Tilted Dirac Fermions
Topological metals from band inversion

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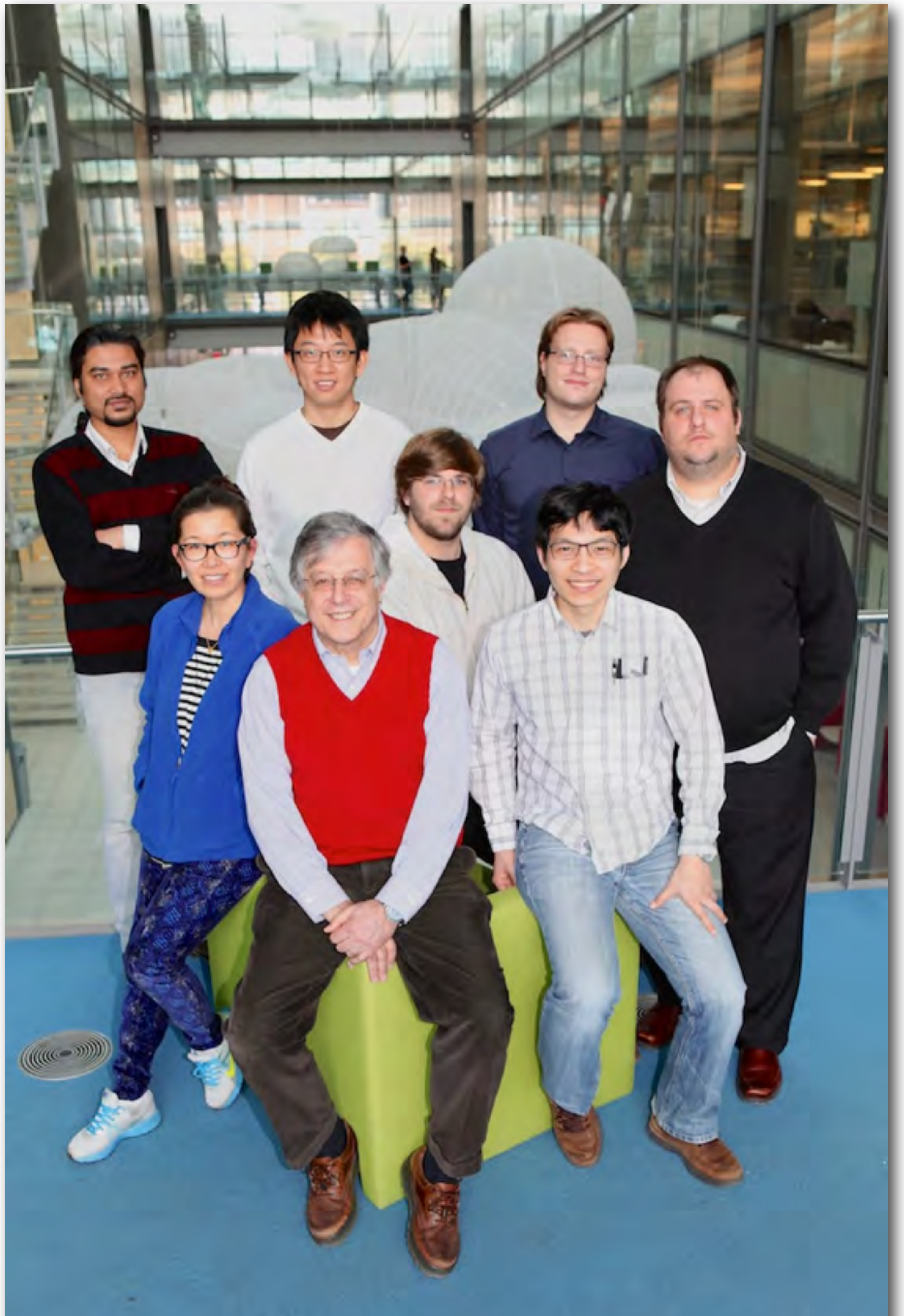
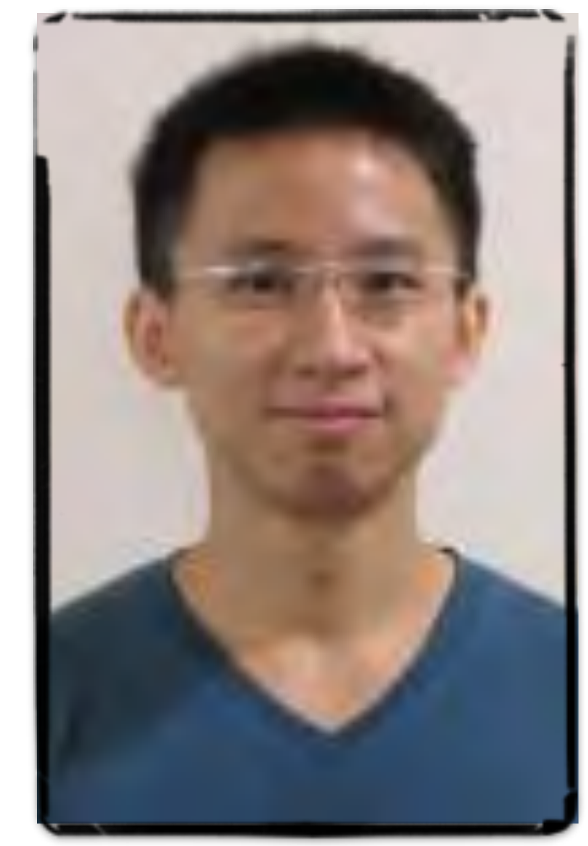
Acknowledgements





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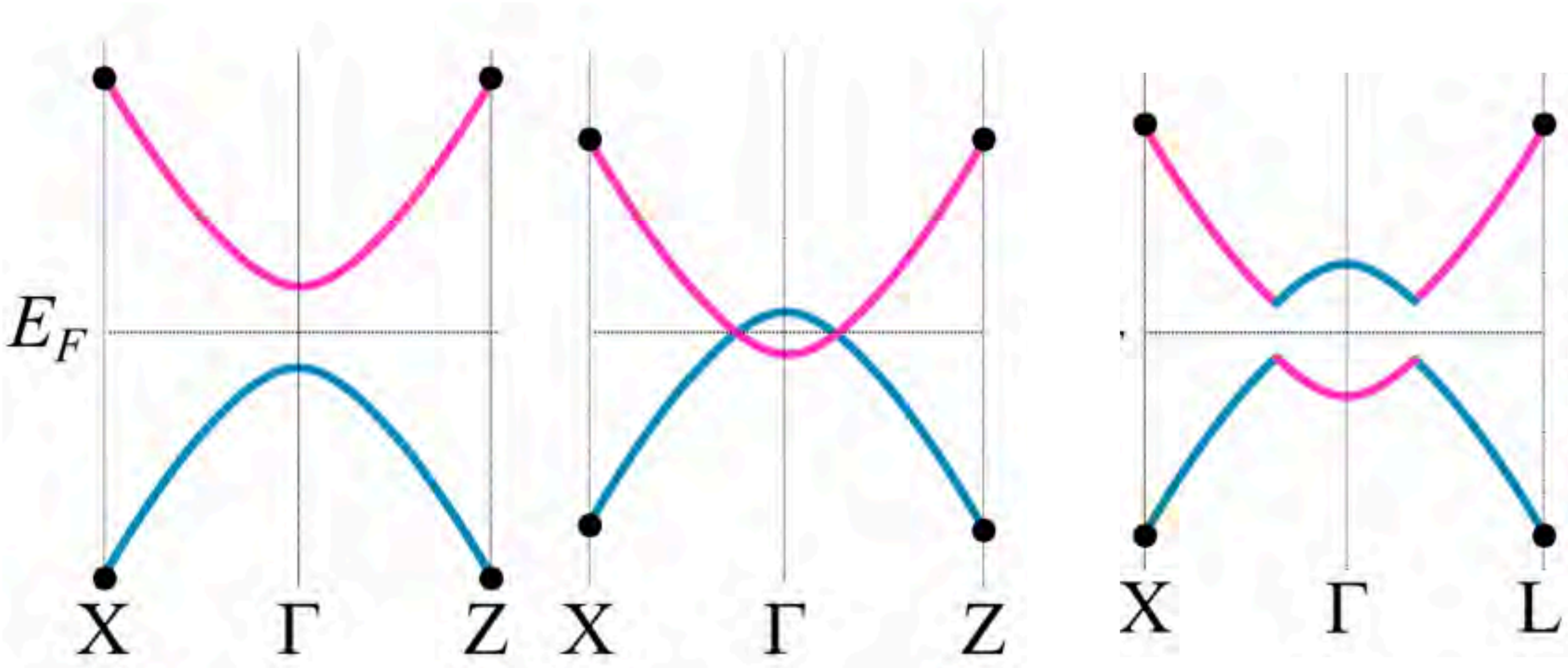
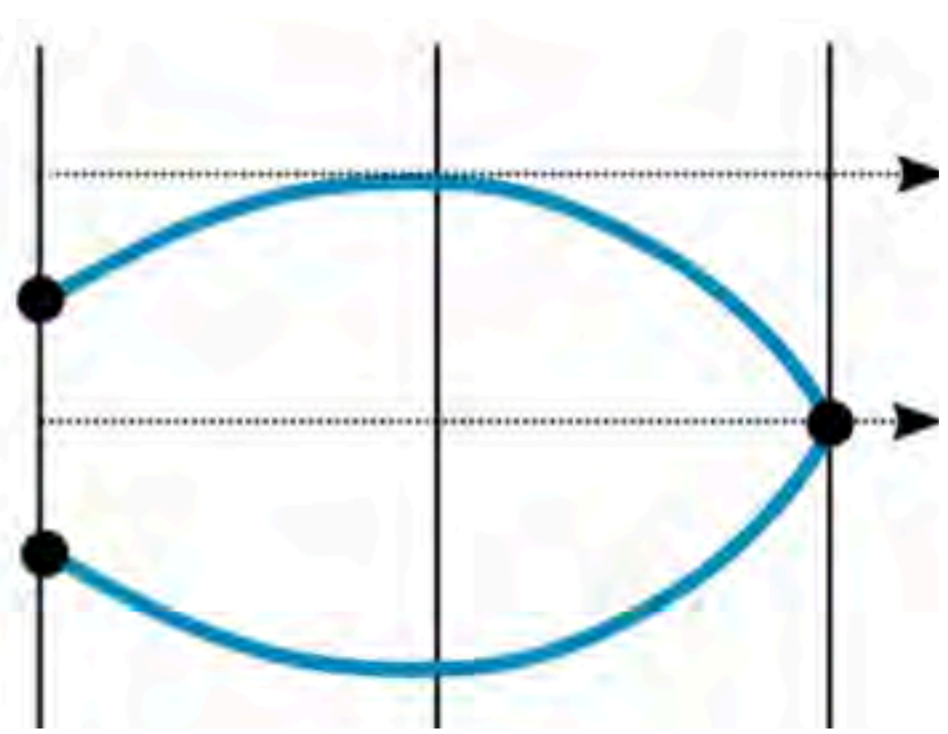
Noninteracting SPTs



Topological (crystalline) Insulators

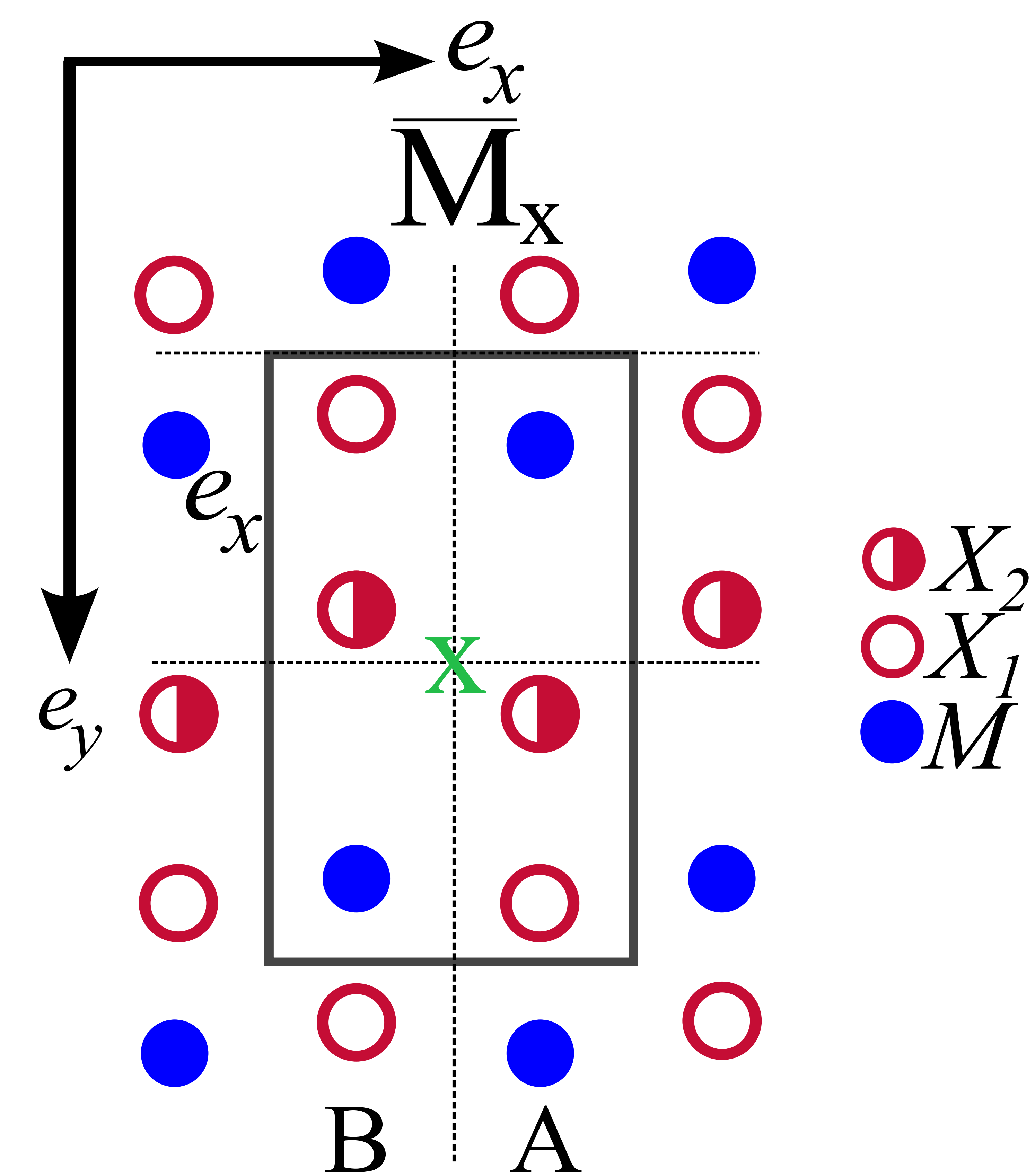


Gaplessness guaranteed by nonsymmorphic symmetries at certain electron fillings

Non-symmorphic symmetries

Two types of symmetries

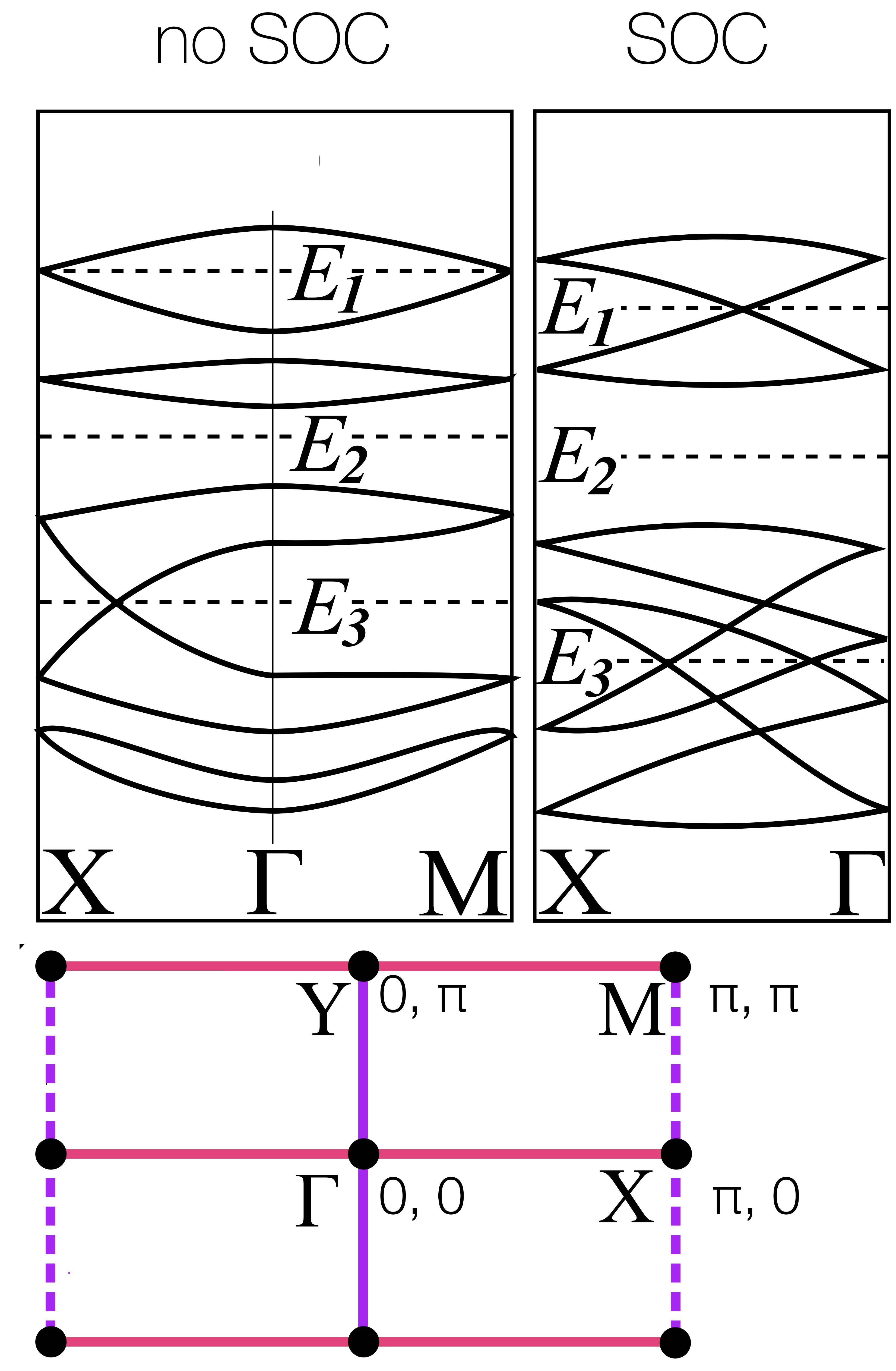
- symmorphic symmetries preserve origin
- non-symmorphic symmetries unavoidably translate spatial origin
- Examples: MX_2 monolayers (ZrI_2,$MoTe_2$,WTe_2)
- Three symmetries: Screw rotation, Glide-reflection and inversion symmetry



Band structures

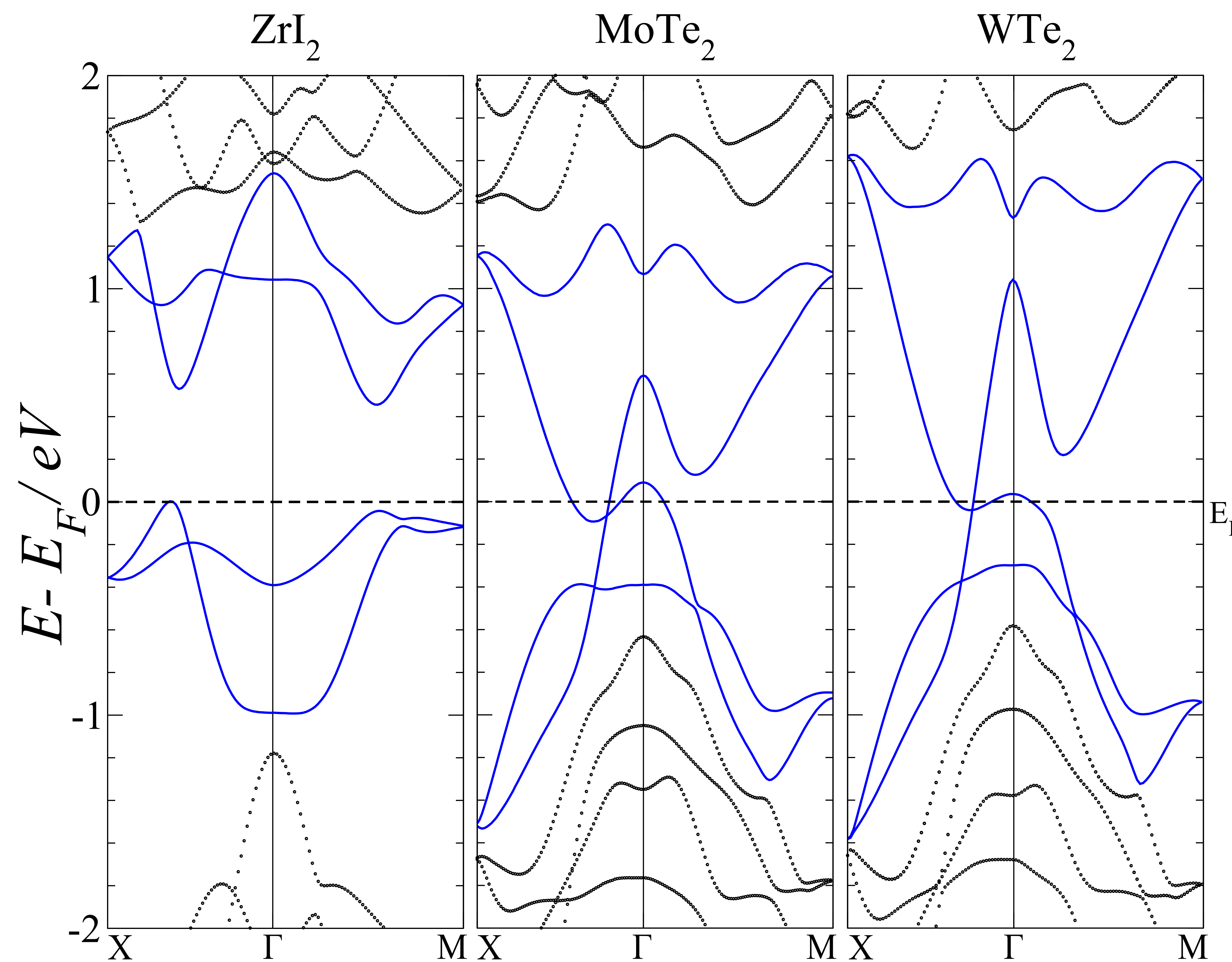
Three different types of band structures

- Filling enforced semimetal (E_1)
- Band insulators (E_2)
- topological semimetal due to band inversion (E_3)



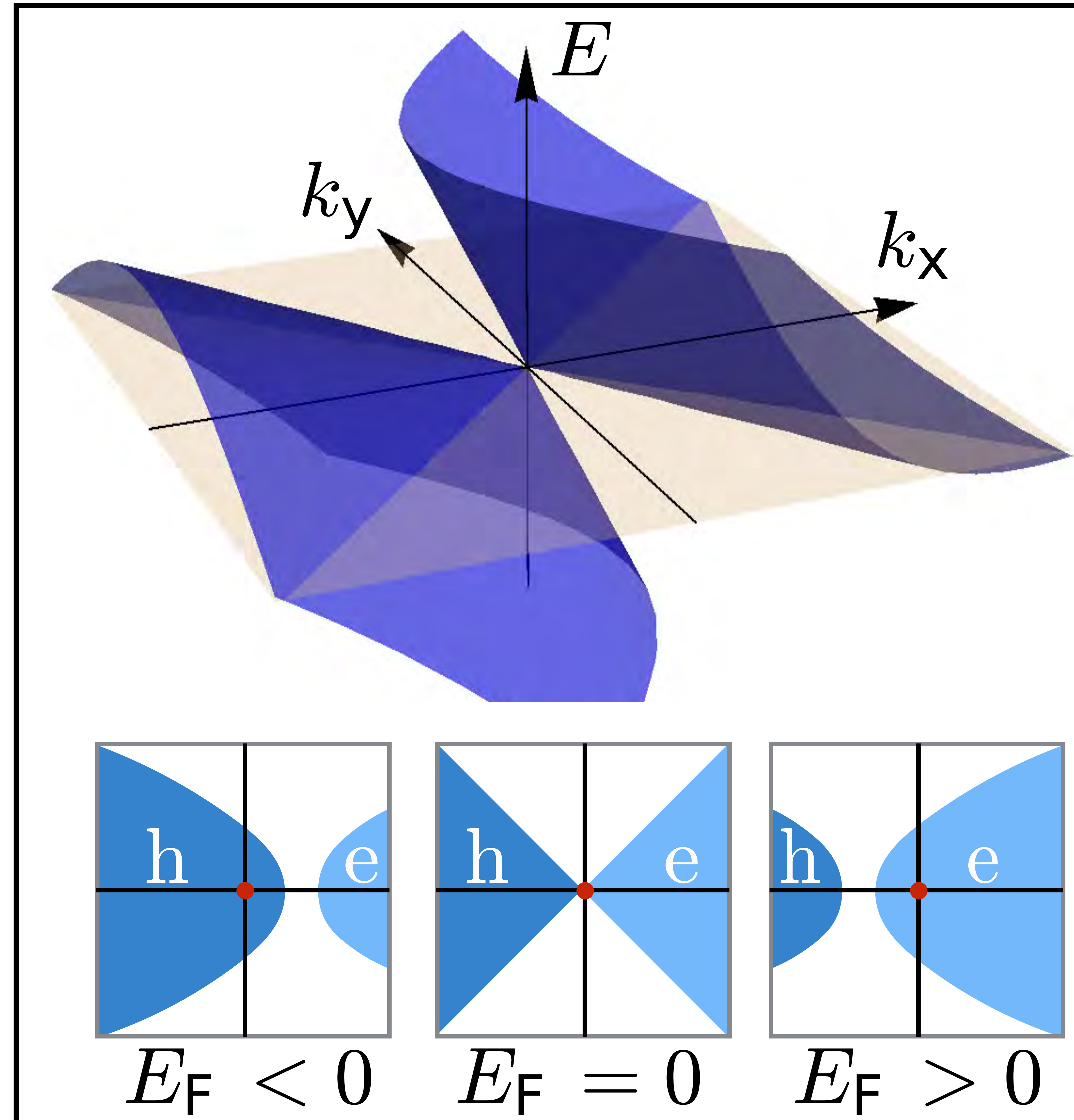
Material examples

- New class of band-inverted topological semimetals
- Band inversion of orthogonal screw representations leads to robust Dirac crossing along ΓX
- Type-II Dirac cones



Type-II Dirac fermions

- Dirac cone tilts over to produce electron- and hole-like Fermi surfaces
- Only Fermi-surfaces that encircle the Dirac node carry Berry phase of π



$$\mathcal{H}_{\mathrm{II}}(\boldsymbol{k}) = u_x k_x \sigma_0 + v_x k_x \sigma_1 + v_y k_y \sigma_2$$

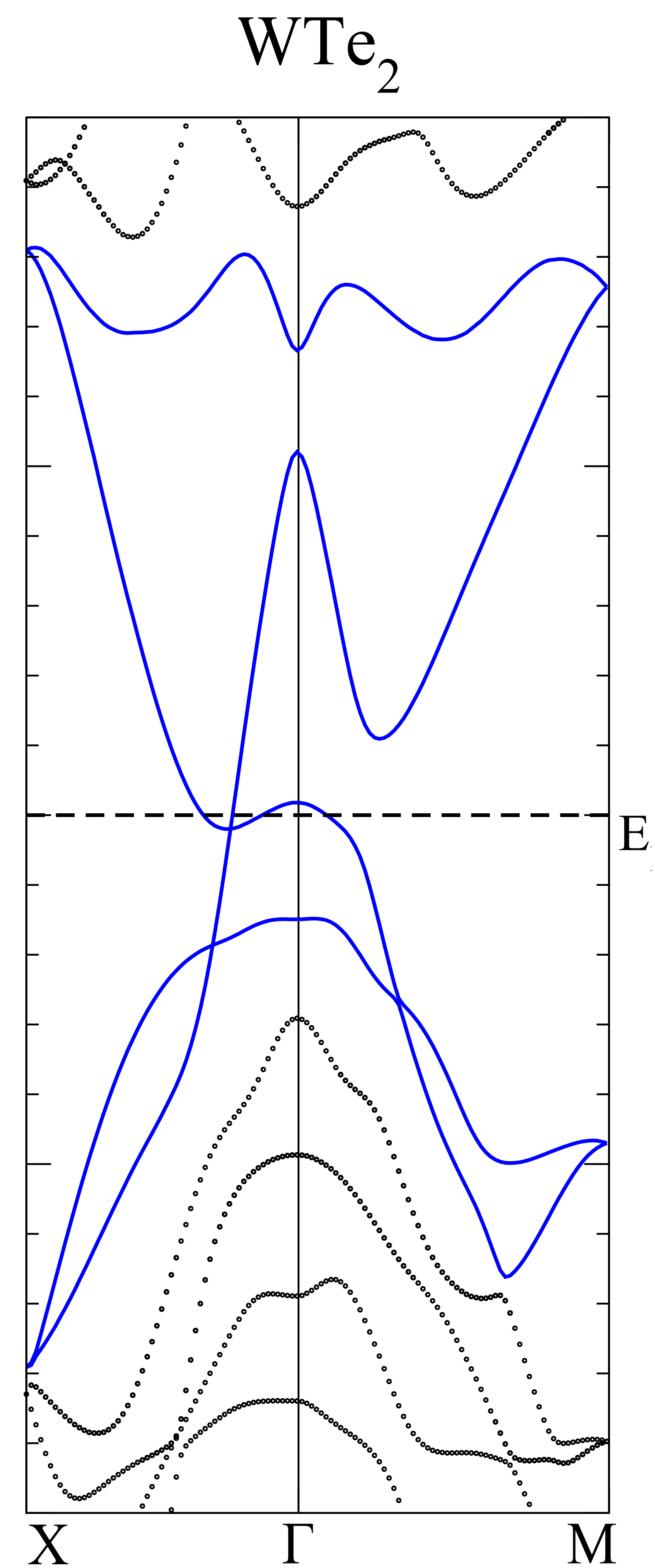
Topological classification

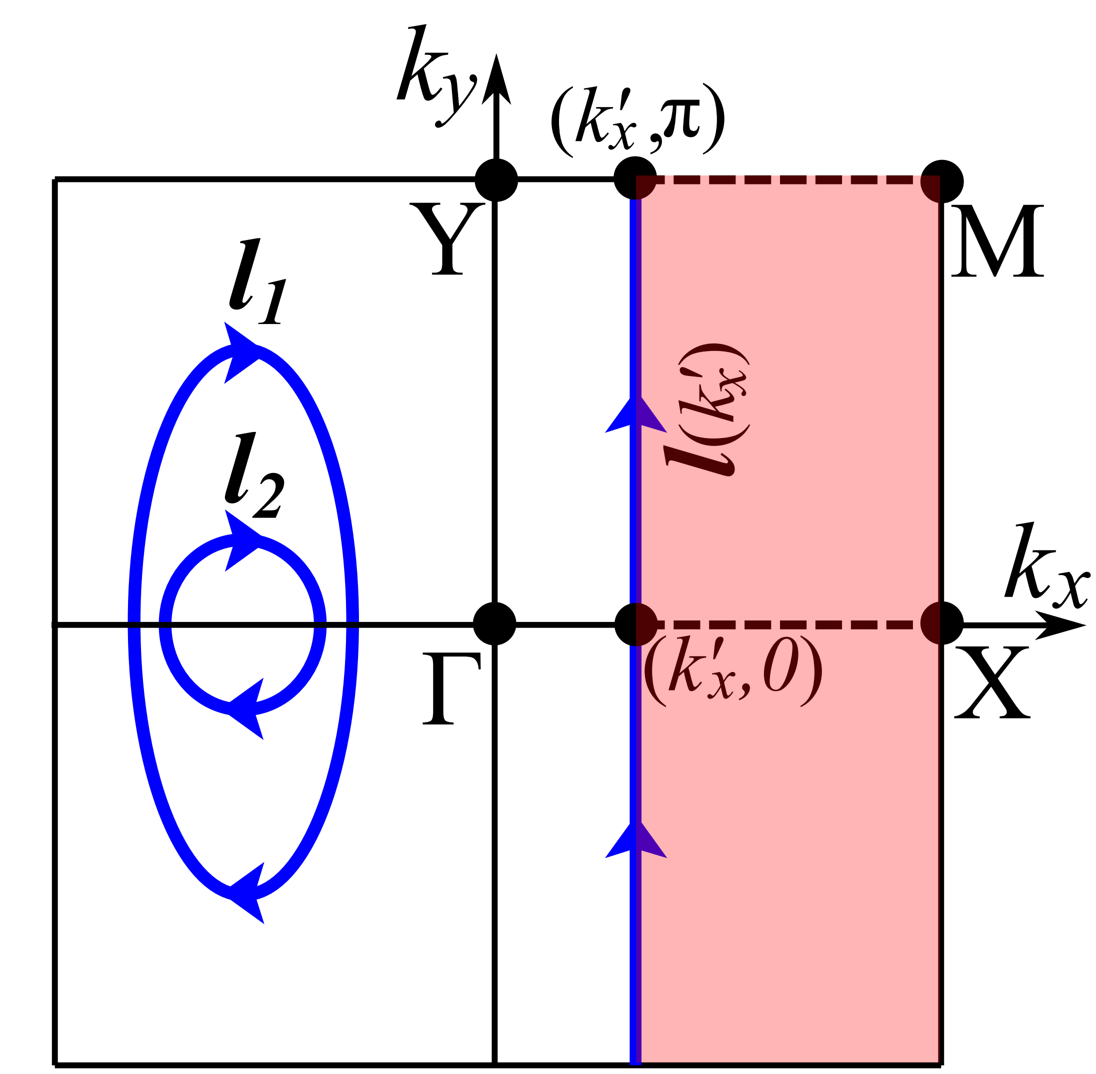
$$\mathcal{W}[l] = \overline{\exp}\left[-\int_l d\boldsymbol{k}\cdot\boldsymbol{A}(\boldsymbol{k})\right]$$

$$\boldsymbol{A}(\boldsymbol{k})_{ij} = \langle u_{i,\boldsymbol{k}}|\nabla_{\boldsymbol{k}} u_{j,\boldsymbol{k}}\rangle$$

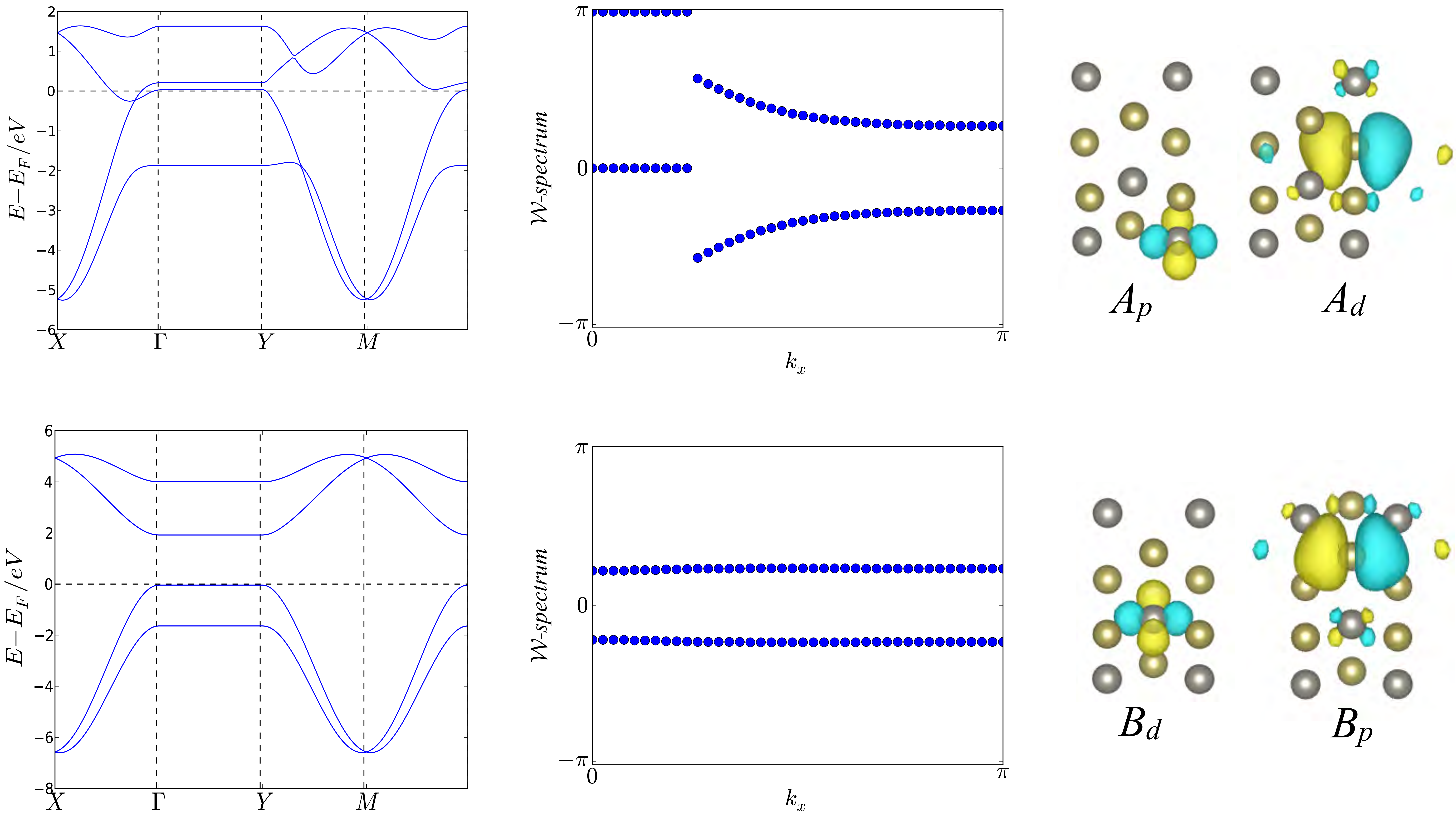
$$e^{i\Phi_{U(1)}[l]} \equiv \exp\left[-\int_l d\boldsymbol{k}\cdot \mathrm{Tr}[\,\boldsymbol{A}(\boldsymbol{k})\,]\right] = \det[\,\mathcal{W}[l]\,]$$

$N_{+,\boldsymbol{k}_1}$	$N_{-,\boldsymbol{k}_2}$	$\mathcal{W}(k_x)$	$\bar{D}_{l(k_x)}$	$D_{\boldsymbol{k}_1} - D_{\boldsymbol{k}_2}$ mod 2
1	1	$[\lambda_1\lambda_1^*]$	0	0
2	1	$[+-]$	1	1
2	0	$[--]$	2	0
2	2	$[++]$	2	0





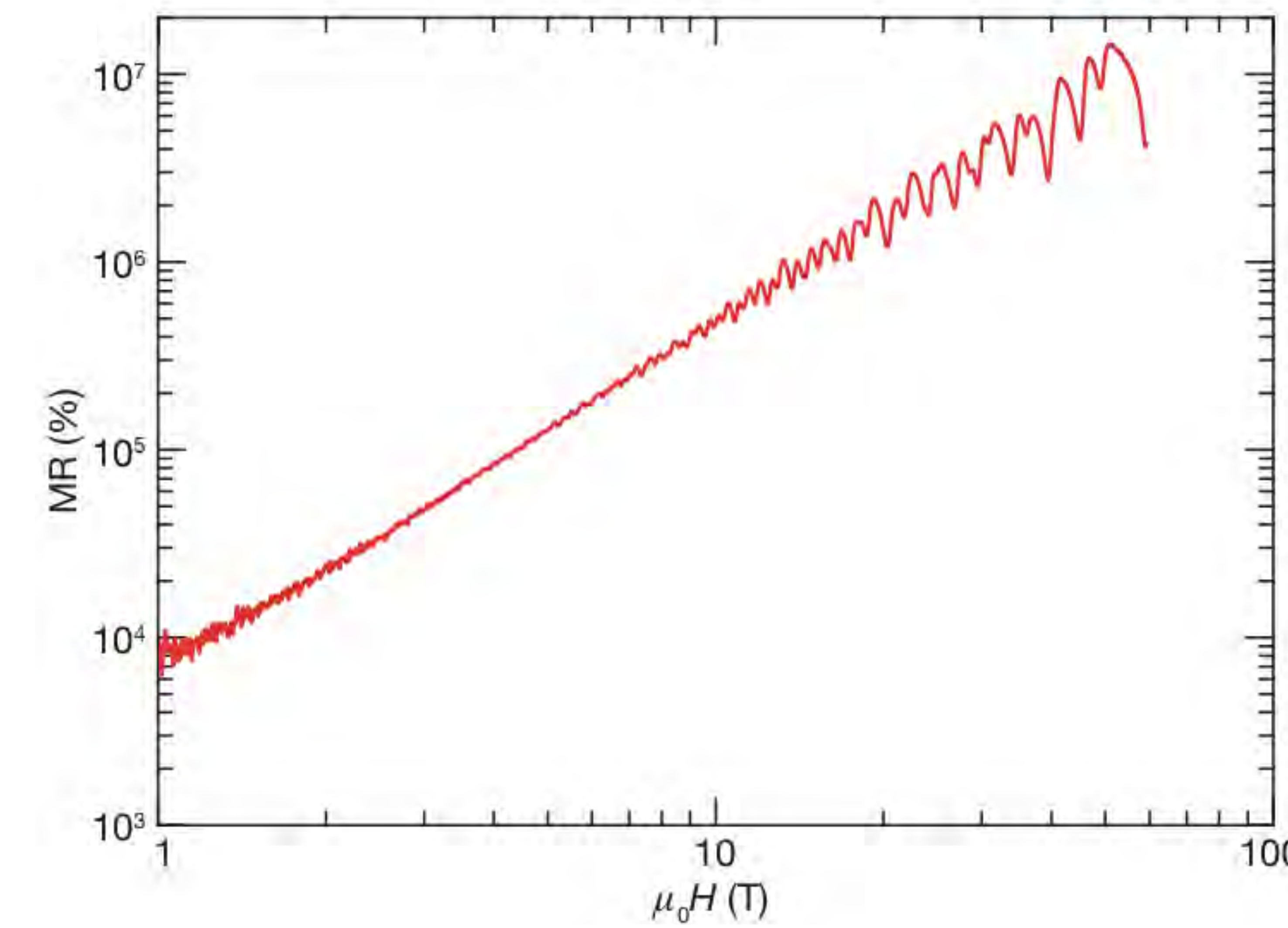
Tight-binding model: WTe_2

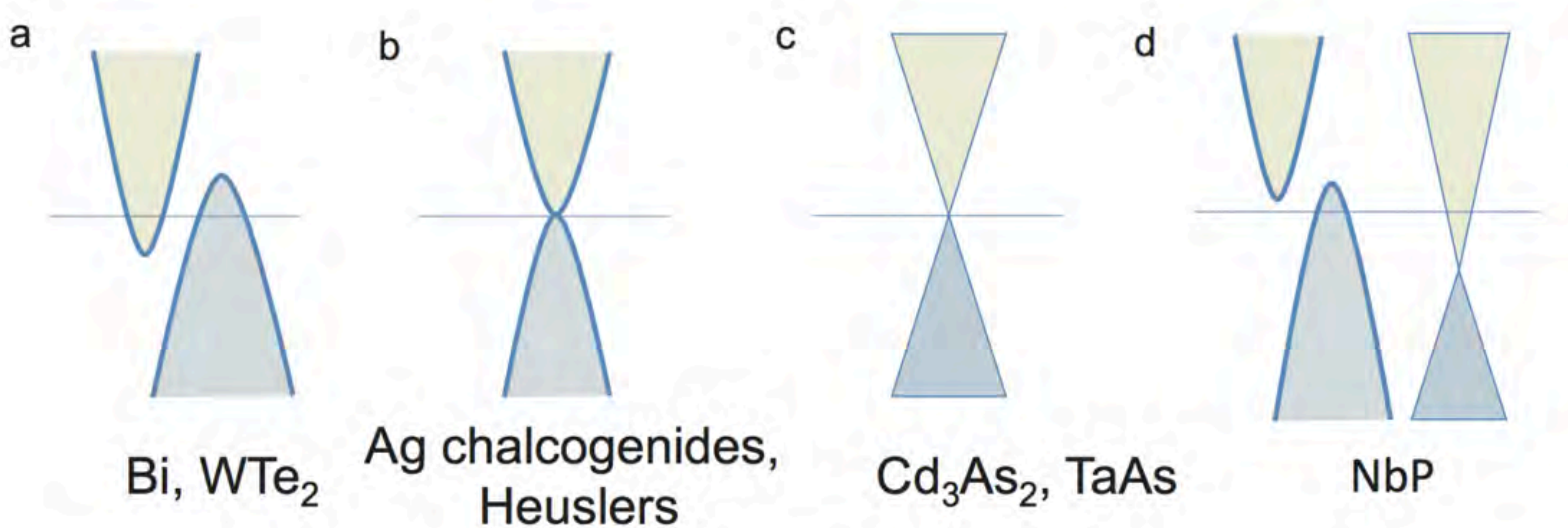


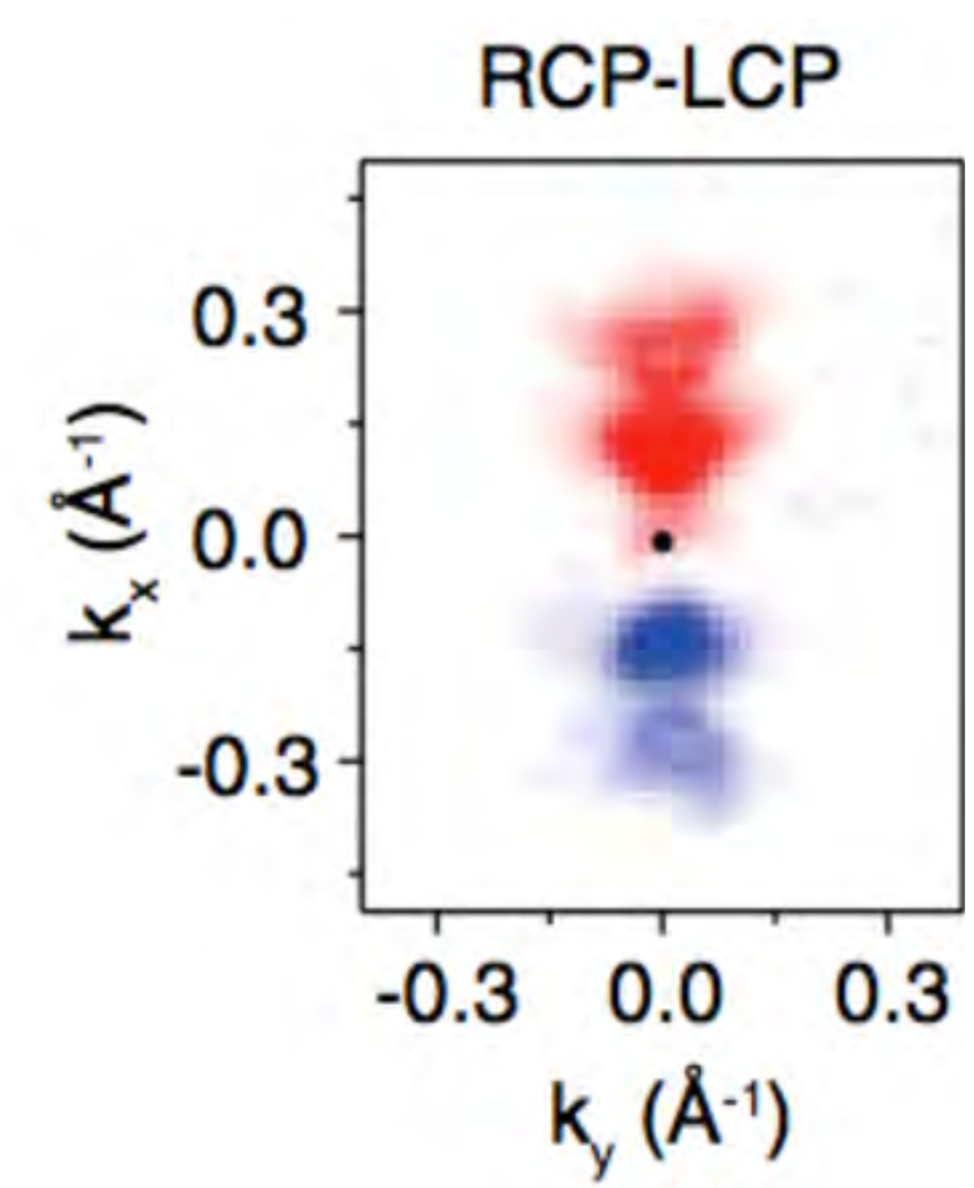
Consequences for 3D material

WTe$_2$: ludicrous magnetoresistance

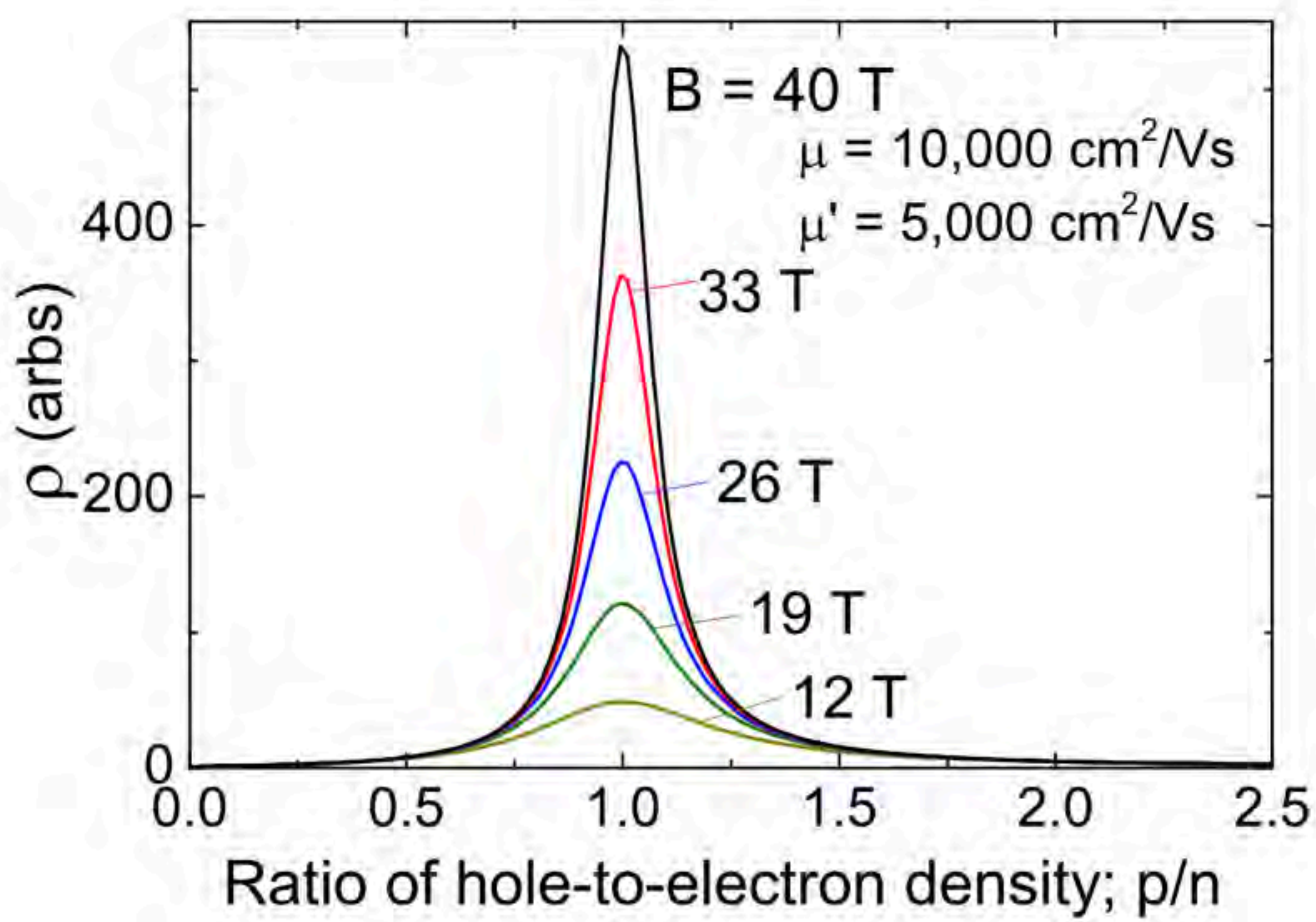
- 1.7 x 10^6 % at 2K and 9T
- Mobilities up to 167 000 cm^2/Vs
- (compensated) electron and hole pockets
- Circular Dichroism in ARPES experiments

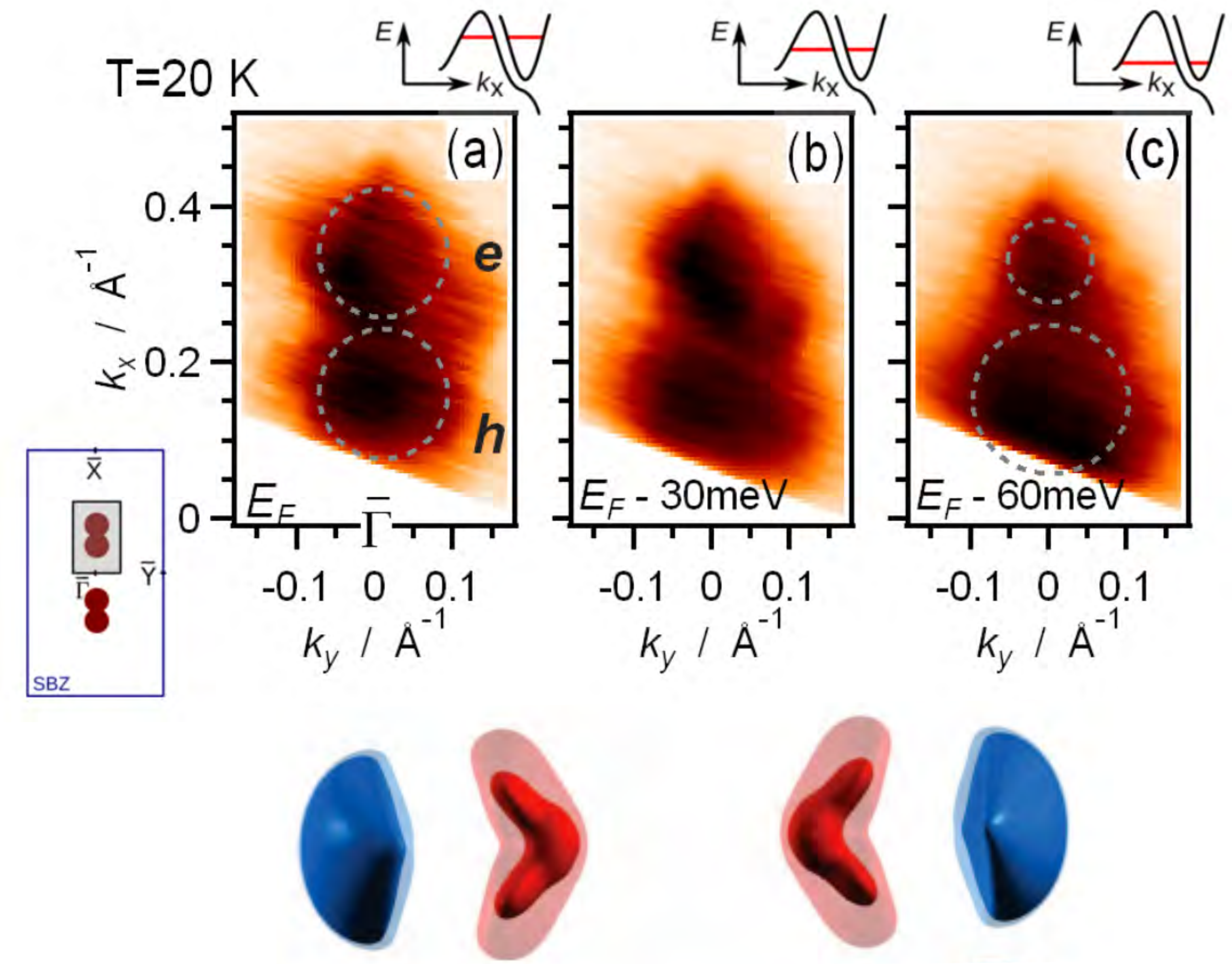






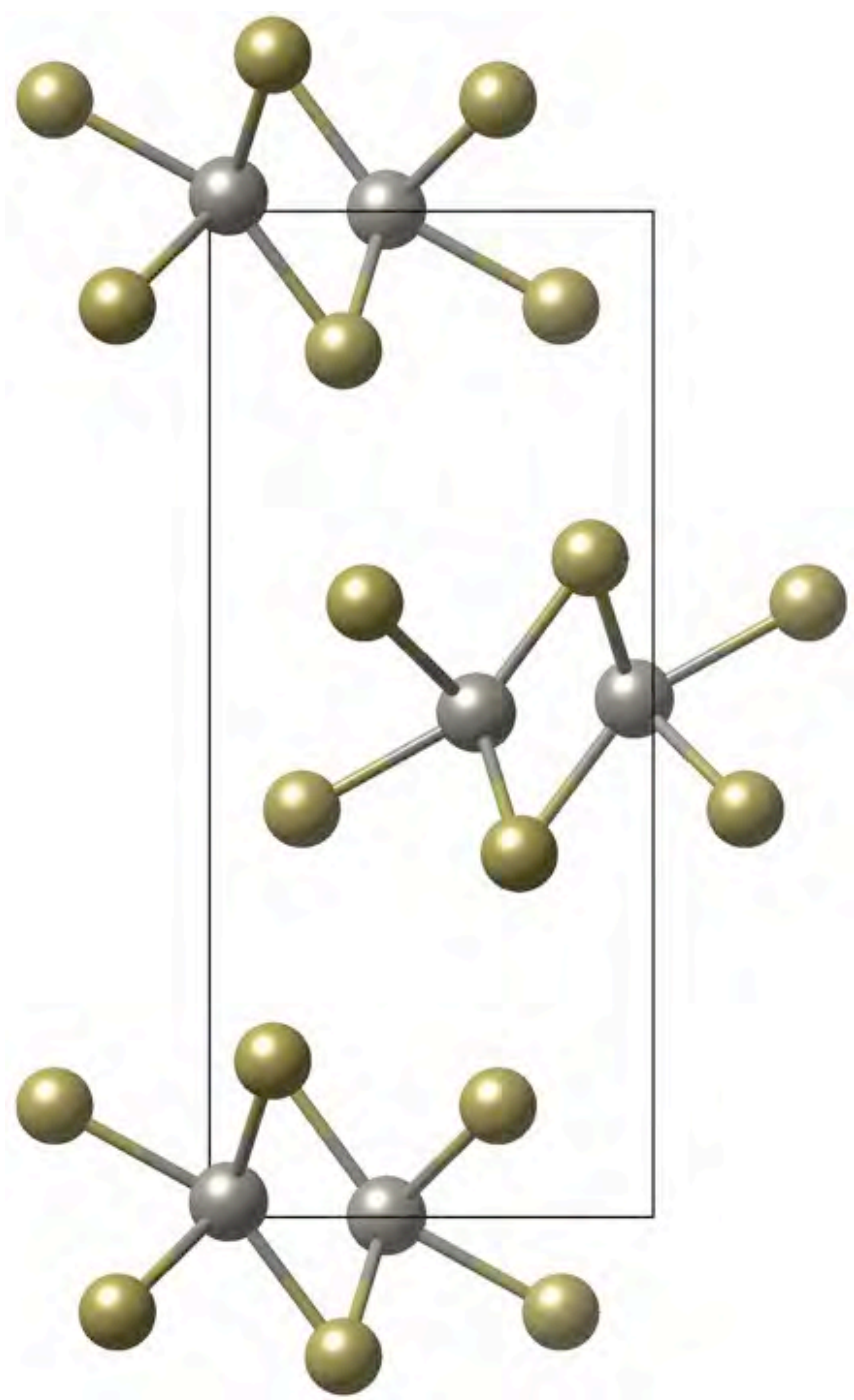
High-MR theory

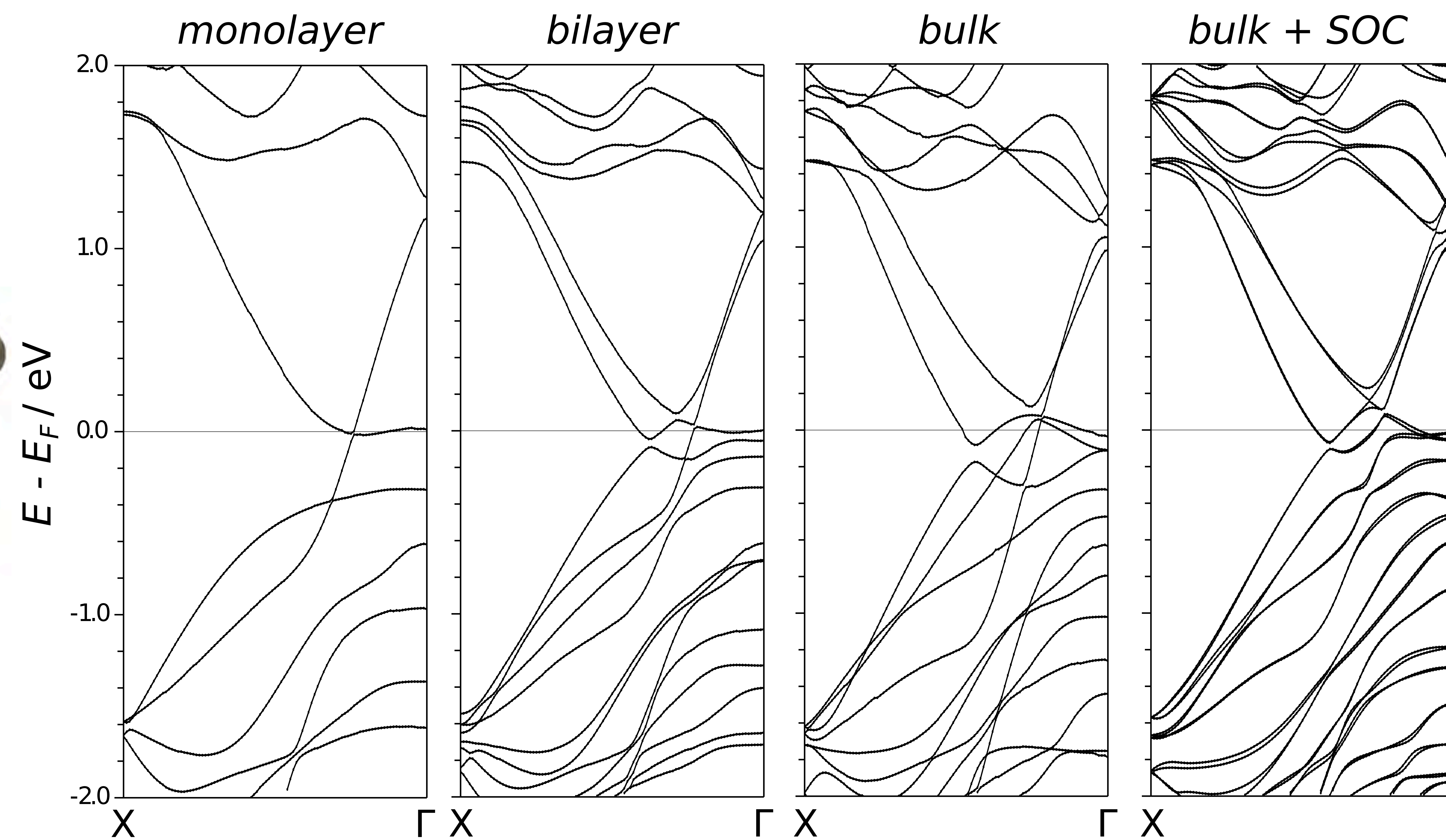




$$[\rho(H) - \rho(0)]/\rho(0) \ = \ \mu_e \mu_h B^2$$

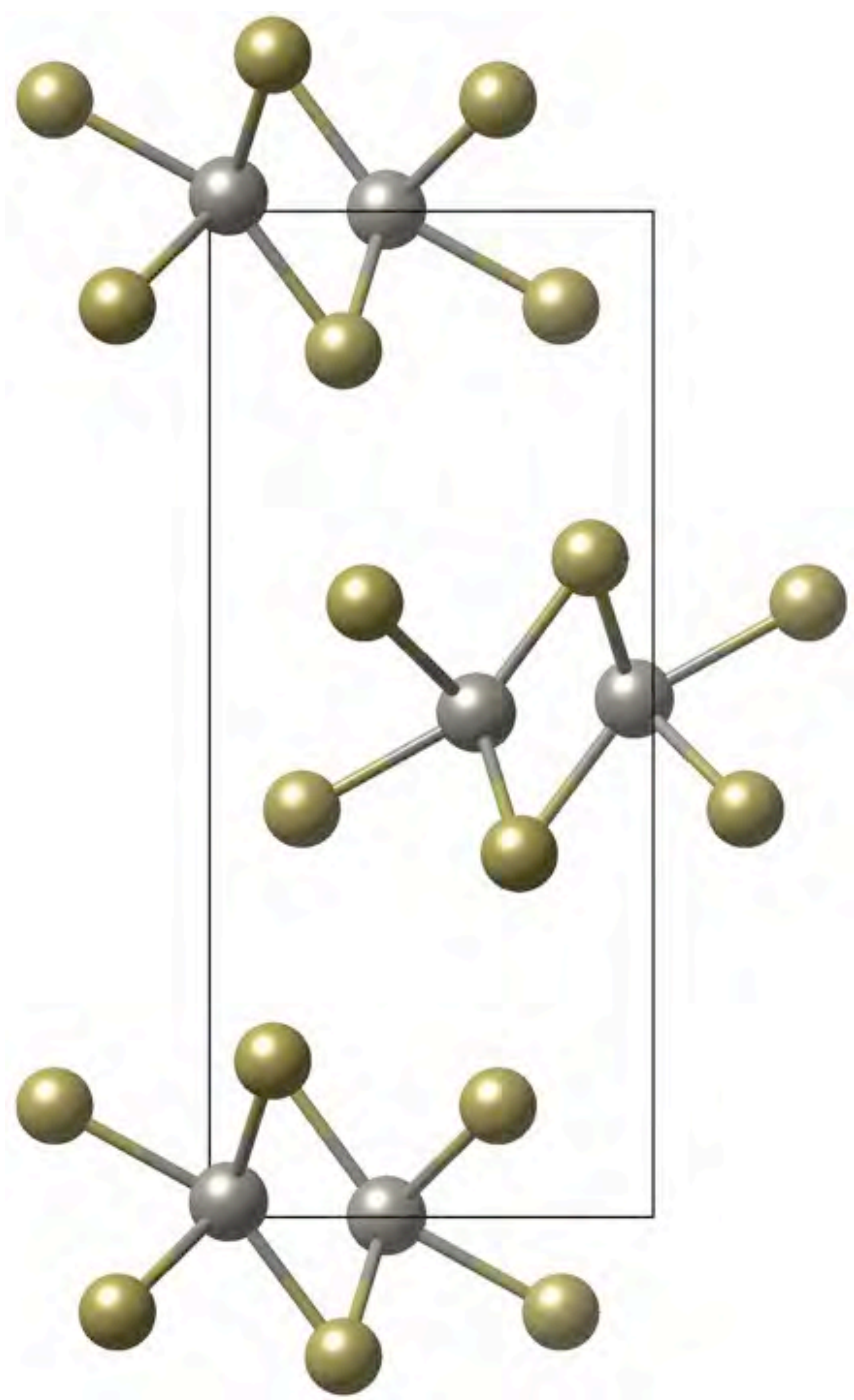
WTe_2 / $MoTe_2$

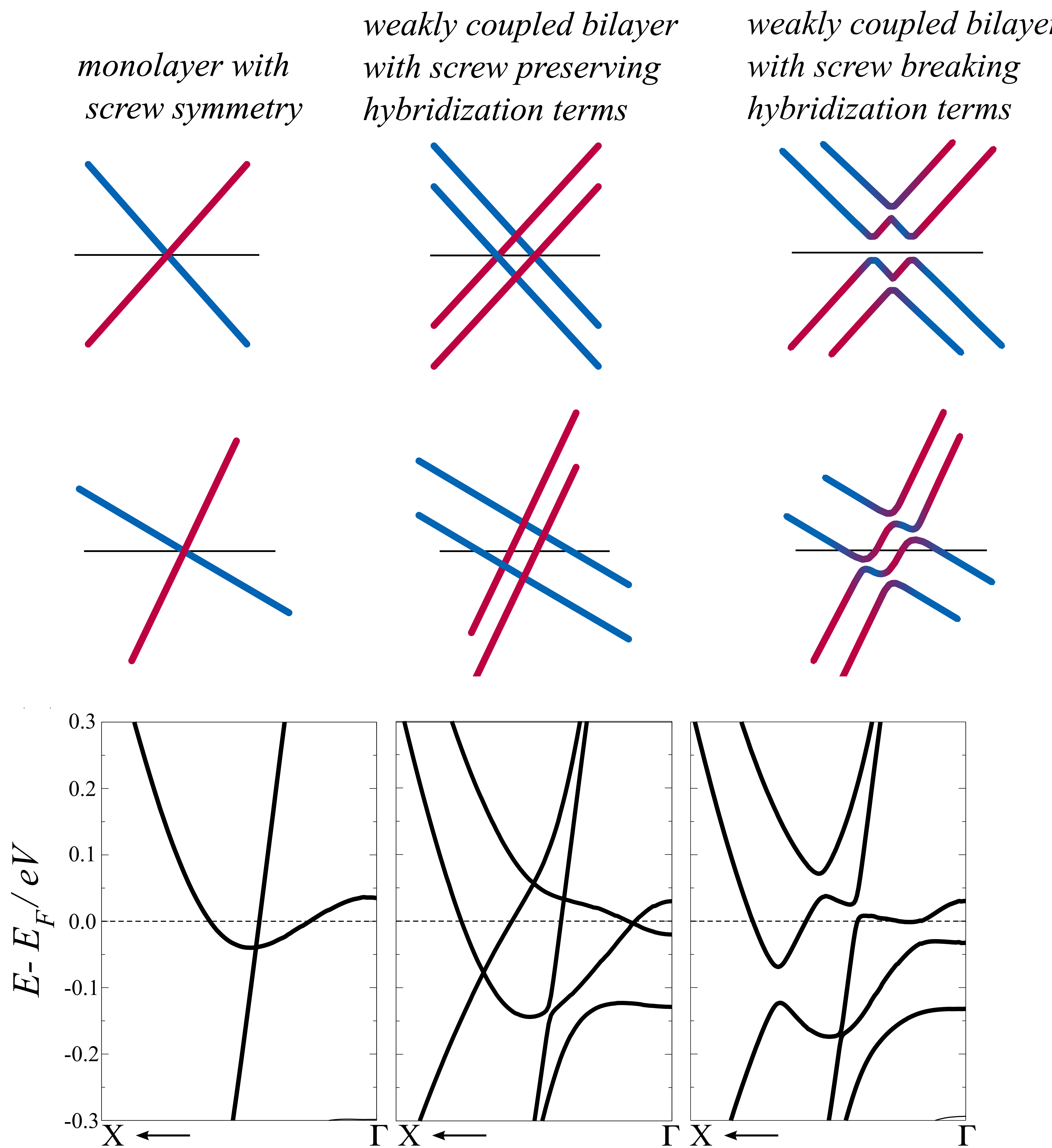




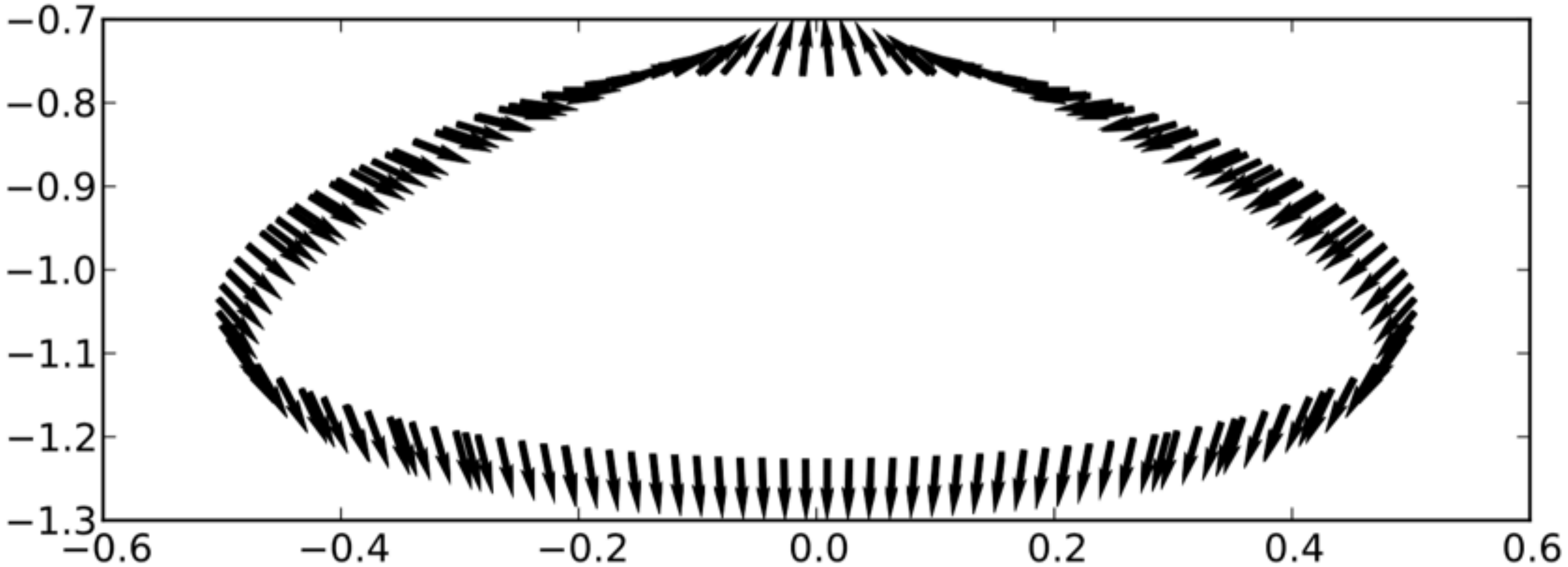
monolayer
bilayer
bulk
bulk + SOC
E - E_F / eV
2.0
1.0
0.0
-1.0
-2.0
X
Γ
X
Γ
X
Γ
X
Γ

Electron and hole pockets

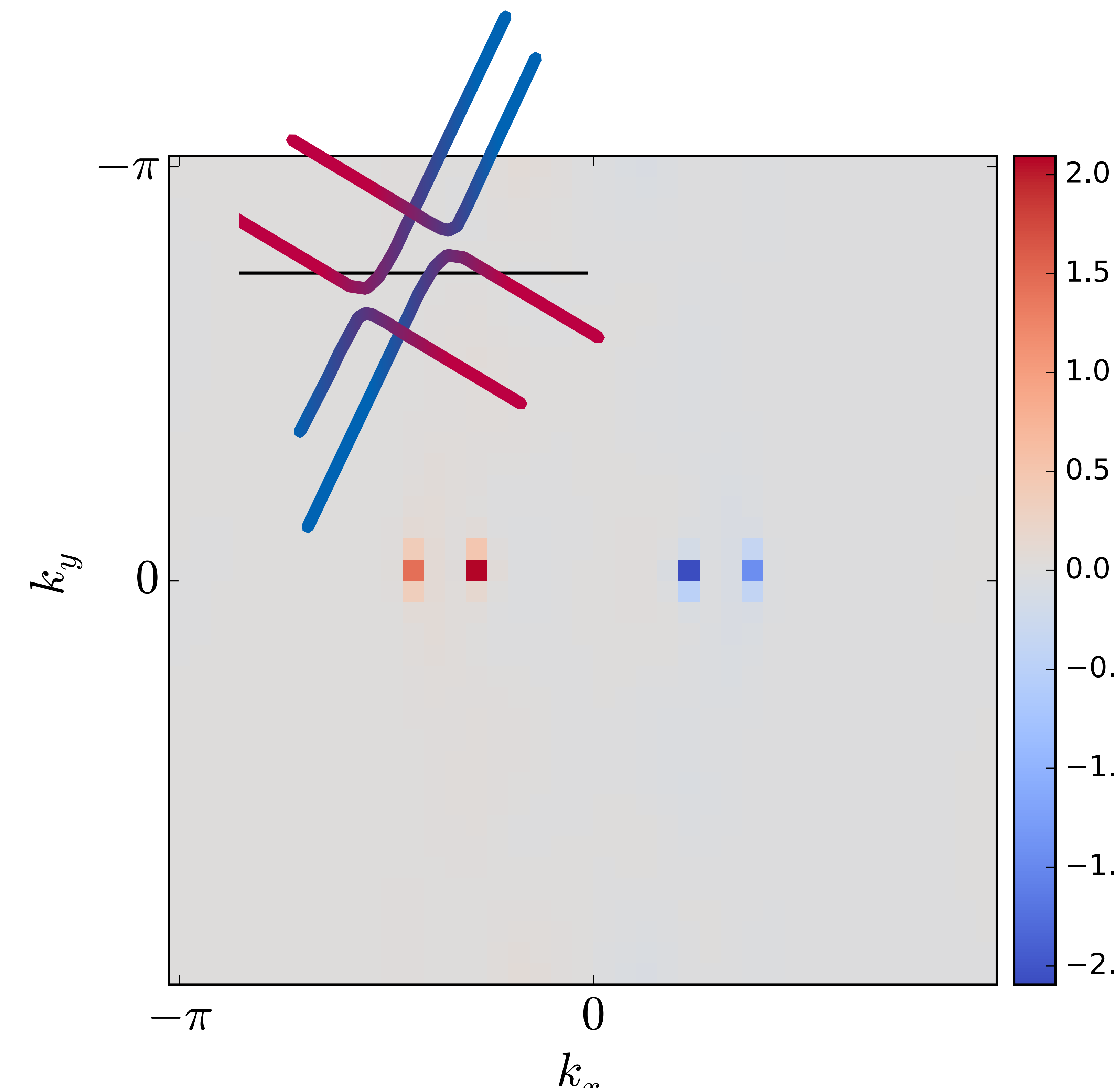




Consequences: transport



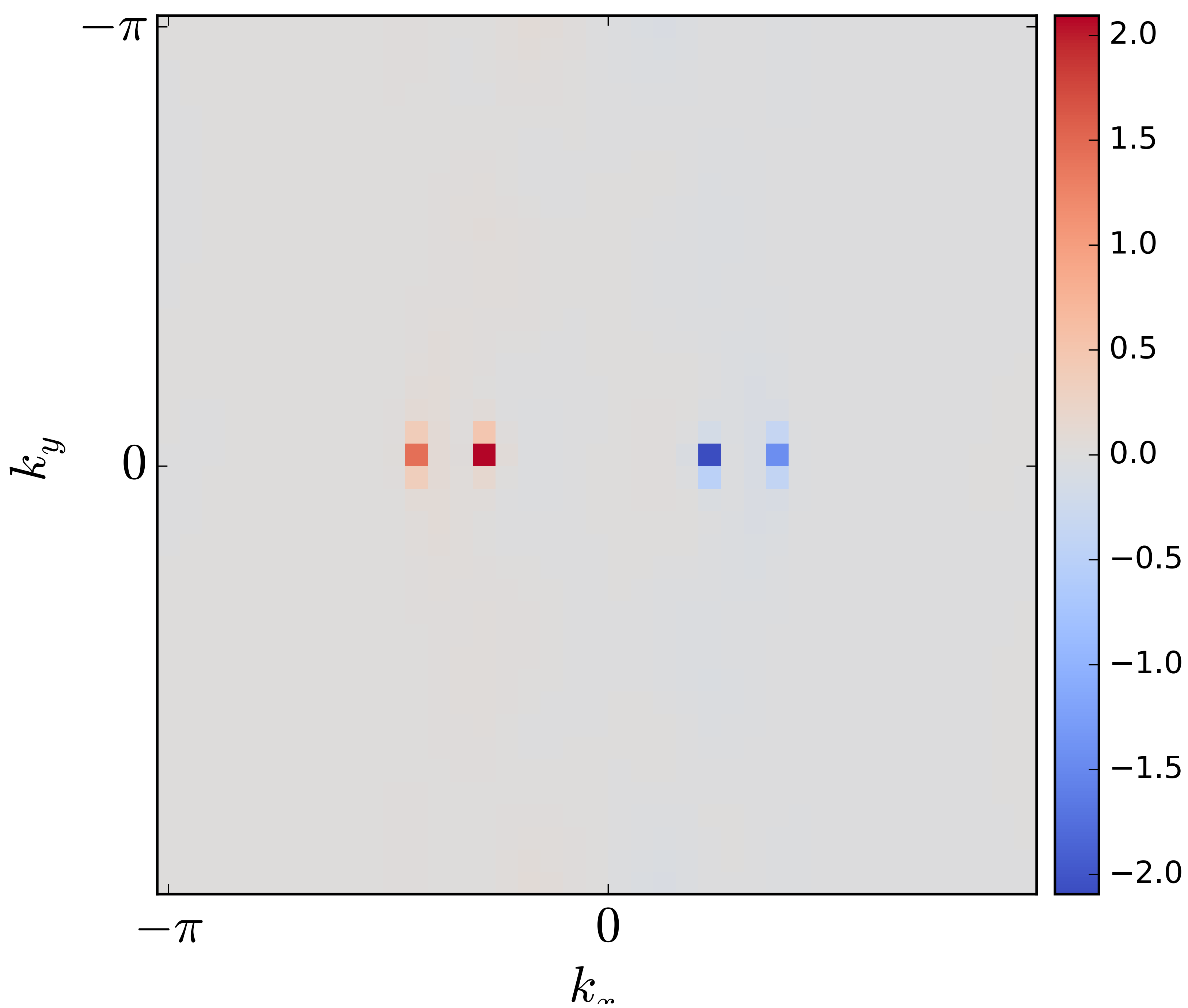
Pseudospin winding in monolayer



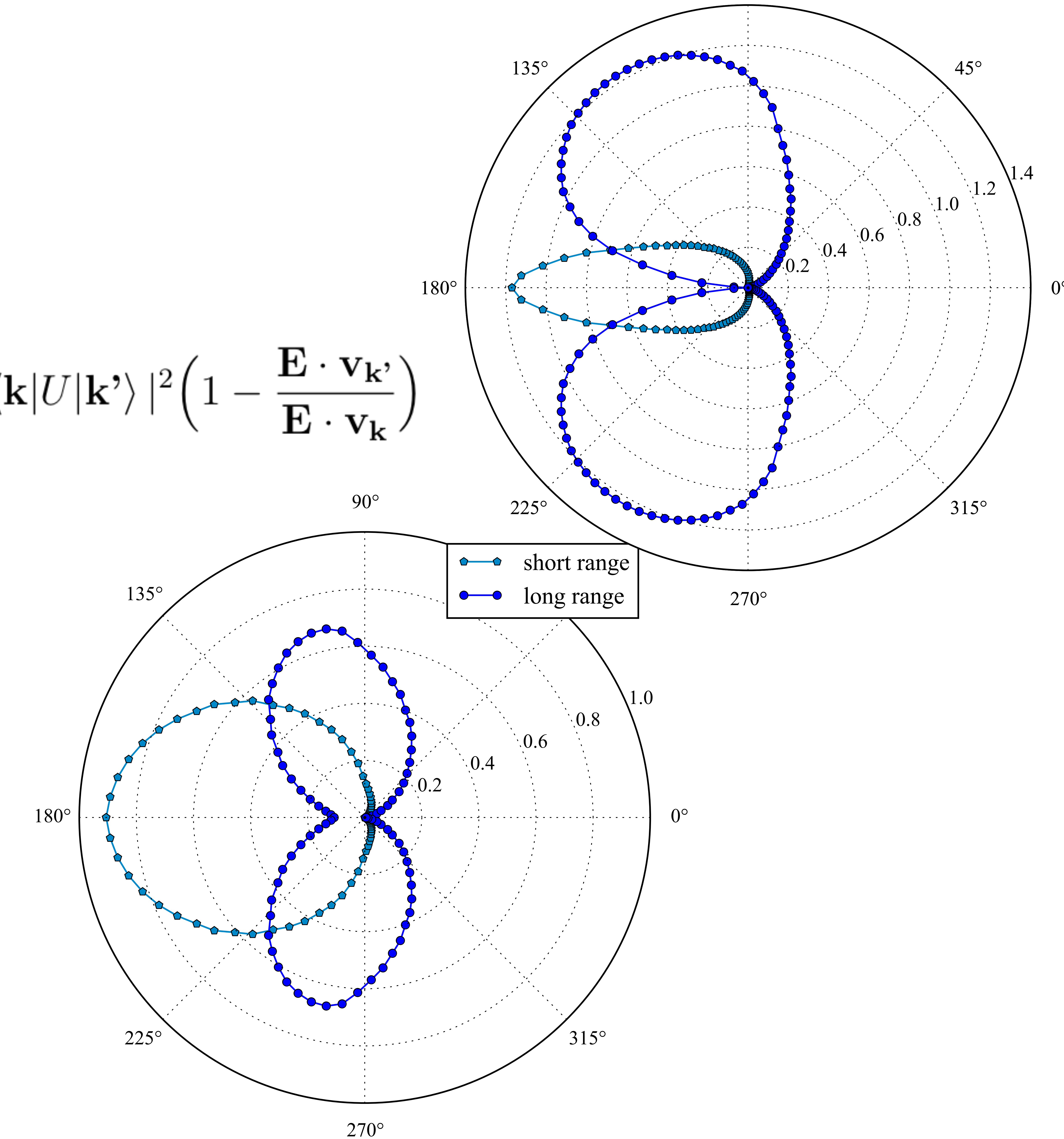
Berry curvature around electron and hole pockets in bilayer WTe_2

Consequences: transport

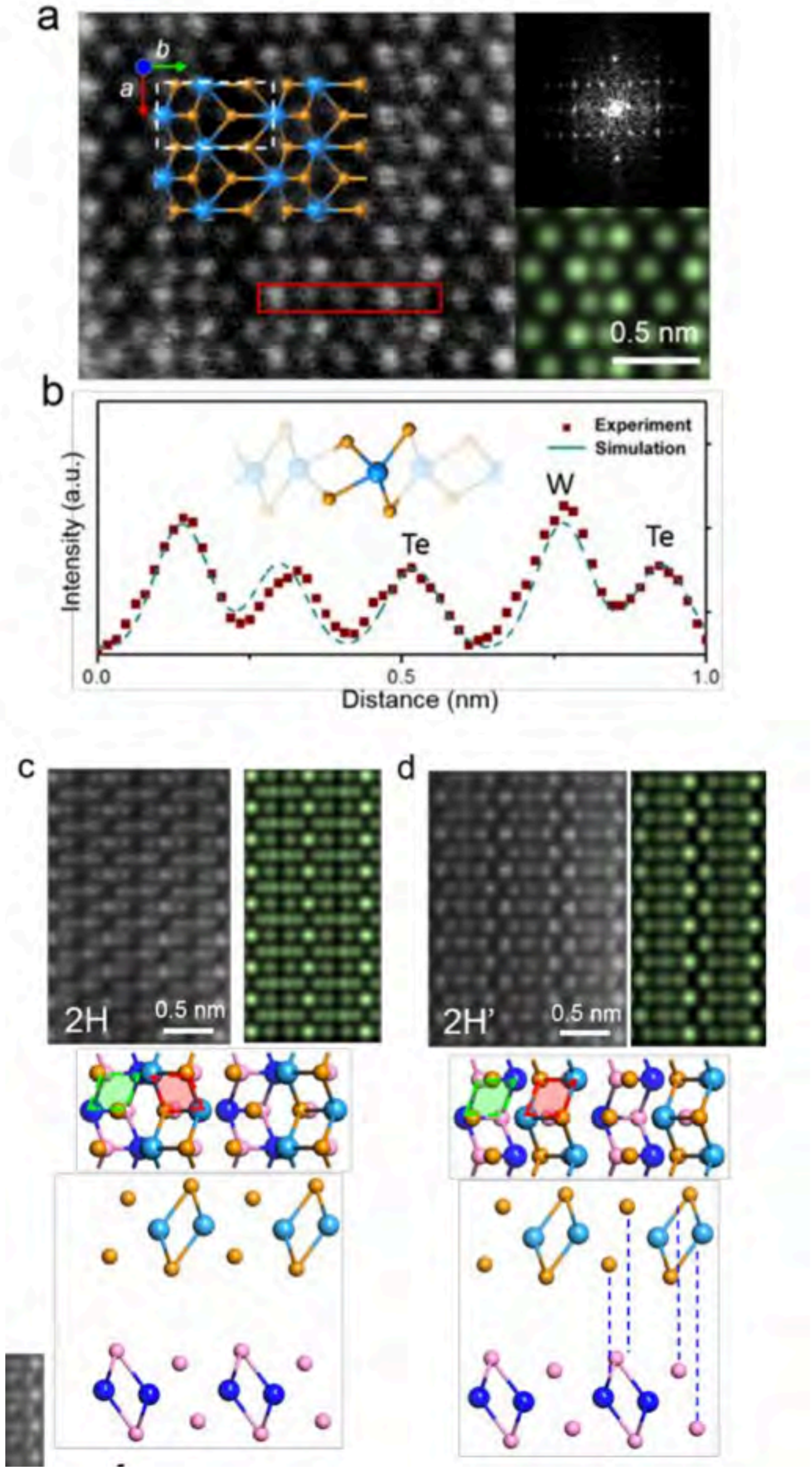
Berry curvature around electron and hole pockets in bilayer WTe_2

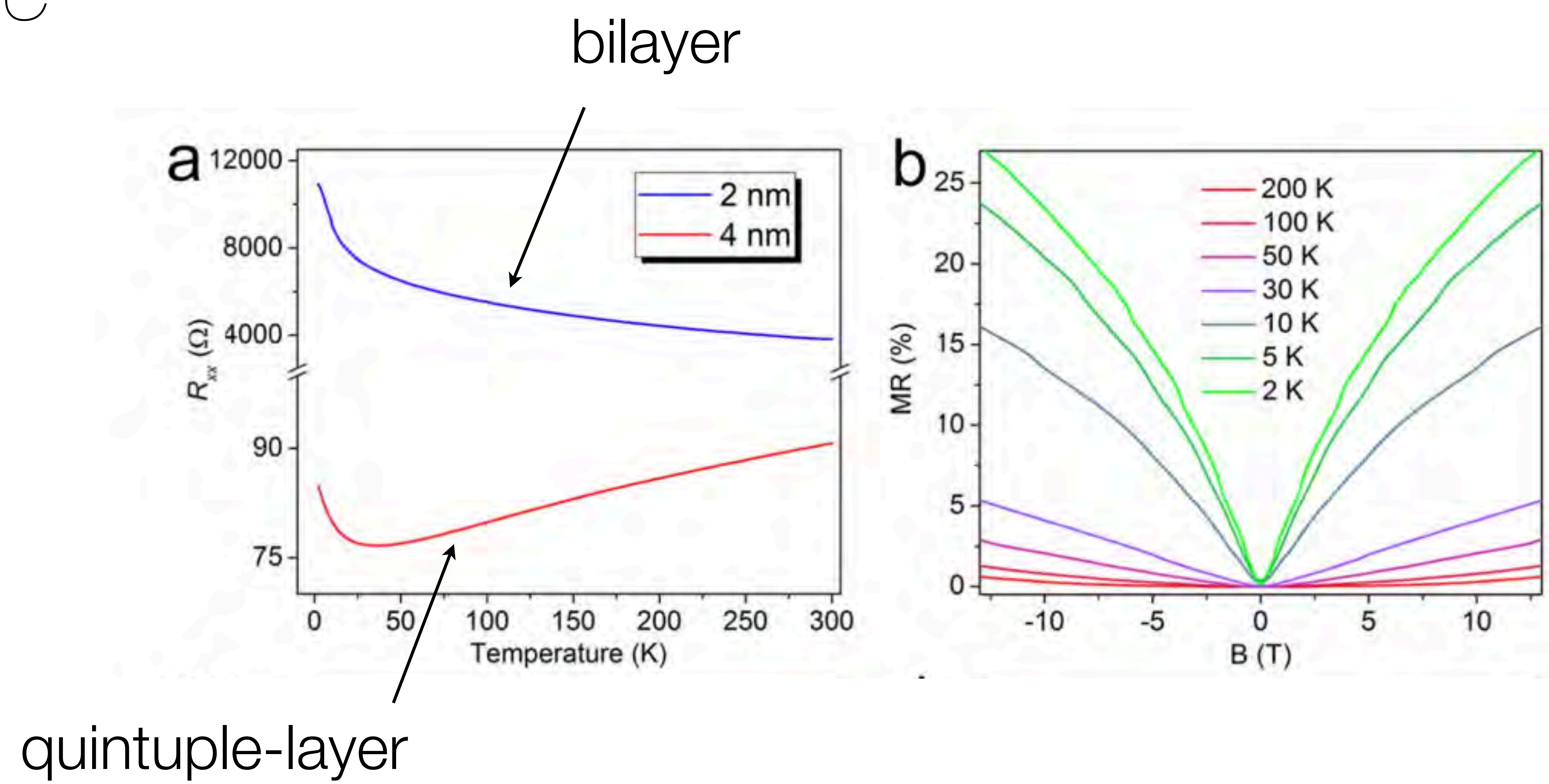


$$\langle \mathbf{k}|U|\mathbf{k'}\rangle\,|^2\left(1-\frac{\mathbf{E}\cdot\mathbf{v_{k'}}}{\mathbf{E}\cdot\mathbf{v_k}}\right)$$



Experimental evidence

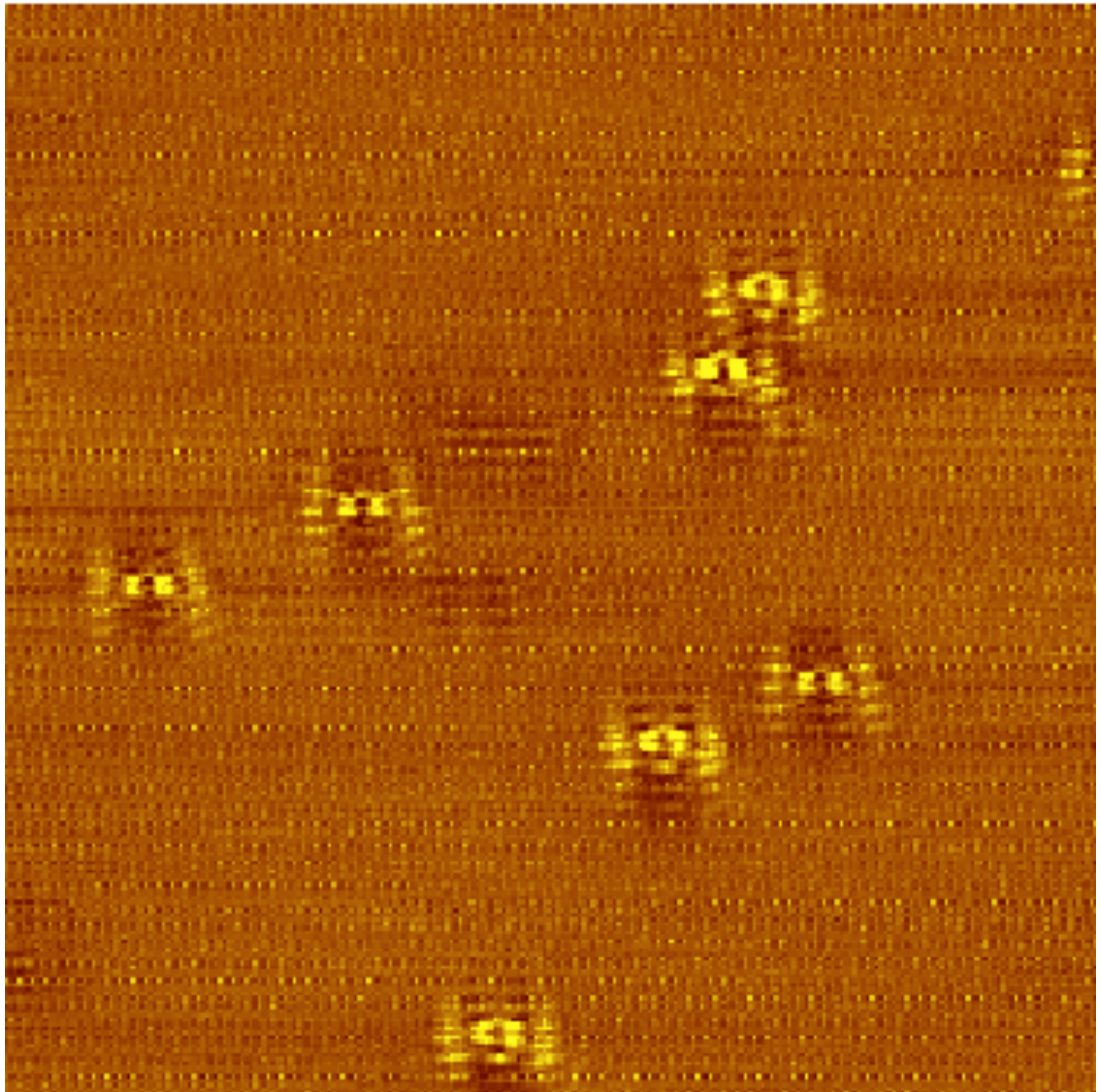




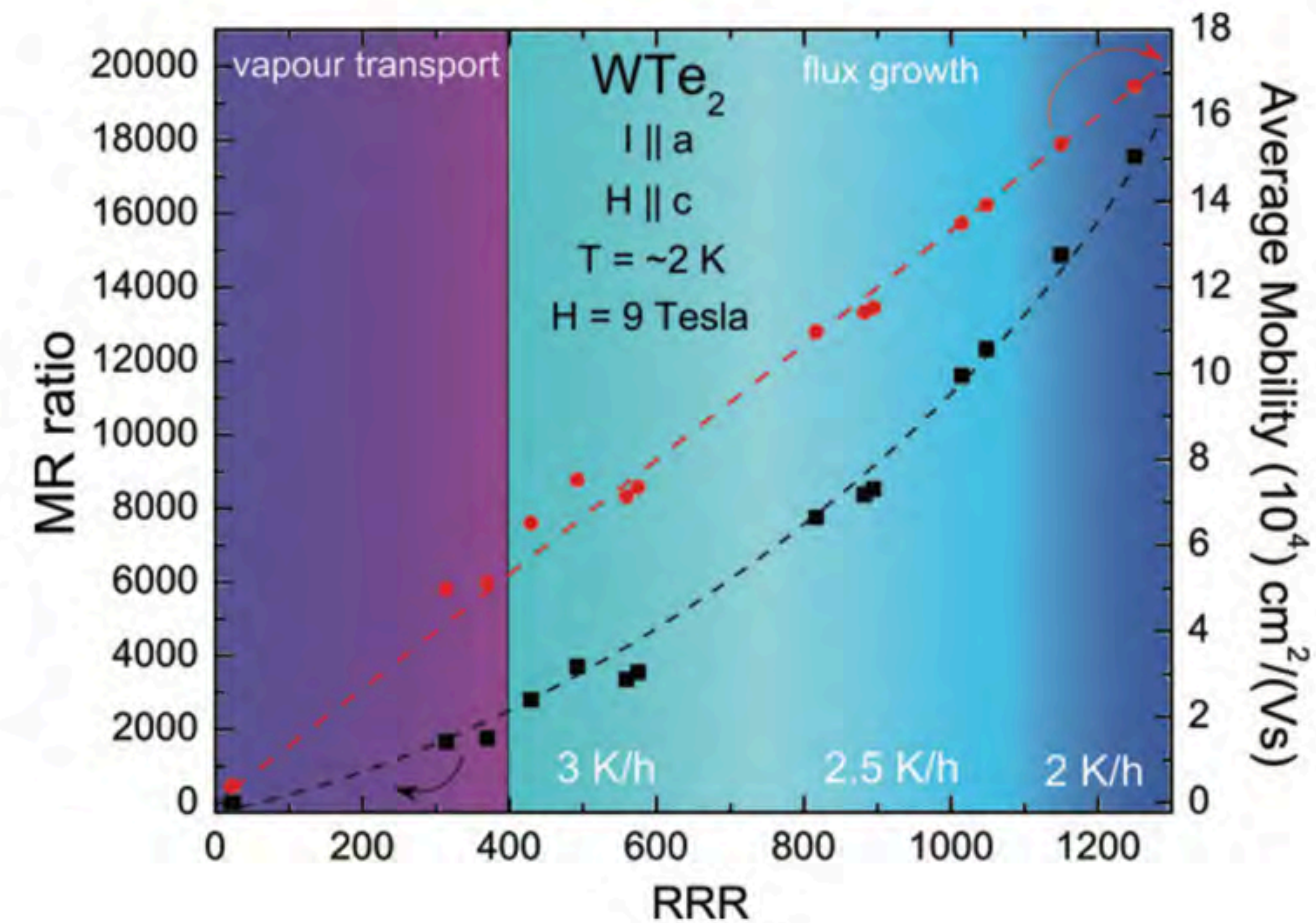
in Fig. 4b. These results show that large and non-saturating magnetoresistance is preserved in our CVD-grown WTe_2 even down to a bilayer sample, which further demonstrates their high quality. The MR reaches a maximum value of 28% at 2 K. For the thick WTe_2 flakes (12 nm), the MR is about 2000% at 25K in a field of 10T, which is shown in Supplementary Fig. S16. These values

arxiv:1606.00126

Experimental evidence



30 x 30 nm (Yazdani group)

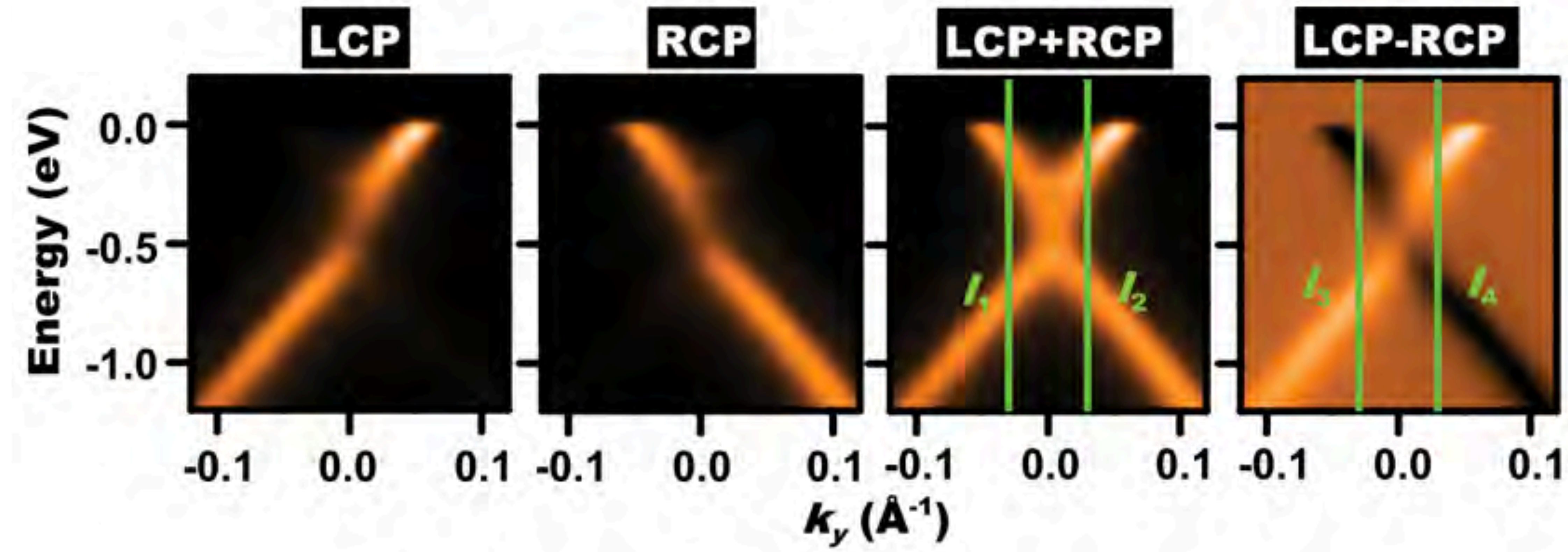


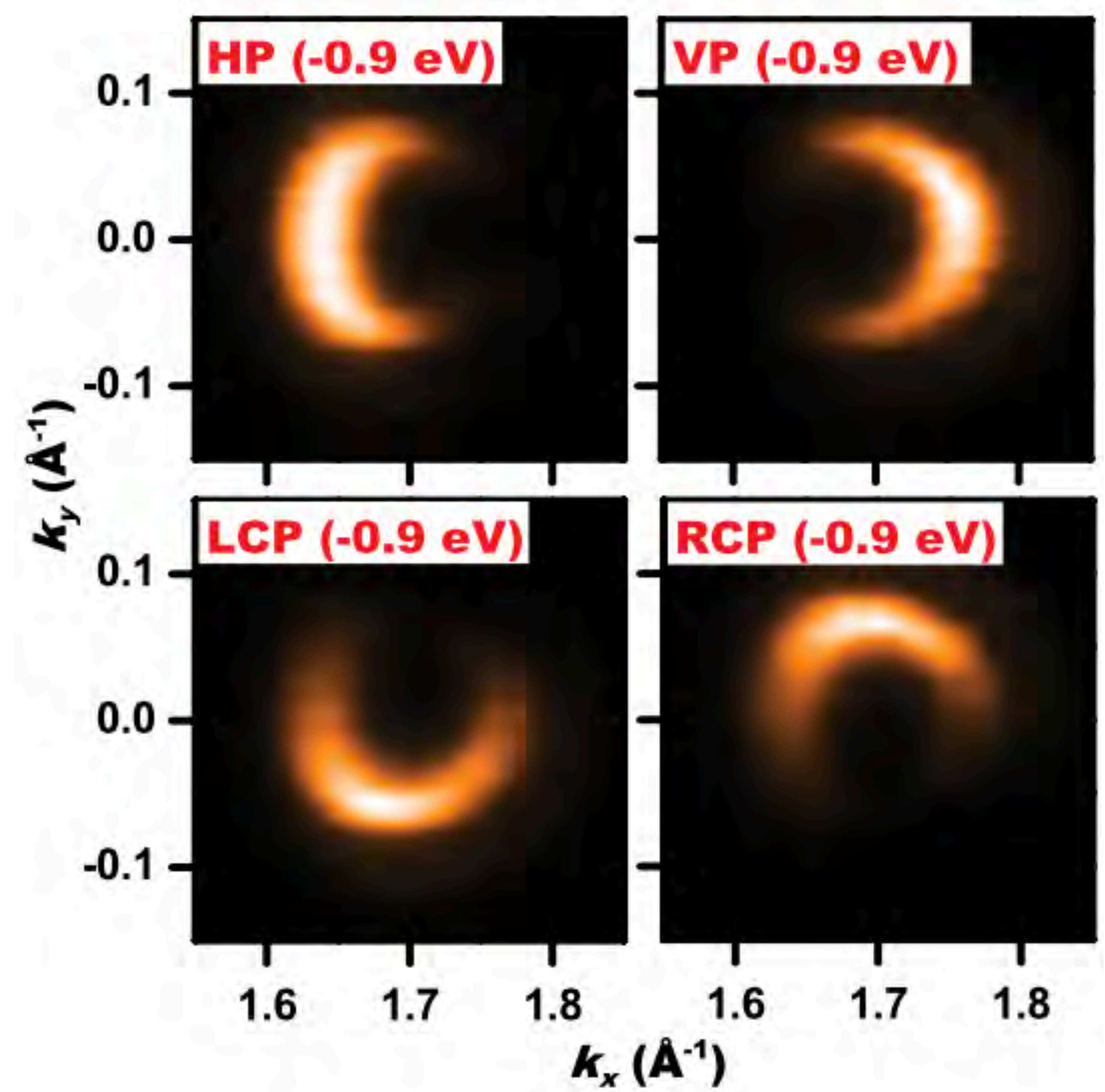
Circular Dichroism

- phase sensitive tool to probe electronic structure
- Can capture effects of Berry's Phase
- $I_{\boldsymbol{\lambda}}(\boldsymbol{k}, E_{\text{kin}}, \hbar\omega)$

  $$\propto \sum_{i,f} |P^{if}_{\boldsymbol{\lambda}}(\boldsymbol{k})|^2 \delta(E_f - E_i - \hbar\omega)\ \delta(E_{\text{kin}} - [E_f - \phi])$$

- $P^{if}_{\pm}(\boldsymbol{k}) = \boldsymbol{\lambda}_{\pm} \cdot \langle f, \boldsymbol{k}|\boldsymbol{p}|i, \boldsymbol{k}\rangle$
- $D_s(\boldsymbol{k}) \ := \ I_+(\boldsymbol{k}, E_f) \ - \ I_-(\boldsymbol{k}, E_f)$



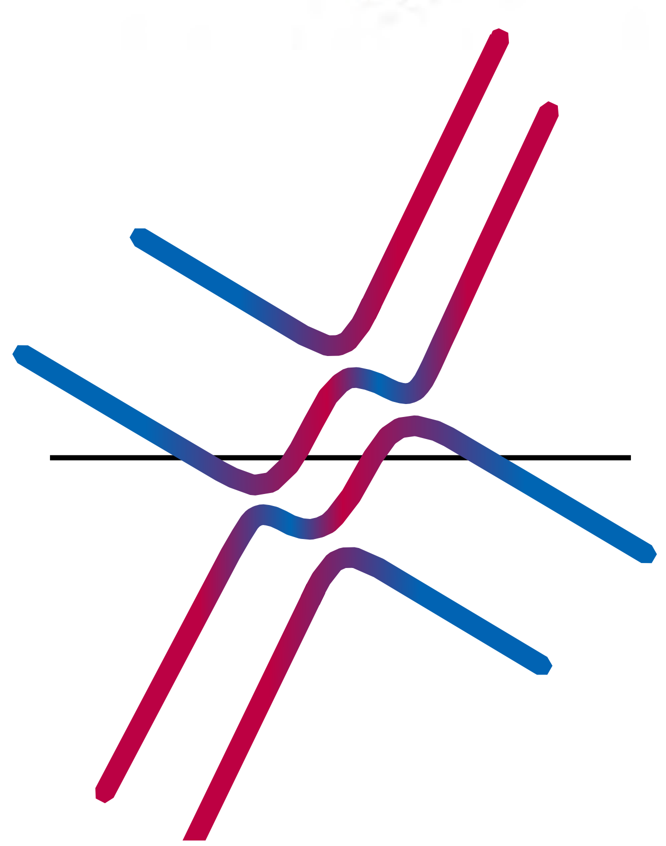


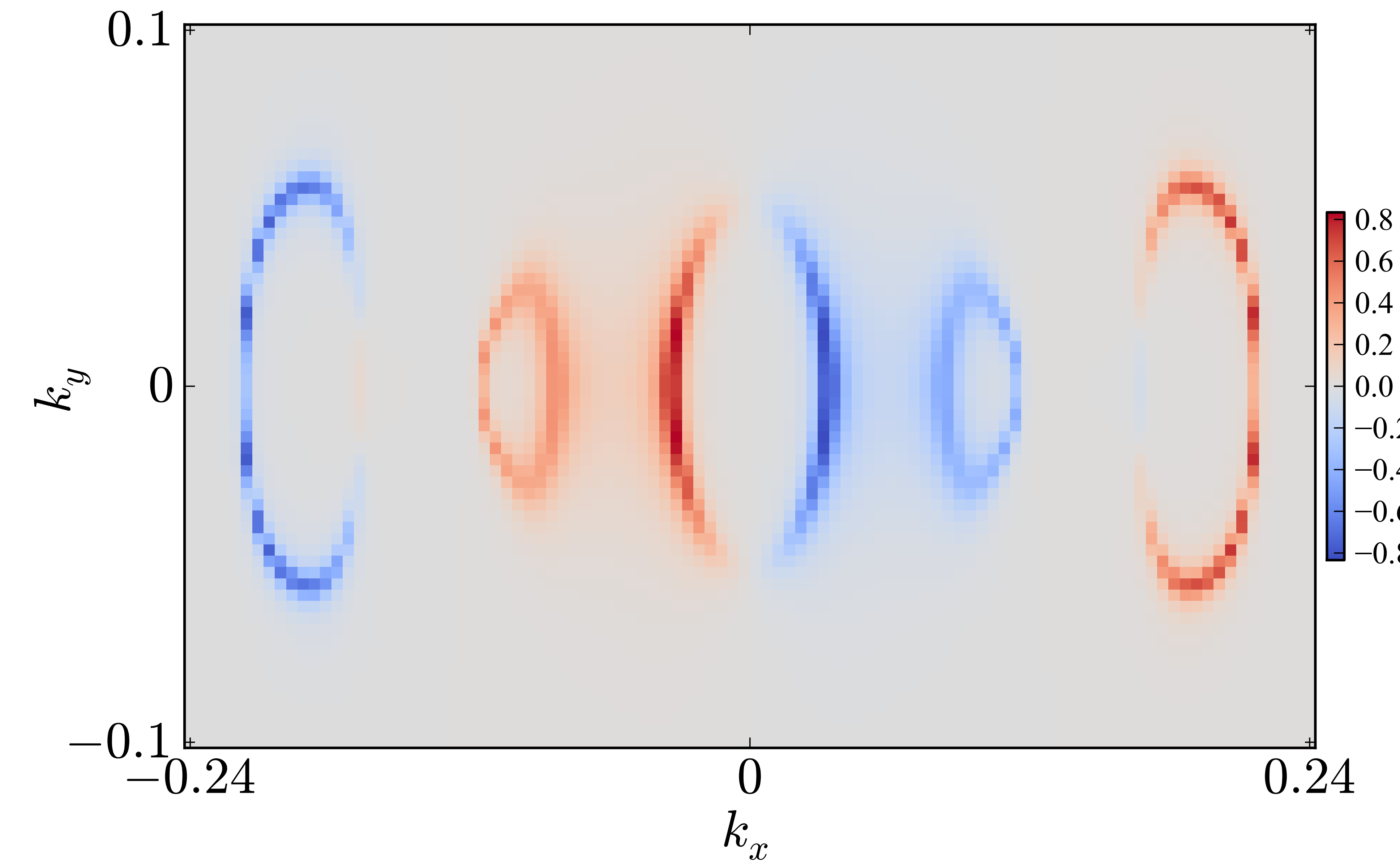
PRL 107, 166803 (2011)

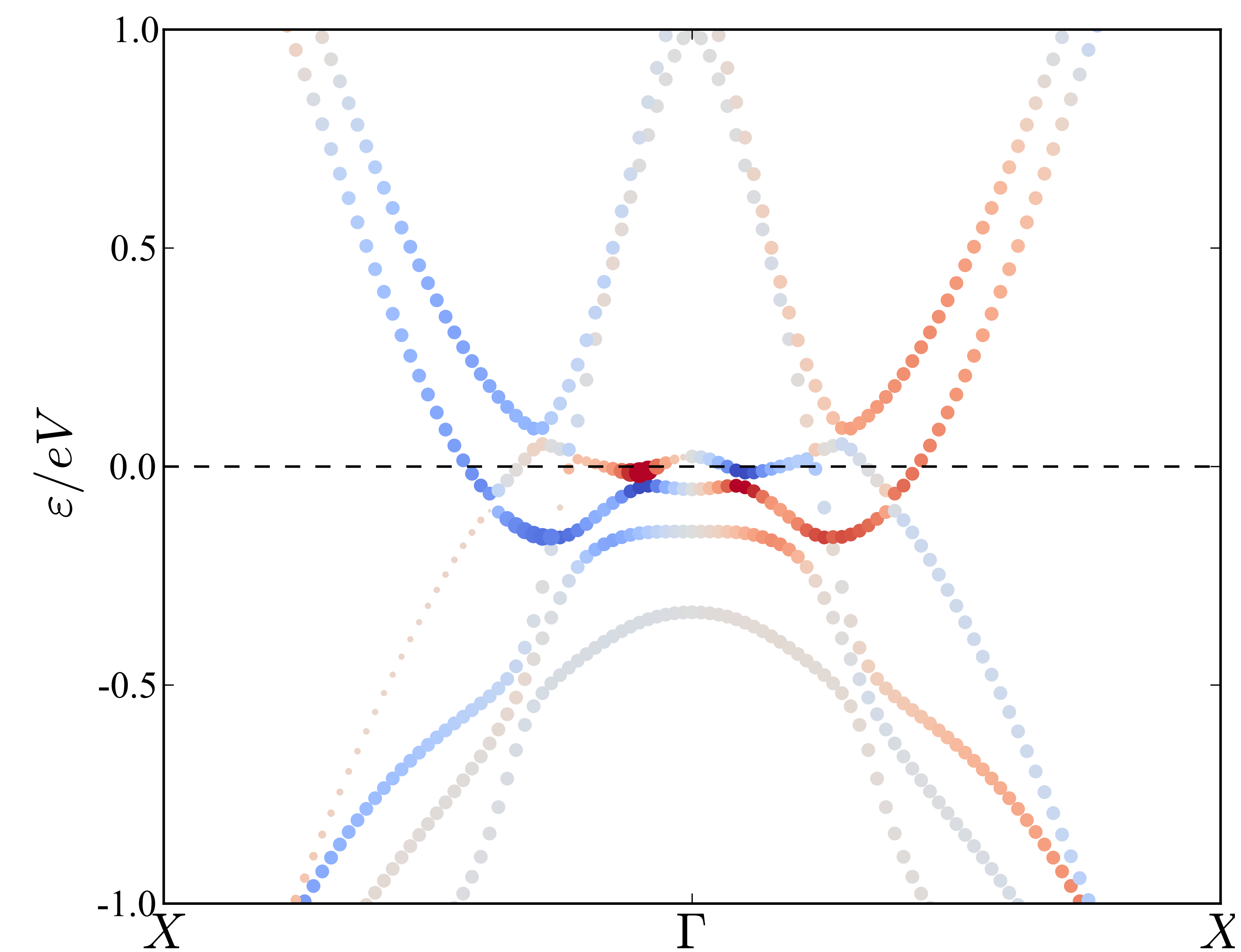
Circular Dichroism

- use of ab-initio wavefunctions for initial states at Fermi level
- Final state is totally symmetric combination of plane waves with longest wavelengths (most simple approximation possible)

$$P_{\pm}^{if}(\boldsymbol{k}) = \boldsymbol{\lambda}_{\pm} \cdot \sum_{\boldsymbol{G}} \boldsymbol{G}\; c_{\boldsymbol{Gk}}^{[f]*} c_{\boldsymbol{Gk}}^{[i]}$$







Summary

- New topological band inverted 2D semimetal in non-symmorphic crystal structures
- Topological classification using non-abelian Wilson loops along non-contractible loops
- Monolayers $MoTe_2$/WTe_2 without SOC as material examples
- Non-trivial monolayer structure has consequences for the 3D materials

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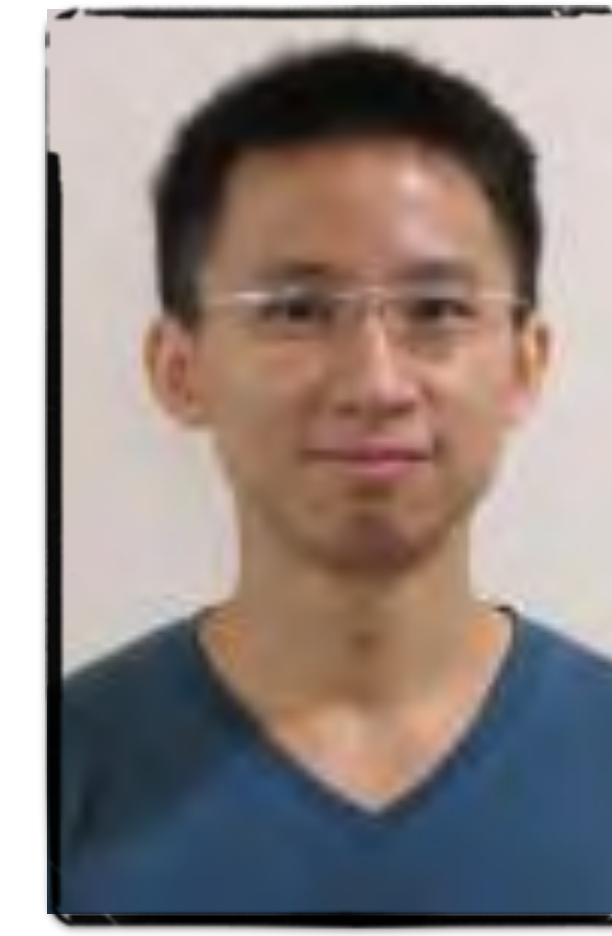

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