-edge mirror eigenvalues





Band-edge states have **definite mirror parity:**

$$M_x|n\rangle = \pm|n\rangle$$

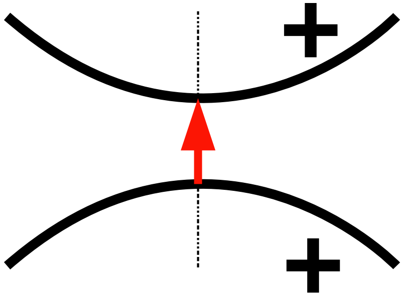
two possible eigenvalues

Microscopic matrix element

$$\sigma^{abb}(\omega) \propto \int_{\mathrm{BZ}} \sum_{n,m} (f_n - f_m)\, r^b_{nm} r^{b;a}_{mn}\, \delta(\omega_{nm} - \omega) d\mathbf{k}$$

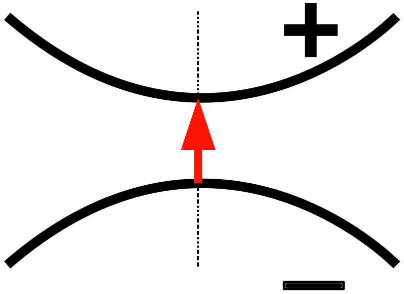
Dipole selection rules, distinguish two cases:

1. States have **same** parity



$$r^x_{nm} = 0$$

2. States have **opposite** parity



$$r^y_{nm} = 0$$

Microscopic matrix element

$$\sigma^{abb}(\omega) \propto \int_{\mathrm{BZ}} \sum_{n,m} (f_n - f_m)\, r^b_{nm} r^{b;a}_{mn}\, \delta(\omega_{nm} - \omega) d\mathbf{k}$$

Dipole selection rules, distinguish two cases:

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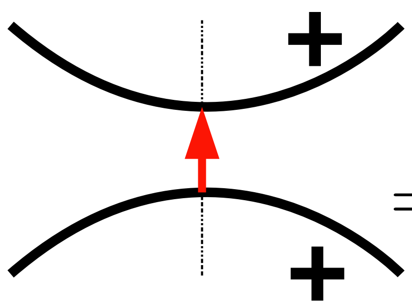
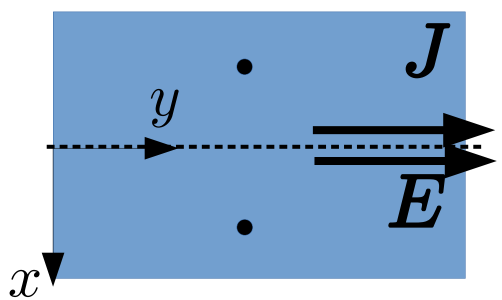


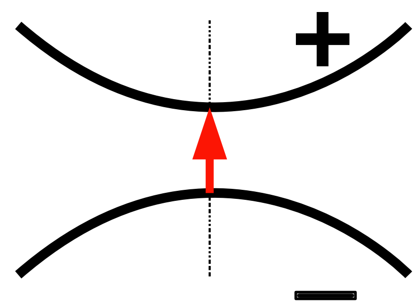
$$r^x_{nm} = 0$$

$$\Rightarrow \sigma^{yxx}(\omega) = 0$$



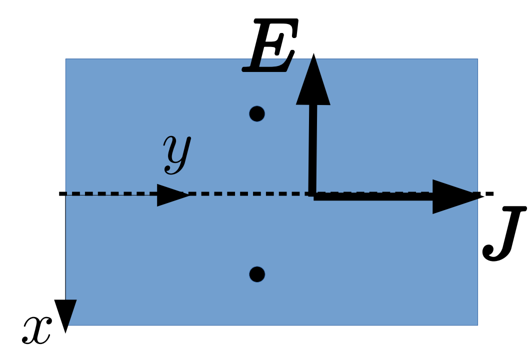
Parallel flow

2. States have **opposite** parity



$$r^y_{nm} = 0$$

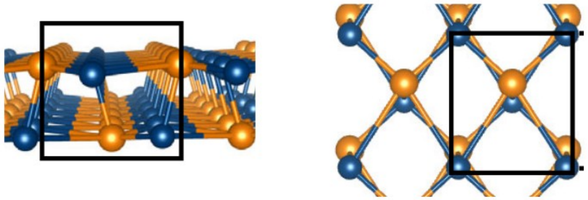
$$\Rightarrow \sigma^{yyy}(\omega) = 0$$



Perpendicular flow

Material realization

Realized in monolayer GeS



Rangel et. al., PRL 2017
Cook et. al., Nat. Comm. 2017

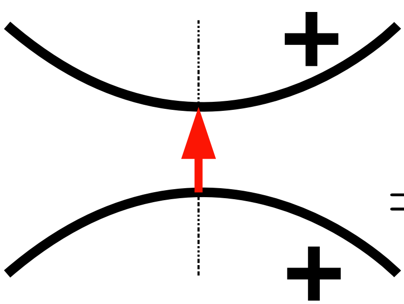
Realized in **graphitic BC_2N**

PHYSICAL REVIEW RESEARCH **2**, 013263 (2020)

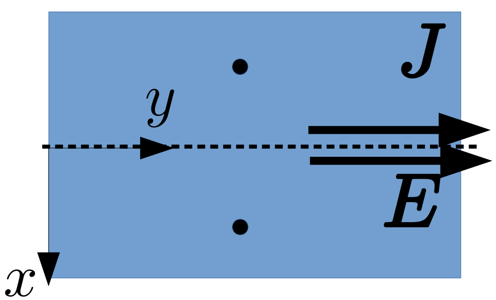
Directional shift current in mirror-symmetric BC_2N

Julen Ibañez-Azpiroz,[1] Ivo Souza,[1,2] and Fernando de Juan[2,3]

1. States have **same** parity

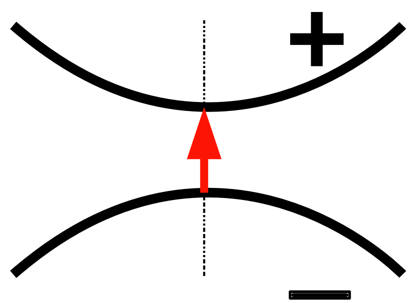


$$r^{x}_{nm} = 0$$
$$\Rightarrow \sigma^{yxx}(\omega) = 0$$



Parallel flow

2. States have **opposite** parity



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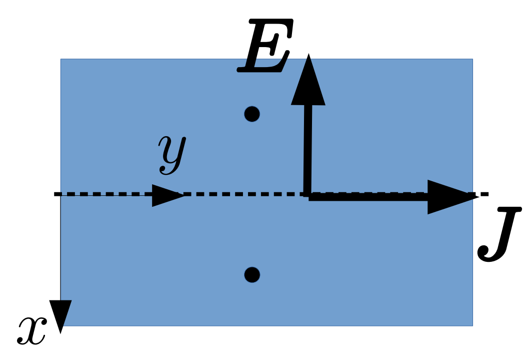


Perpendicular flow

Outline

First-principles scheme:

- *Wannier interpolation of the shift photocurrent*

Applications:

- *Dipole selection rules in graphitic BC_2N*
- *Variety of nonlinear responses in Weyl semimetal $TaIrTe_4$*

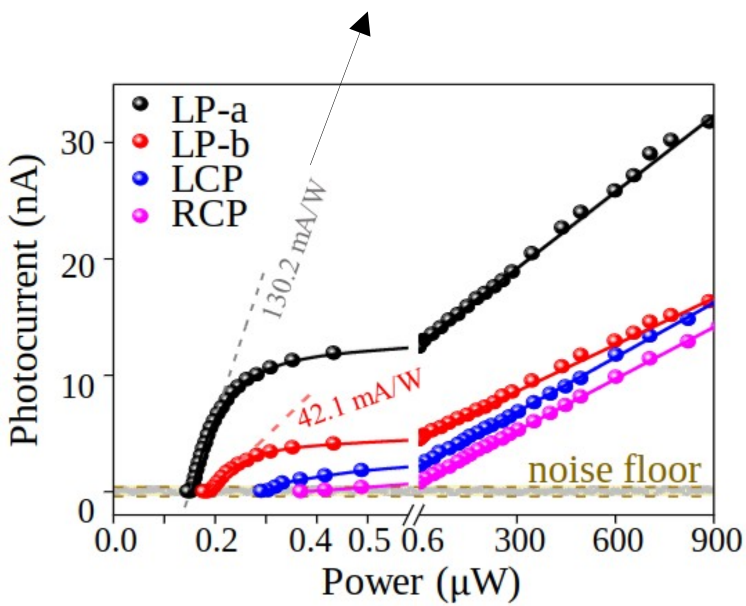
Optical measurements in $TaIrTe_4$

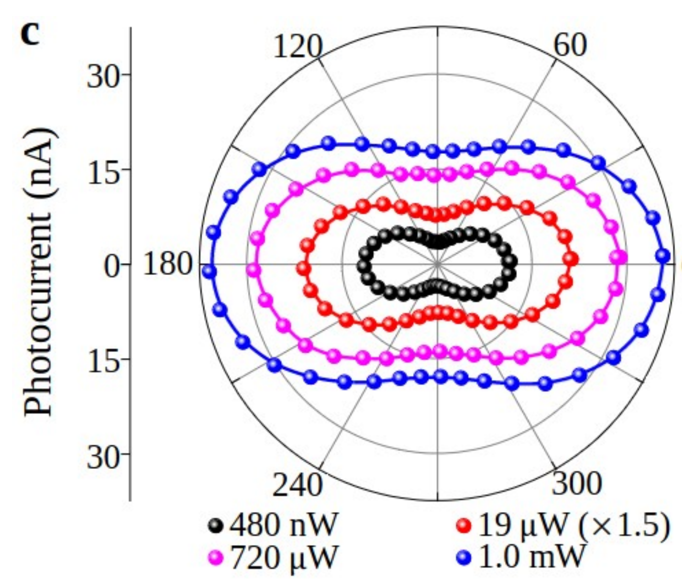
ARTICLES
https://doi.org/10.1038/s41563-019-0296-5
nature materials

Nonlinear photoresponse of type-II Weyl semimetals

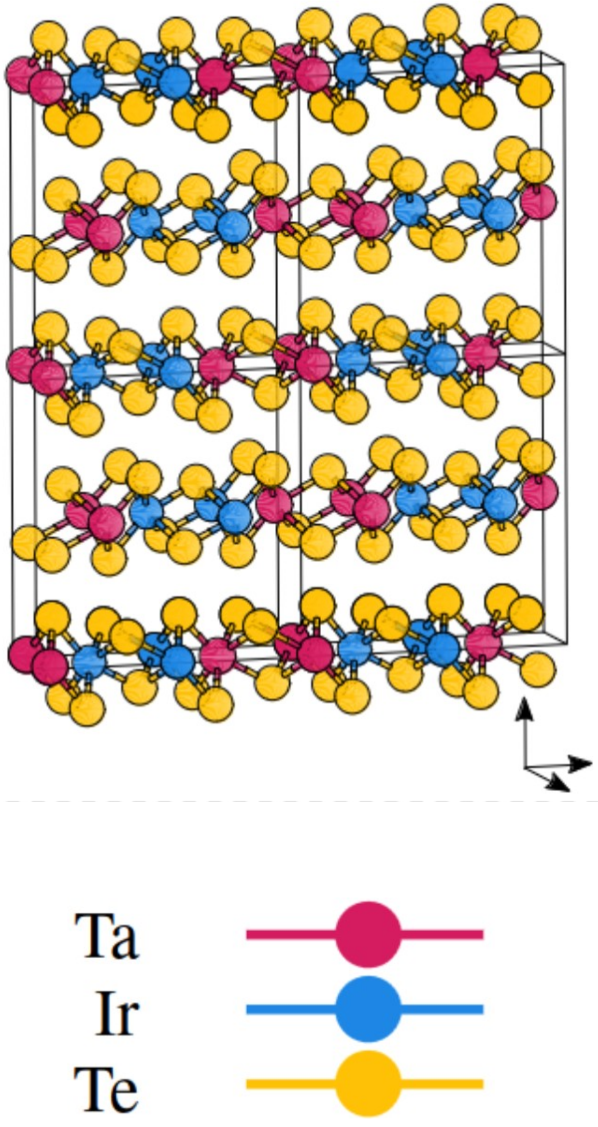
Junchao Ma[1], Qiangqiang Gu[1], Yinan Liu[1], Jiawei Lai[1], Peng Yu[2], Xiao Zhuo[1], Zheng Liu[2], Jian-Hao Chen[1,3]*, Ji Feng[1,3,4]* and Dong Sun[1,3]*

130 mA/W: ranks amongst largest photoresponses reported to date

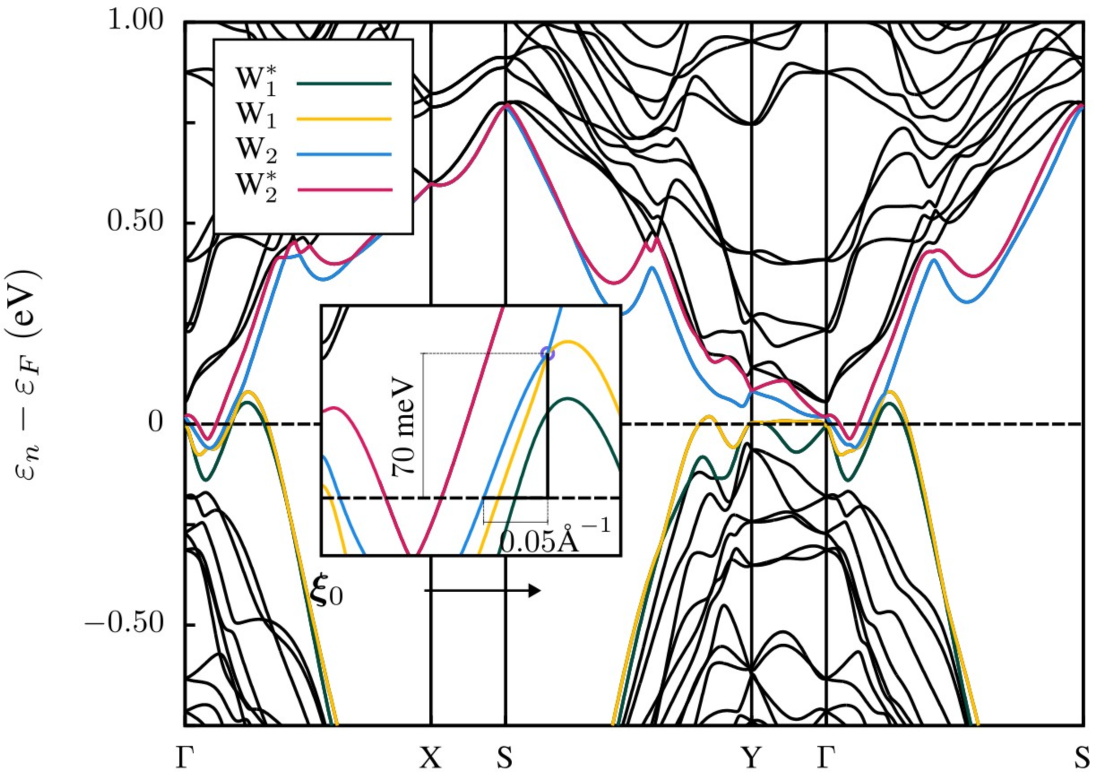




$TaIrTe_4$: basic facts

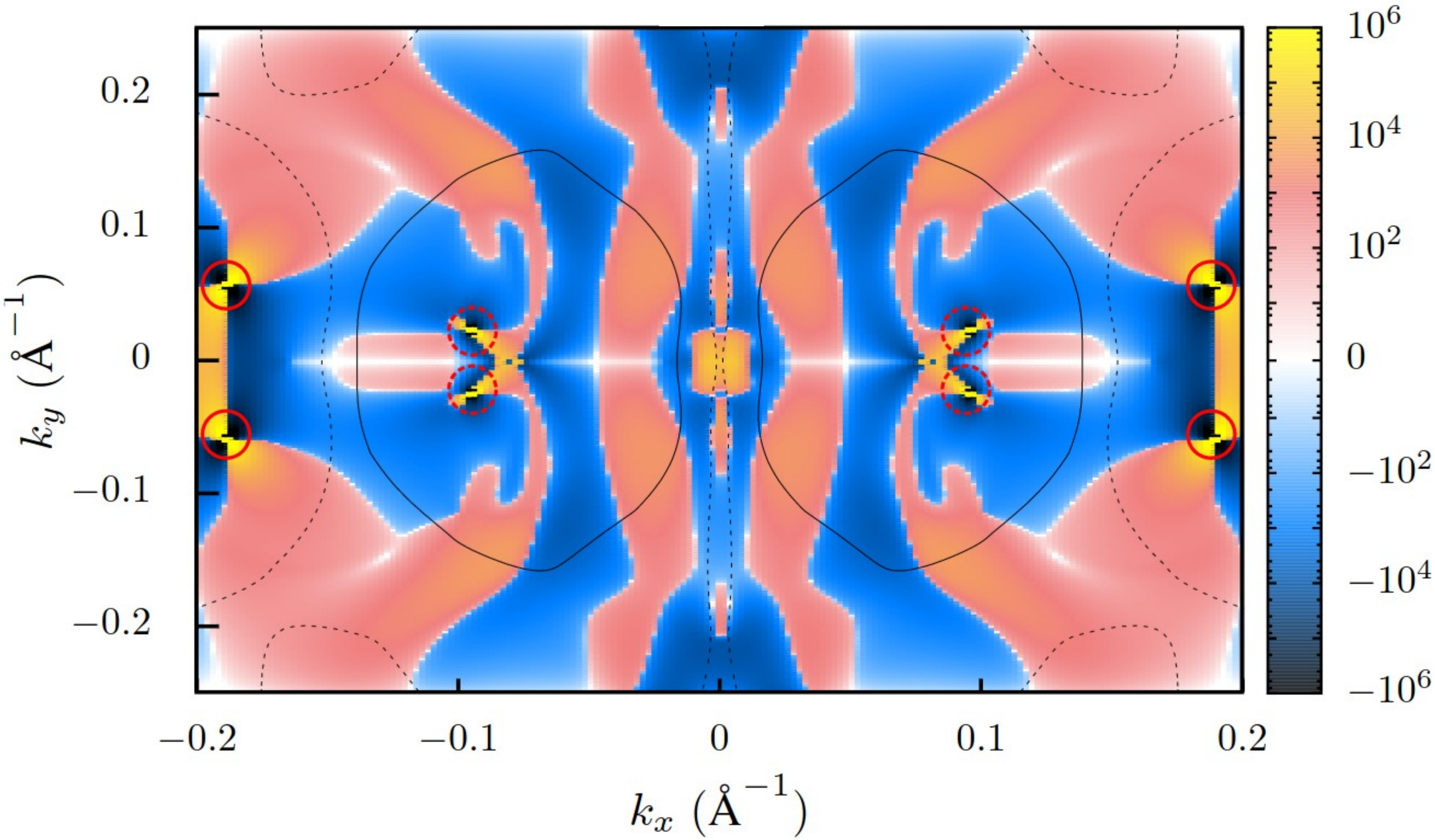


- Type II Weyl semimetal
- Space group *Pmn2₁*, acentric
- 4 metallic bands
- 2 pairs of Weyl points are in the $k_z = 0$ plane, ~70 meV above Fermi level



Shift-current transition matrix element between Weyl bands

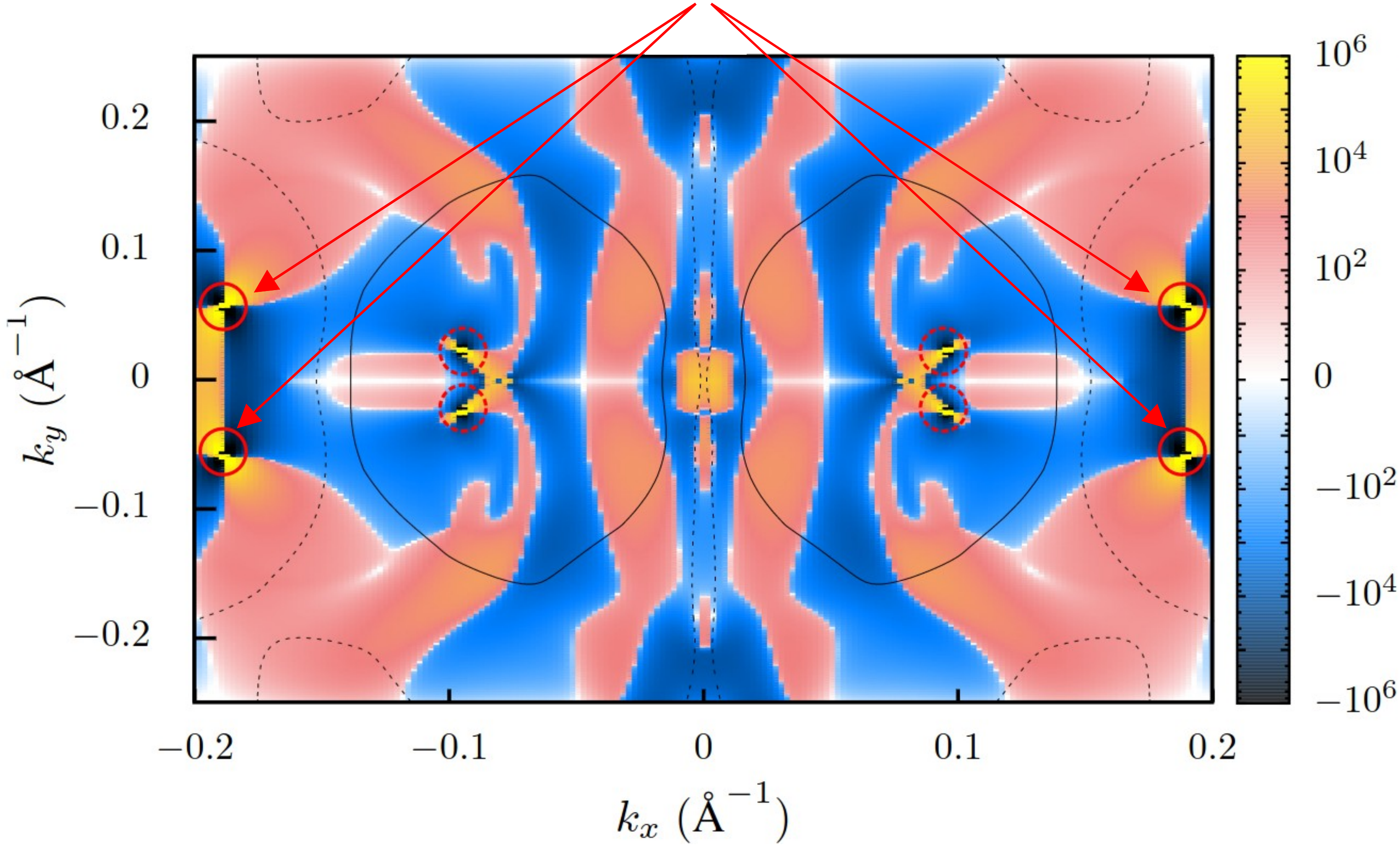
$$r^x_{W_1,W_2} \cdot r^x_{W_1,W_2;z}$$



(3 x 10^6 k-points employed)

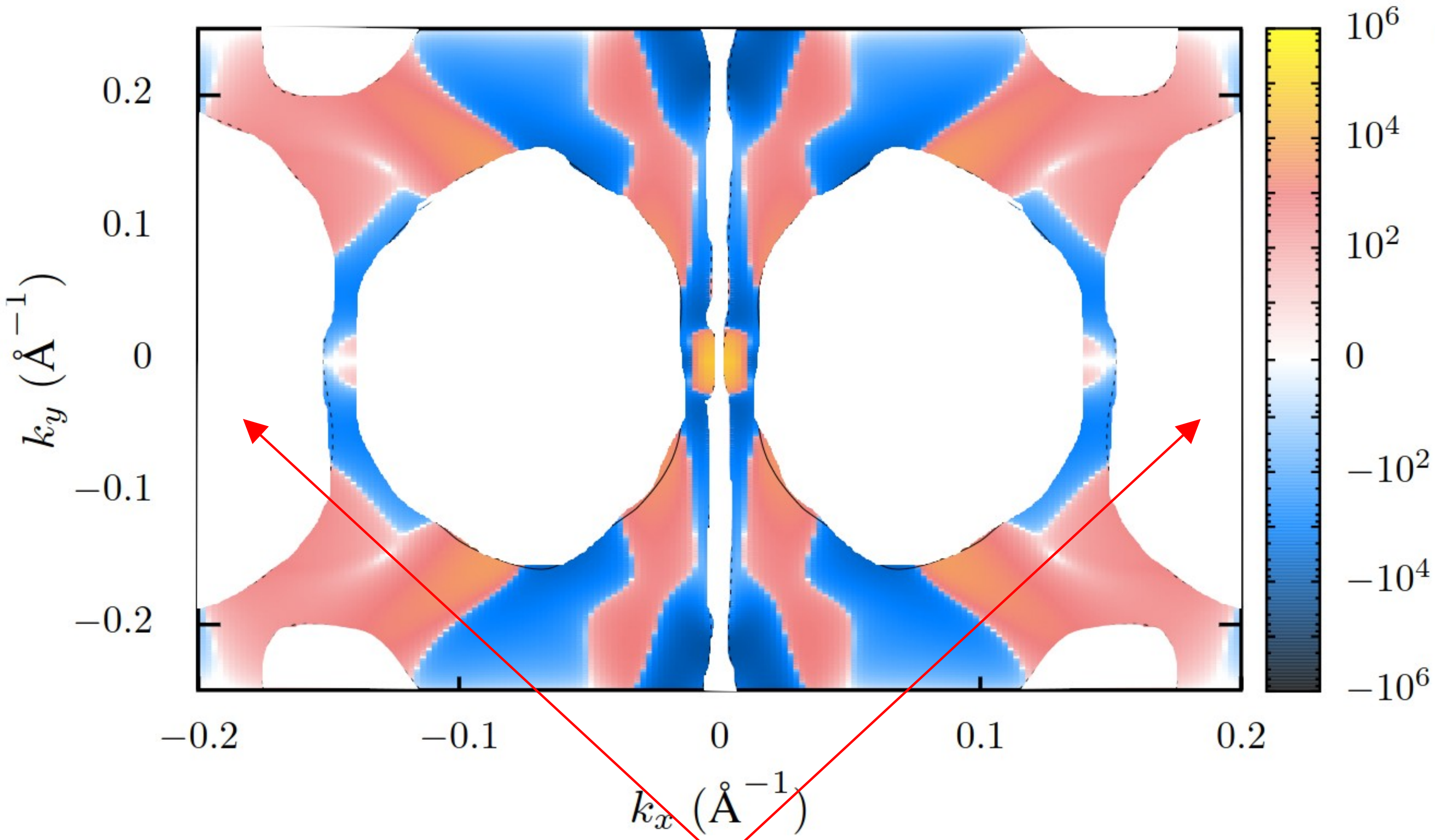
Shift-current transition matrix element between Weyl bands

Pronounced enhancement of integrand at the Weyl points



Shift-current transition matrix element between Weyl bands

Large enhancement of integrand at the Weyl points



$$f_n - f_m = 0$$

<u>... but they do not contribute due to occupation factors</u>

Beyond the quadratic response

Nonlinear photoresponse of type-II Weyl semimetals

Junchao Ma[1], Qiangqiang Gu[1], Yinan Liu[1], Jiawei Lai[1], Peng Yu[2], Xiao Zhuo[1], Zheng Liu[2], Jian-Hao Chen[1,3*], Ji Feng[1,3,4*] and Dong Sun[1,3*]

The experimental manifestation of topological effects in bulk materials is attracting enormous research interest. However, direct experimental evidence of the effective *k*-space monopole of the Weyl nodes has so far been lacking. Here, signatures of the singular topology of the type-II Weyl semimetal $TaIrTe_4$ are revealed in the photoresponses, which are related to divergence of the Berry curvature. $TaIrTe_4$ exhibits a large photoresponsivity of 130.2 mA W^{-1}—with 4 μm excitation in an unbiased field-effect transistor at room temperature—arising from the third-order nonlinear optical response, approaching the performance of commercial low-temperature detectors. In addition, the circularly polarized galvanic response is enhanced at 4 μm, possibly due to the same Berry curvature singularity enhancement. Considering the optical selection rule of chiral Weyl cones, this may open the door for studying and controlling the chiral polarization of Weyl fermions with an electric field in addition to the optical helicities.

Third-order contribution: d.c. electric field (“built-in”)

$$J_a(0) \propto E_b(\omega) E_c(-\omega) \cdot E_d(0)$$

Accounting for a d.c. field: competing effects

- Semiclassical prescription:

$$f_n(\mathbf{k}) \to f_n(\mathbf{k} + \frac{e\tau\mathbf{E}(0)}{\hbar}) \simeq f_n(\mathbf{k}) + \frac{e\tau\mathbf{E}(0)}{\hbar} \cdot \frac{\partial f_n(\mathbf{k})}{\partial\mathbf{k}}$$

→ ”current-induced” <u>shift</u> and <u>injection</u> currents

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→ ”current-induced” shift and injection currents

- Intrinsic third-oder d.c. current: the **jerk current**

$$J^a_{\text{jerk}}(0) = \tau^2 \cdot \iota^{(3)}_{abcd}(\omega) \cdot E_b(\omega)E_c(-\omega) \cdot E_d(0)$$

PHYSICAL REVIEW LETTERS **121,** 176604 (2018)

Jerk Current: A Novel Bulk Photovoltaic Effect

Benjamin M. Fregoso,[1] Rodrigo A. Muniz,[2,3] and J. E. Sipe[3]
[1]*Department of Physics, Kent State University, Kent, Ohio 44240, USA*
[2]*Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan 48109 USA*
[3]*Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada*

Accounting for a d.c. field: competing effects

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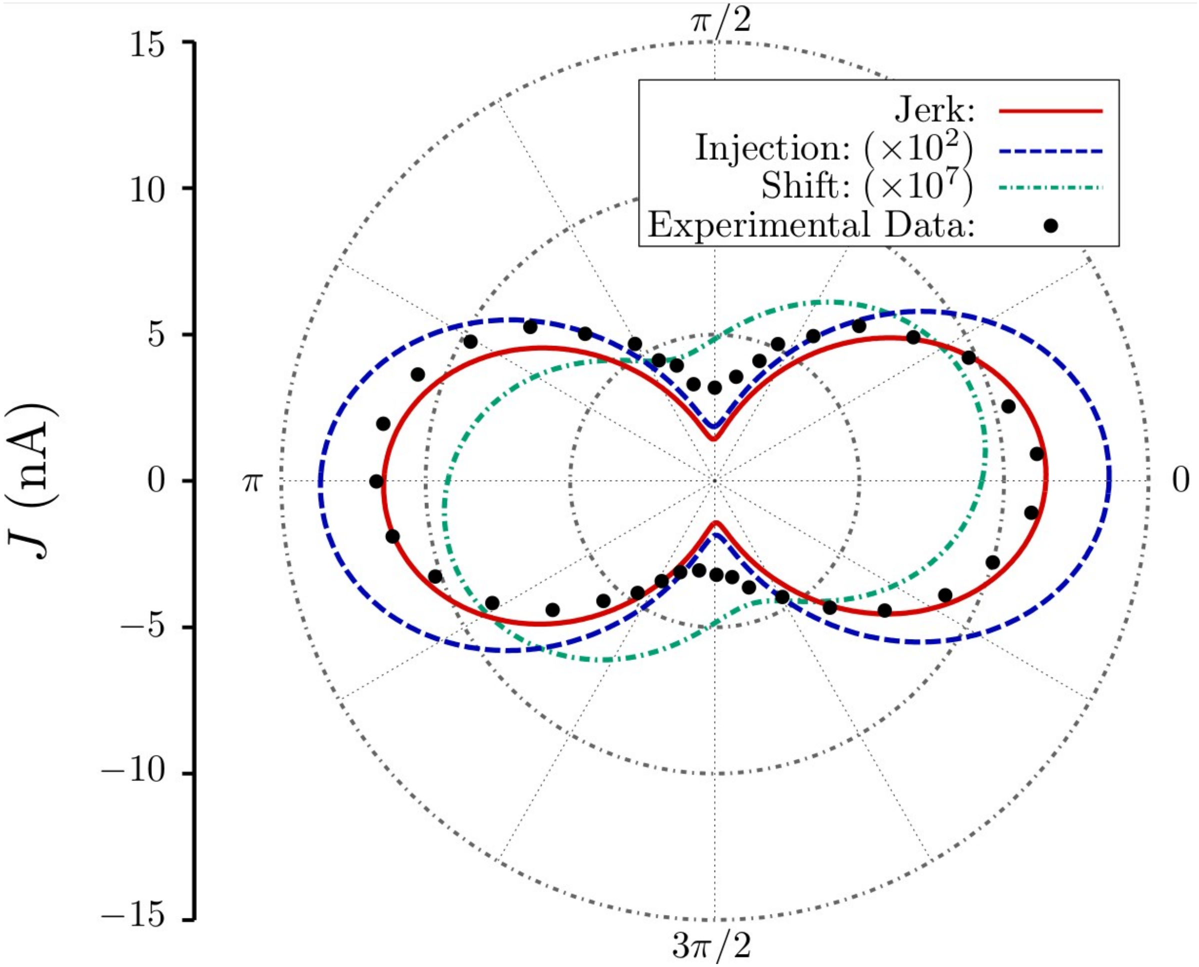
$$\iota^{(3)}_{abcd}(\omega) = \frac{2\pi e^4}{\hbar^3} \int_k \sum_{n,m} f_{nm} \frac{\partial^2 \omega_{nm}}{\partial k_a \partial k_d} r^b_{nm} r^c_{mn} \delta(\omega_{nm} - \omega)$$

Size and polar distribution of the various third-order terms

Estimates for the d.c. field and relaxation time:

$$|\mathbf{E}(0)| \sim 10^5 \text{ V/m}, \quad \tau \sim 10^{-14} \text{ s}$$



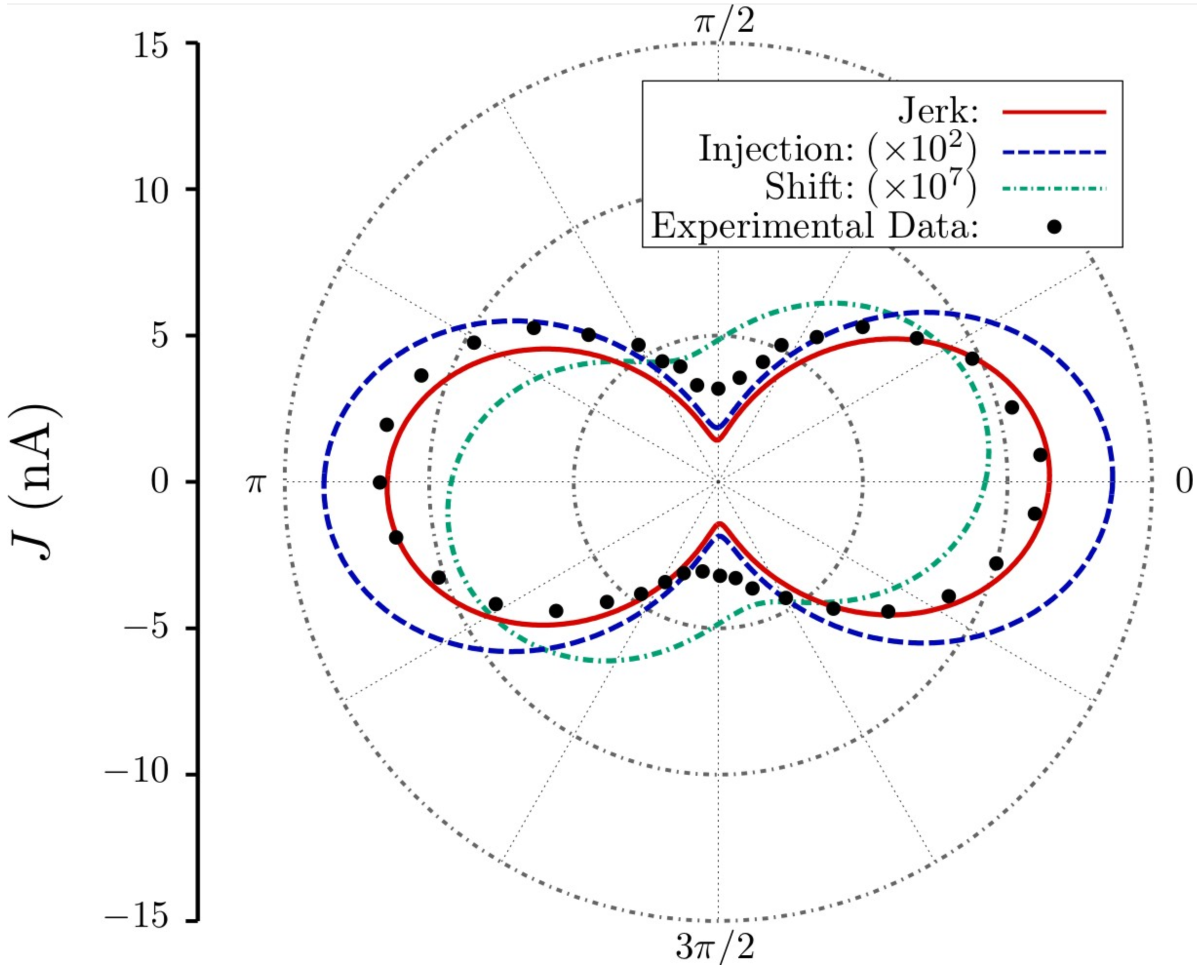
Size and polar distribution of the various third-order terms

PHYSICAL REVIEW B **107**, 205204 (2023)

Editors' Suggestion

***Ab initio* study of the nonlinear optical properties and dc photocurrent of the Weyl semimetal $TaIrTe_4$**

Álvaro R. Puente-Uriona,[1,*] Stepan S. Tsirkin,[1,2] Ivo Souza,[1,2] and Julen Ibañez-Azpiroz[1,2]



Bonus!

First-principles scheme:

- *Wannier interpolation of the shift photocurrent*

Applications:

- *Dipole selection rules in graphitic BC_2N*
- *Variety of nonlinear responses in Weyl semimetal $TaIrTe_4$*
- ➡ *Many body effects*

- KS and MB microscopic conductivity tensors are linked through the chain rule:
  - 1^{st} order:

$$\sigma_1{}^{ab}(1,2) = \int \sum_c \sigma_1^{\mathsf{KS}\,ac}(1,3)\epsilon^{-1\,cb}(3,2)d3$$

$$\epsilon^{ab}(1,2) = \delta(1,2)\delta_{ab} - \int \sum_c F_{\mathsf{Hxc}}{}^{ac}(1,3)\sigma_1^{\mathsf{KS}\,cb}(3,2)d3$$

  - 2^{nd} order:

$$\sigma_2{}^{abc}(1,2,3) = \sum_{def} \iiint \epsilon^{-1\,T\,ad}(1,4)\sigma_2^{\mathsf{KS}\,def}(4,5,6)\epsilon^{-1\,eb}(5,2)\epsilon^{-1\,fc}(6,3)d4d5d6$$
$$+ \sum_{def} \iiint \sigma_1{}^{ad}(1,4)G_{\mathsf{xc}}{}^{def}(4,5,6)\sigma_1{}^{eb}(5,2)\sigma_1{}^{fc}(6,3)d4d5d6$$

- Tensorial generalization of the scalar equations of TD-DFT | Luppi *et al.*, PhysRevB.82.235201 (2010)

Garcia-Goiricelaya, Krishna, IA PRB 107, 205101 (2023)