$BaNiS_2$ monolayer as possible Z2 topological insulator

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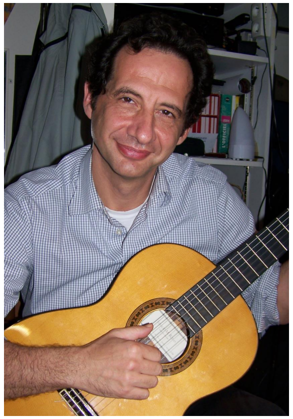
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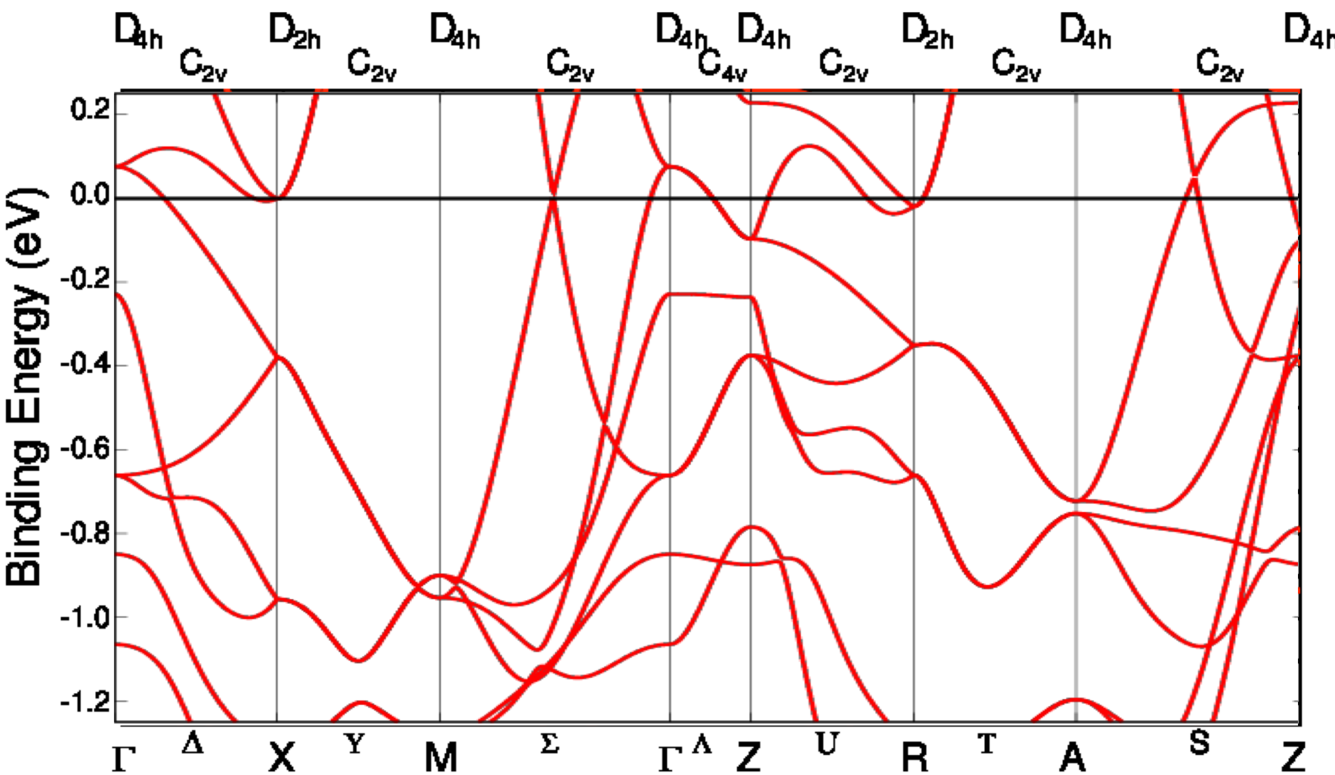
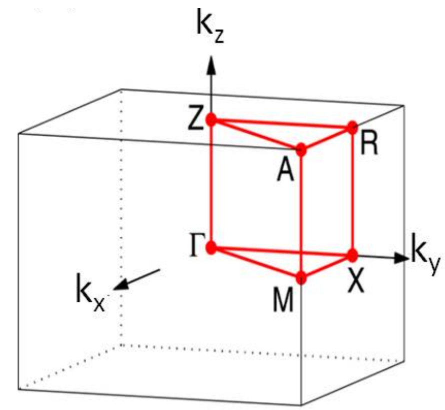
- PRACE

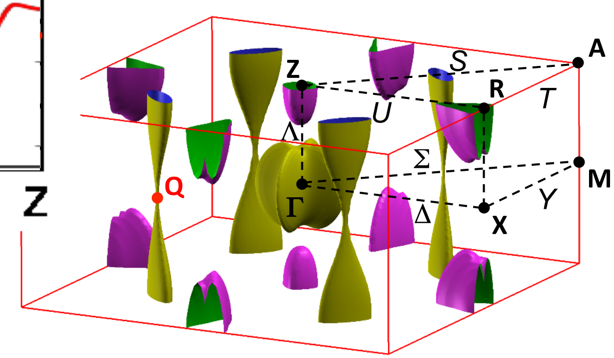
Outline

- Spin-orbit coupling in $BaNiS_2$
- Spin-orbit + Dirac
- Monolayer

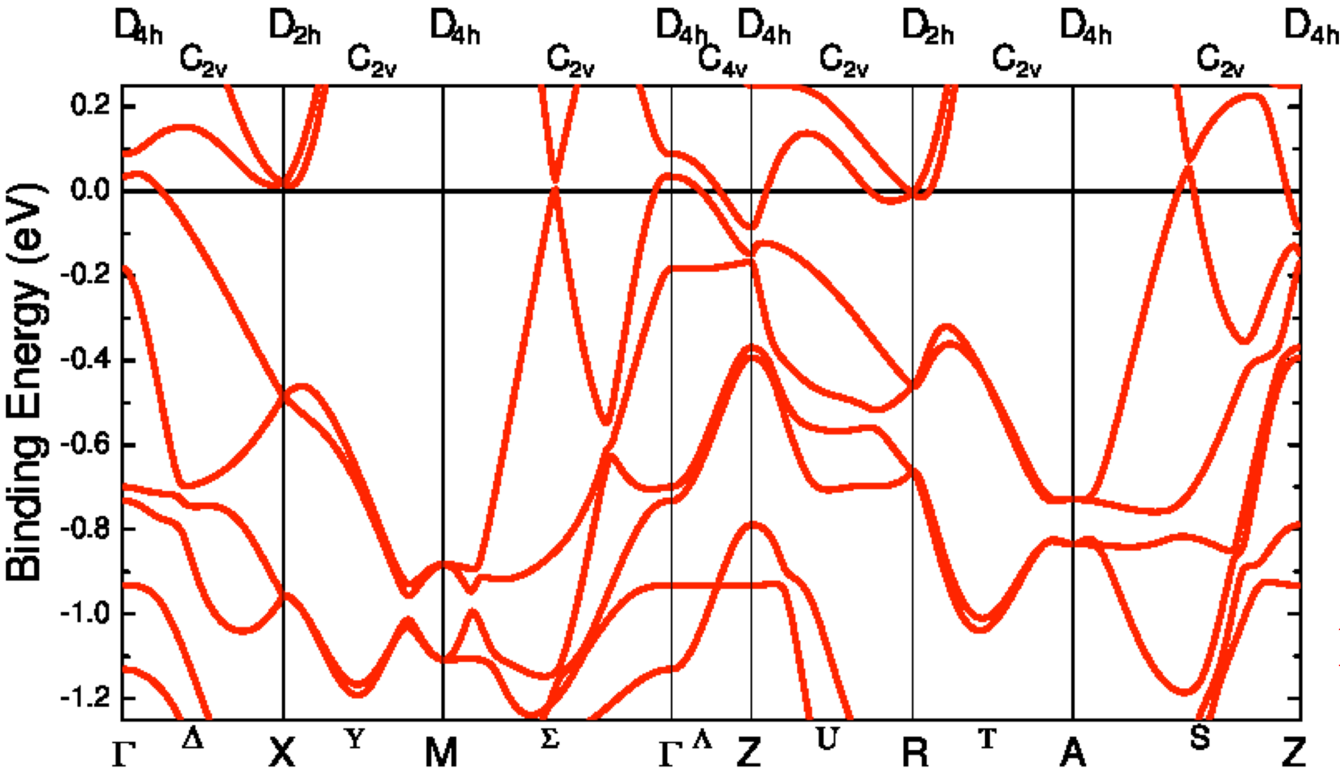
Electronic structure of $BaNiS_2$ (GGA+U)

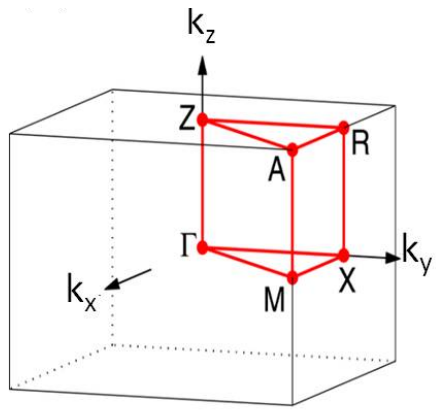


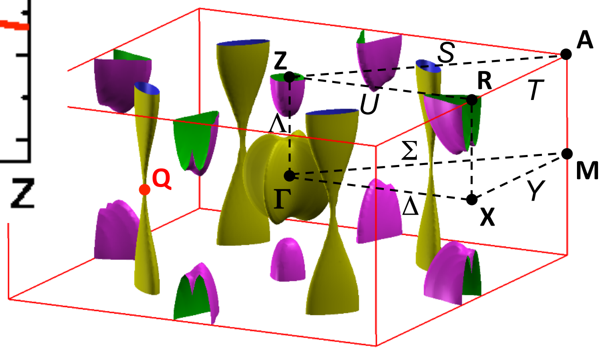




Electronic structure of $BaNiS_2$ (GGA+U+SOC)



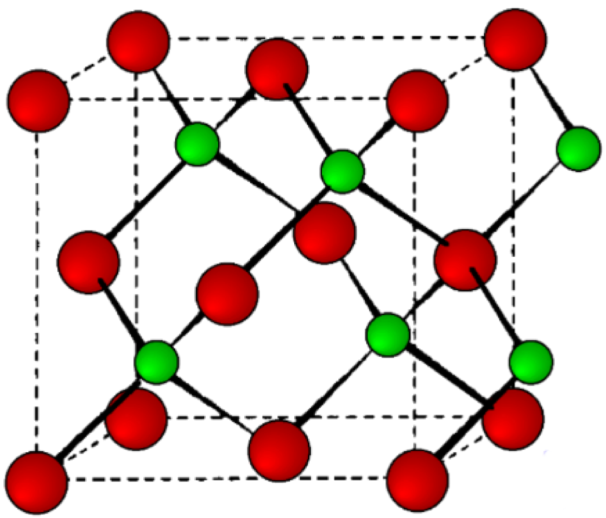




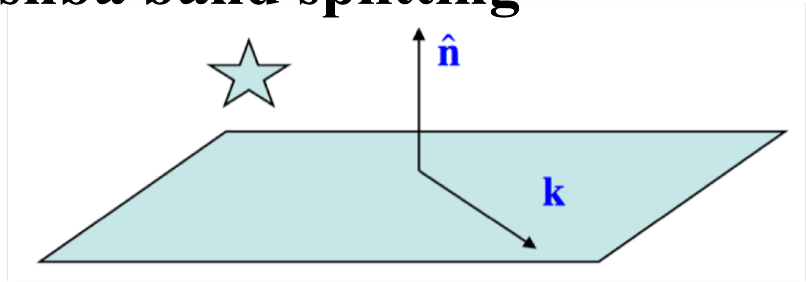
SOC split bands

Usually in crystals with broken inversion symmetry with spin polarized bands

BIA: Bulk Inversion Asymmetry (non-centrosymmetric e.g. GaAs)
Dresselhaus band splitting



SIA: Surface Inversion Asymmetry
(e.g. heterostructures)
Rashba band splitting



Rashba band splitting

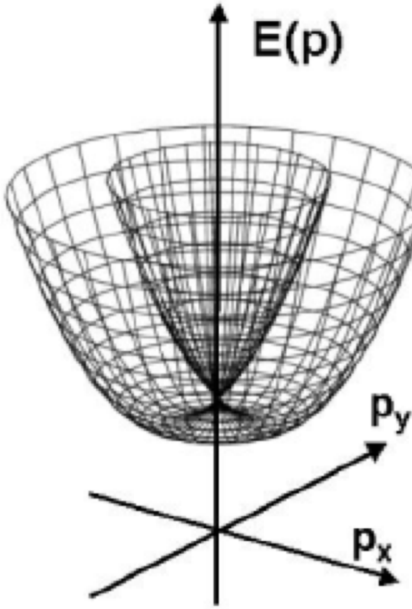
Rashba Hamiltonian: $H_R = \frac{p^2}{2m} - \boldsymbol{\sigma} \cdot \alpha_R \hat{\mathbf{z}} \times \boldsymbol{p}$

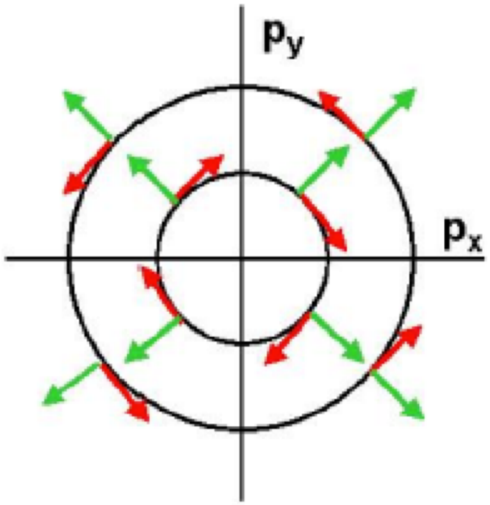
Spin-chiral polarized states:

$$\chi = \boldsymbol{\sigma} \cdot \boldsymbol{p} \times \hat{\mathbf{z}} = \pm 1$$

Rashba spinors:

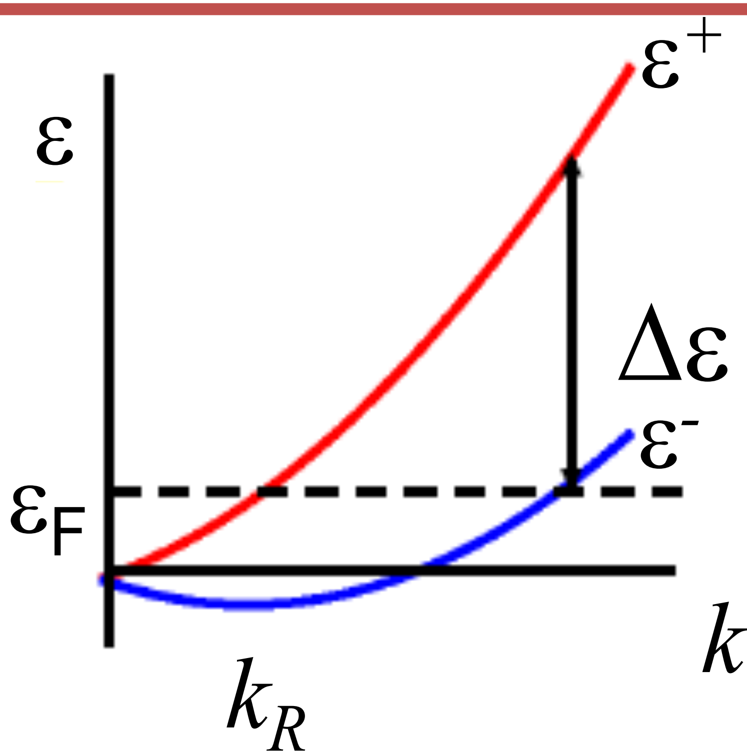
$$\psi_{\mathbf{k}}^{\pm} = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm i e^{-i\phi_{\mathbf{k}}} \\ 1 \end{pmatrix}$$





Sinova et al. (2004)

Rashba parameters



Parabolic bands:

$$\varepsilon^{+} - \varepsilon^{-} = \alpha_{R}\, k$$

α_R: Rashba coupling
k_R: Rashba wave vector
$\Delta\varepsilon$: Rashba splitting

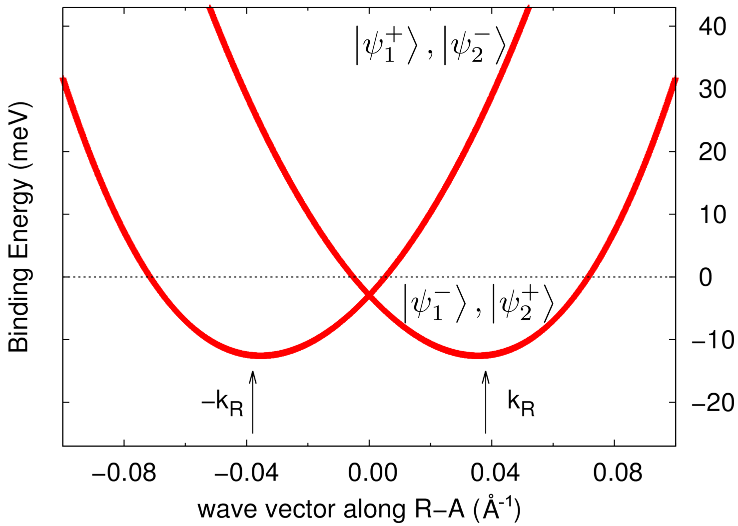
Systems with large Rashba split

Sample	k_0	E_R	α_R
Surface state			
Au(111)	0.012	2.1	0.33
Bi(111)	0.05	14	0.55
1/3 ML Bi on Ag surface alloy	0.13	200	3.05
Interface			
InGaAs/InAlAs	0.028	<1	0.07
QW state			
Pb thin film (6-22 ML)	0.035	$\lesssim 10$	0.04
Bi thin film (7-40 BL)	-	-	-
1 ML Bi on Cu	N/A	N/A	2.5
Bulk			
BiTeI	0.052	100	3.8

Ishikawa et al. (2011)

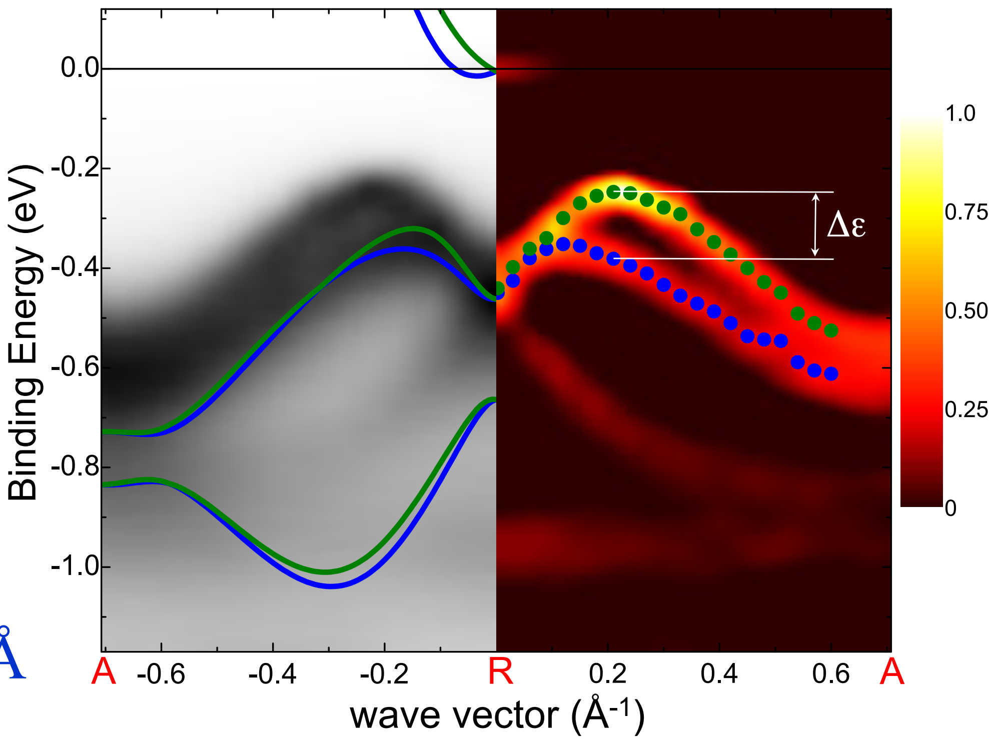
All these systems contain **heavy elements** and are bulk or surface **inversion asymmetric** (BIA or SIA)

Rashba splitting at R point



Conduction bands

Valence bands



- k_R=0.04 $Å^{-1}$
- Rashba splitting: Δε=150 meV
- Rashba coupling: α_R=0.25 eV Å

→ **very large values!**

Comparison with known literature

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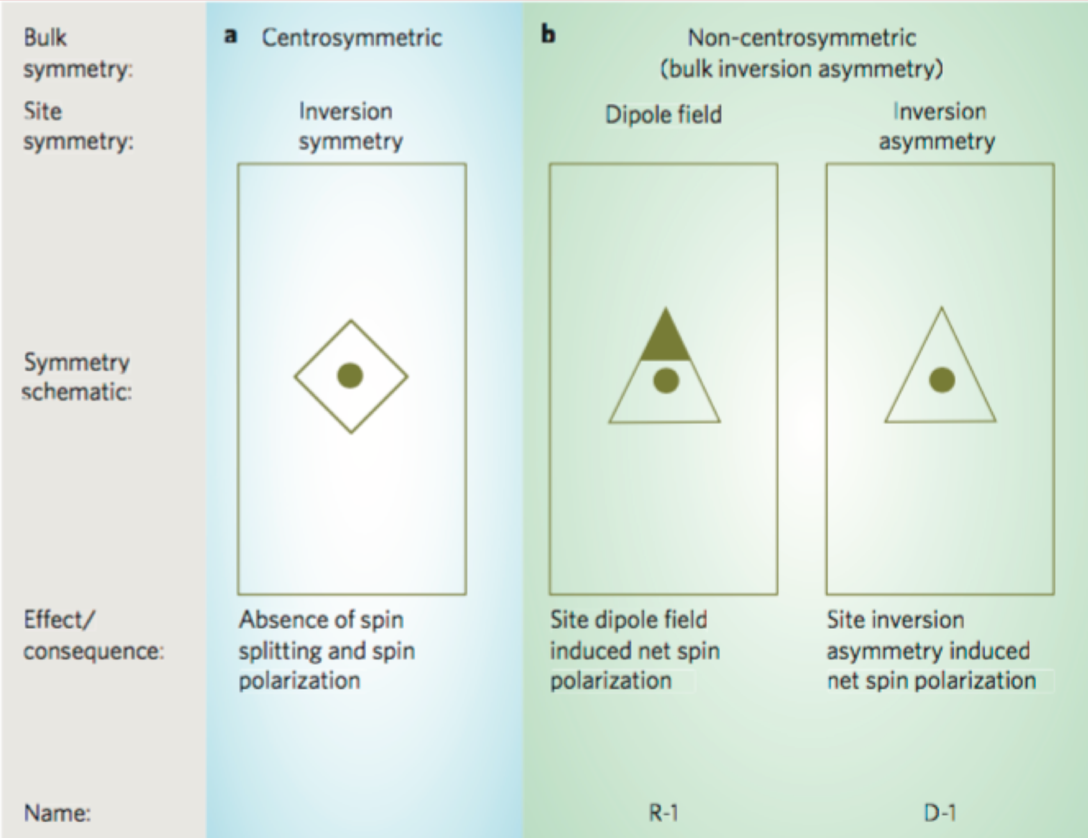
BiTeI	0.052	100	3.8
$BaNiS_2$	0.040	150	0.25

Note that $(Z_{Bi}/Z_{Ni})^4 \sim 100$

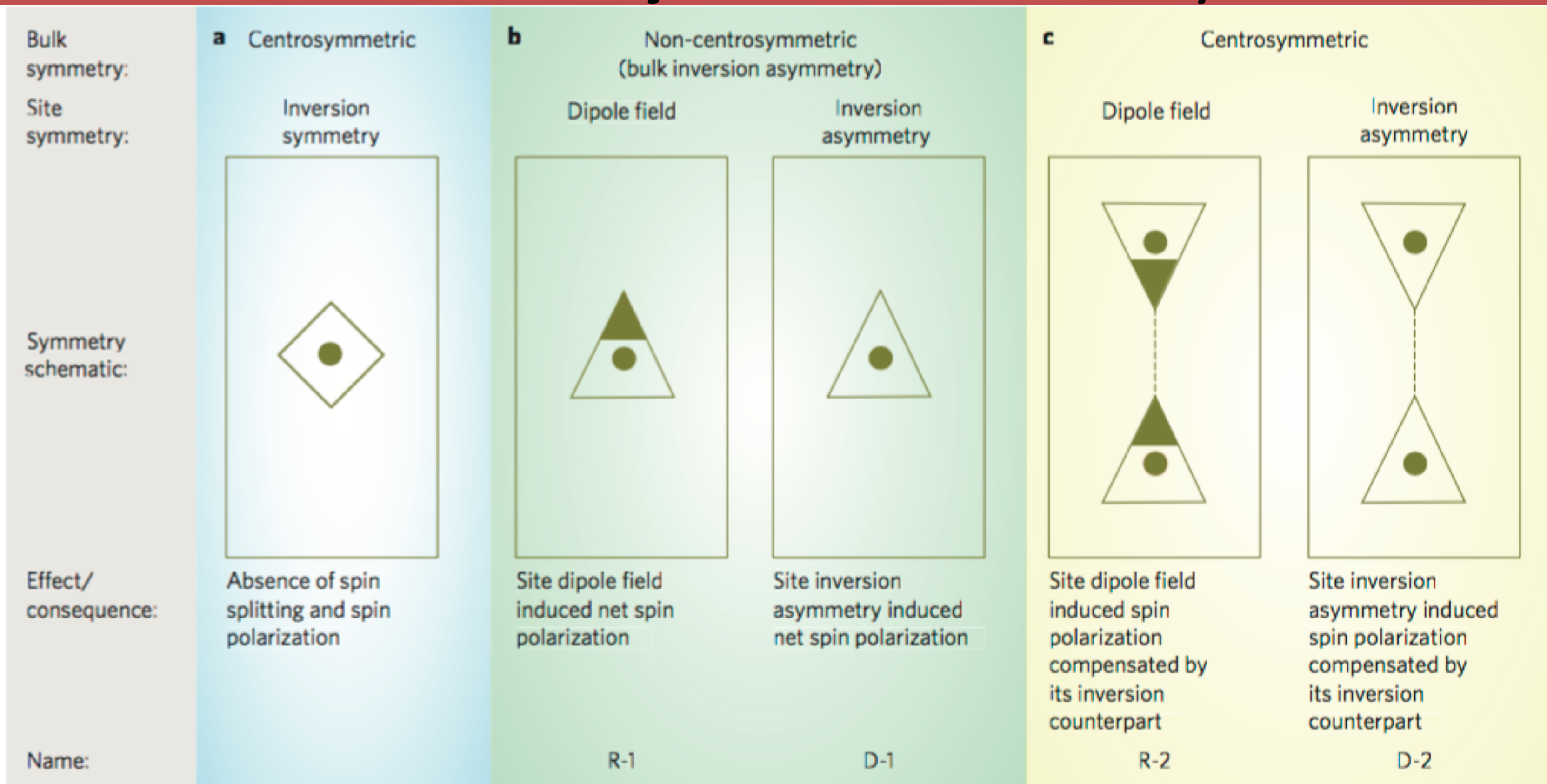
One would have expected spin-orbit effects in $BaNiS_2$ two orders of magnitude smaller!

Hidden spin polarization in inversion-**symmetric** bulk crystals



Zhang et al. (2014)

Hidden spin polarization
in inversion-**symmetric** bulk crystals



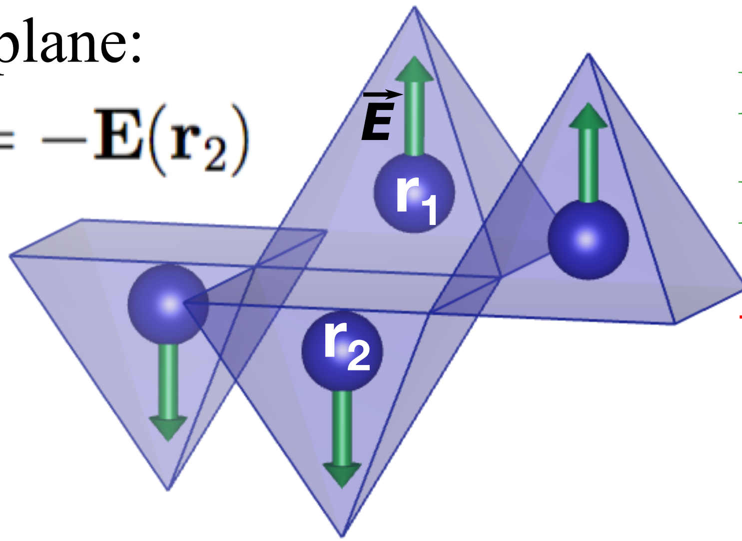
Zhang et al. (2014)

Local Inversion Asymmetry (LIA) counts as well!

Non-symmorphic symmetry and SOC effects

Gliding plane:

$\mathbf{E}(\mathbf{r}_1) = -\mathbf{E}(\mathbf{r}_2)$



Local Inversion Asymmetry

E_z~1.4 V Å: huge crystal field!

→ Rashba coupling enhancement

Without SOC **With SOC**

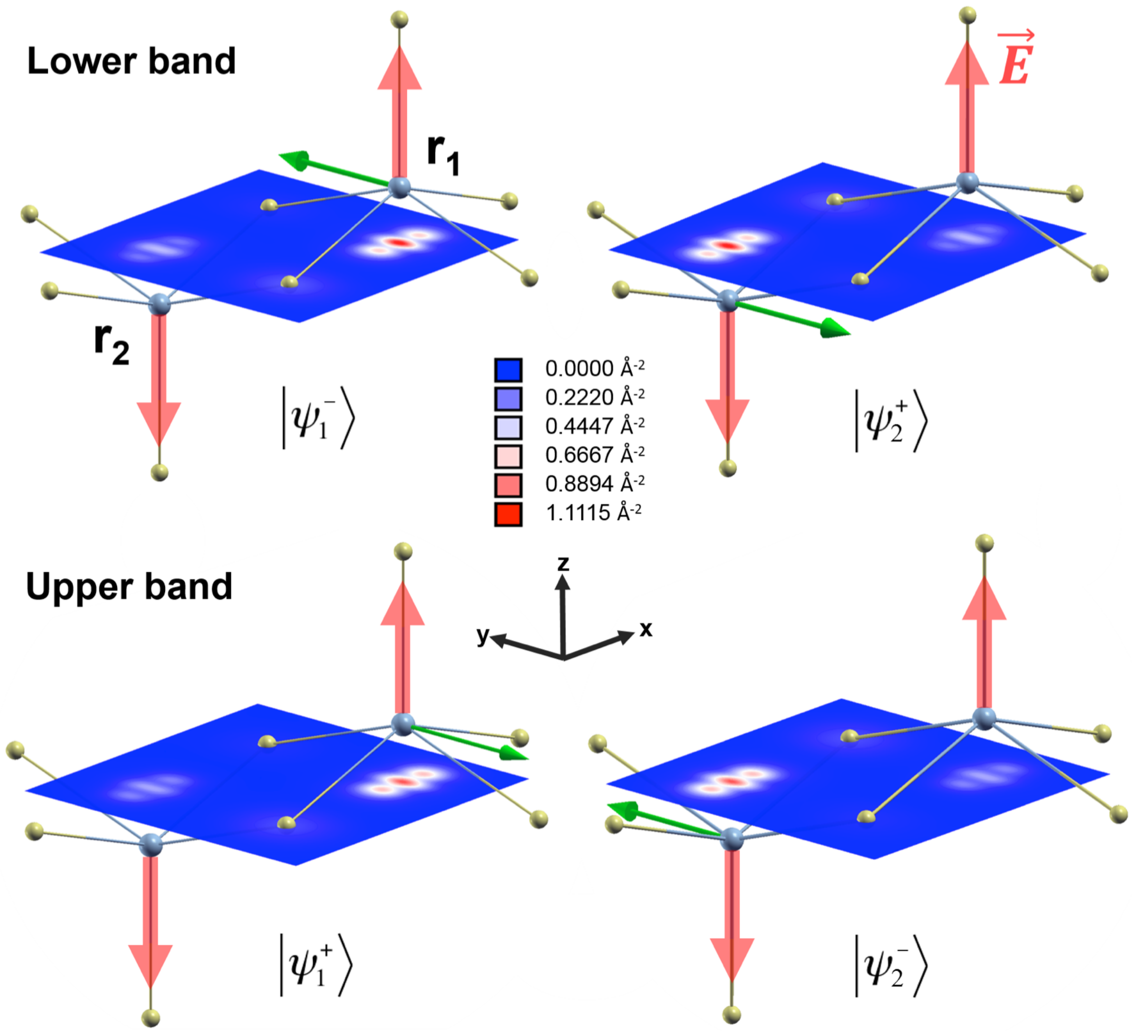
spin degeneracy +
orbital degeneracy

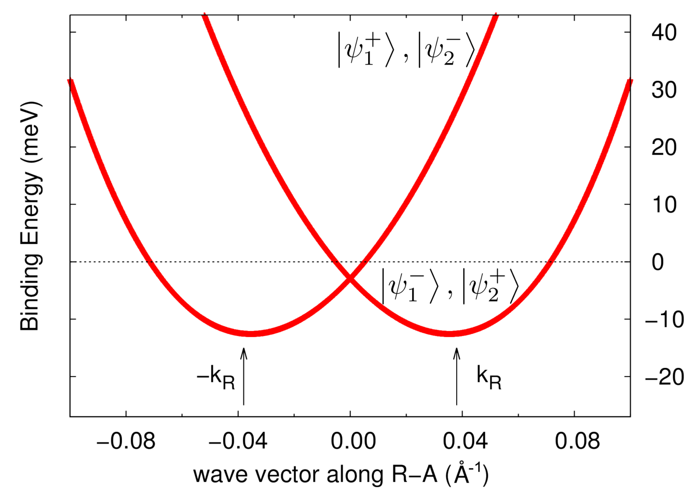
Without SOC: $|\psi_1^{\pm}\rangle, |\psi_2^{\pm}\rangle$

With SOC: $|\psi_1^{-}\rangle, |\psi_2^{+}\rangle$

$|\psi_1^{+}\rangle, |\psi_2^{-}\rangle$

hidden spin-chirality of Bloch states

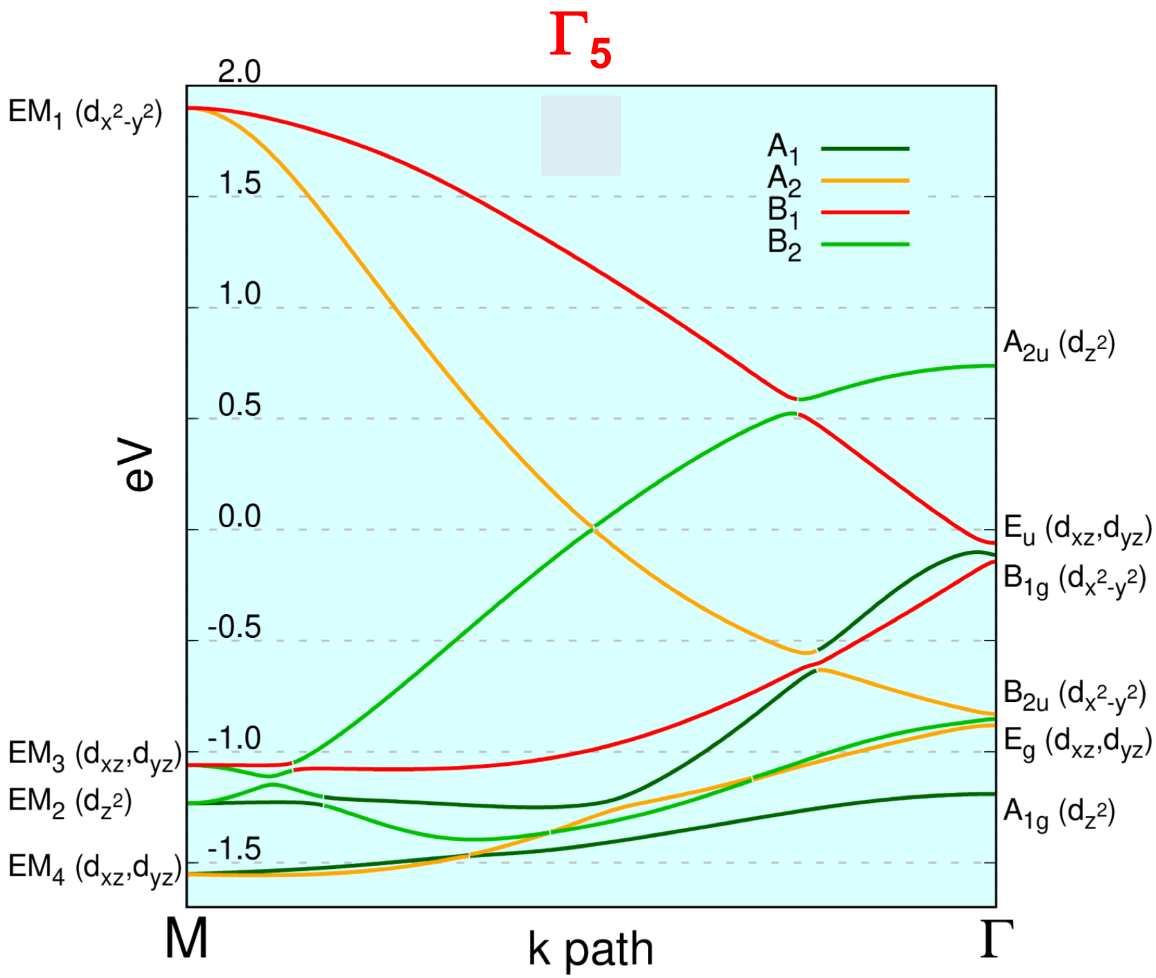




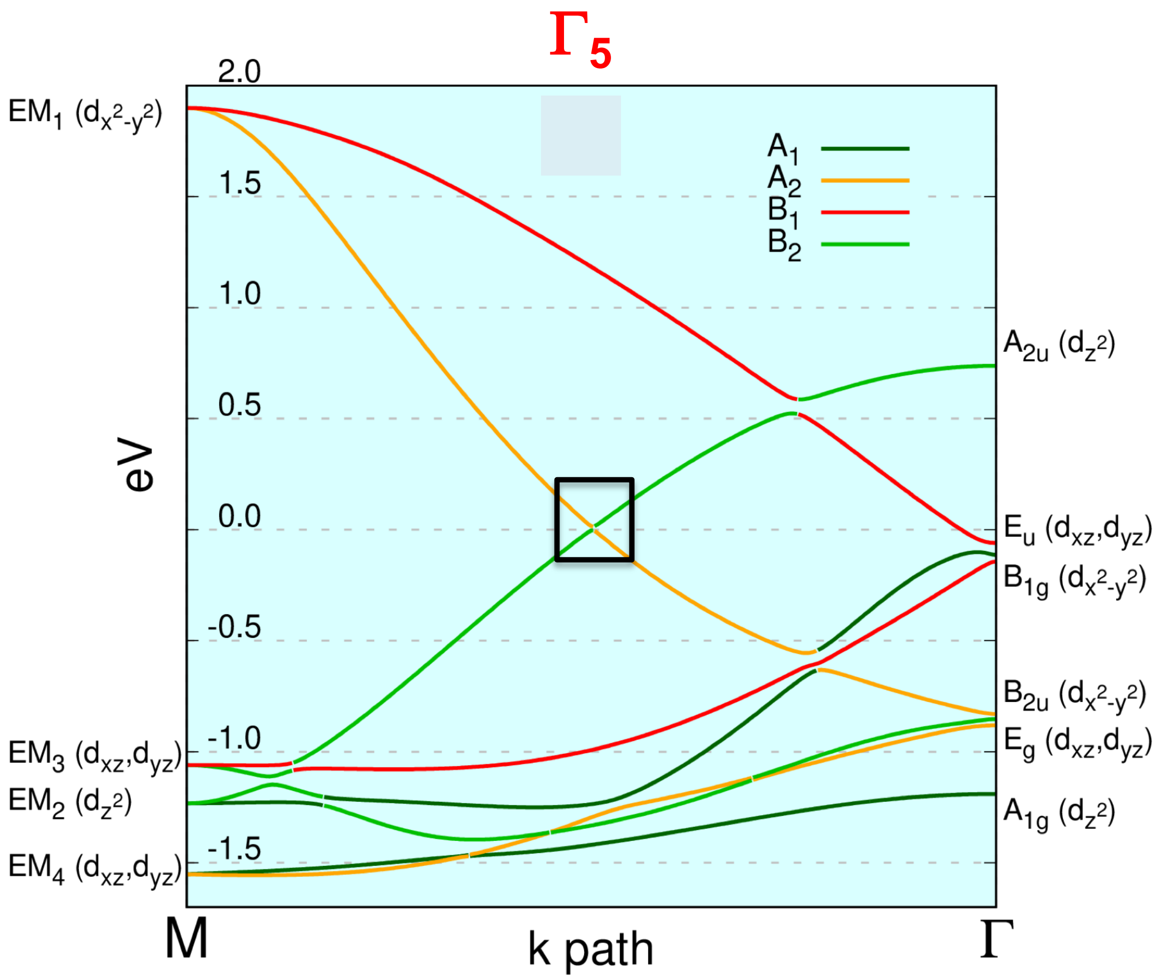
Opposite spin chiralities:

- Degenerate in k-space
- **Separated in real space**

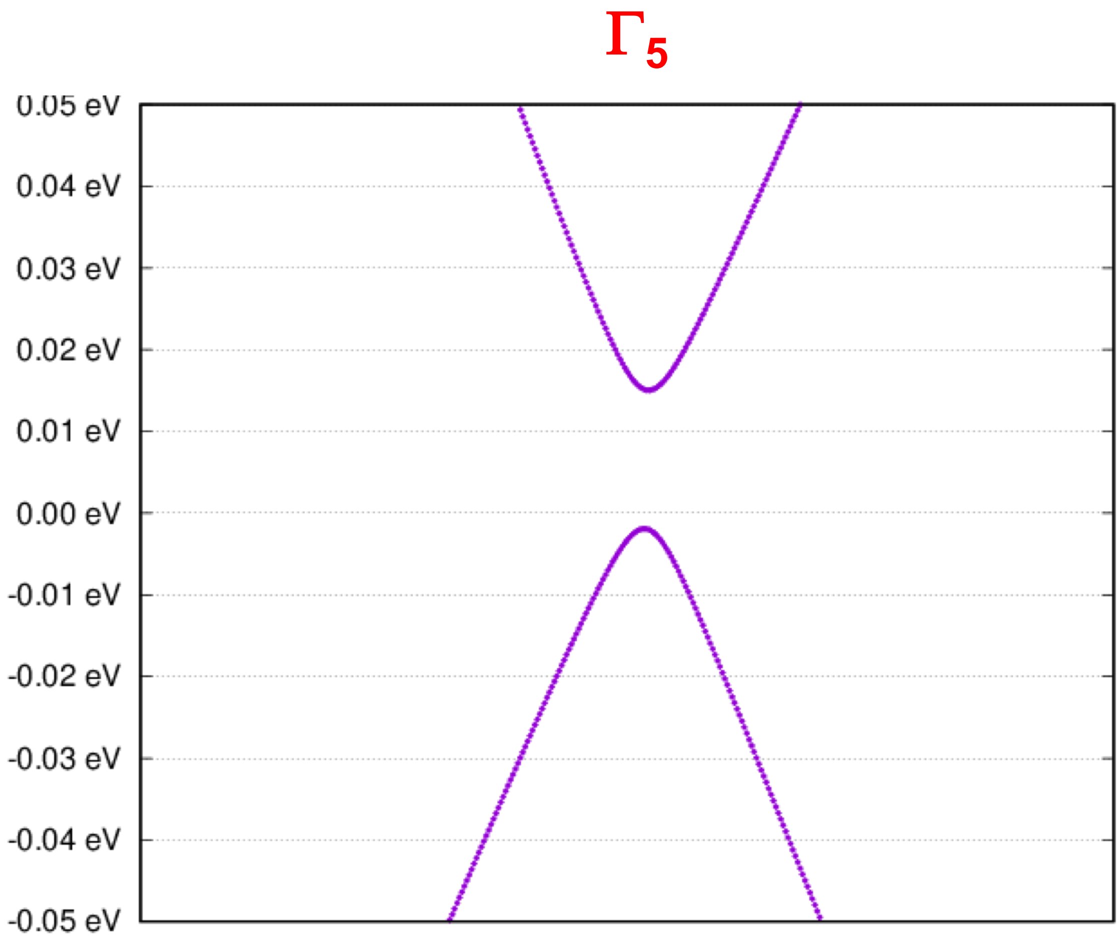
Dirac cones with SOC?



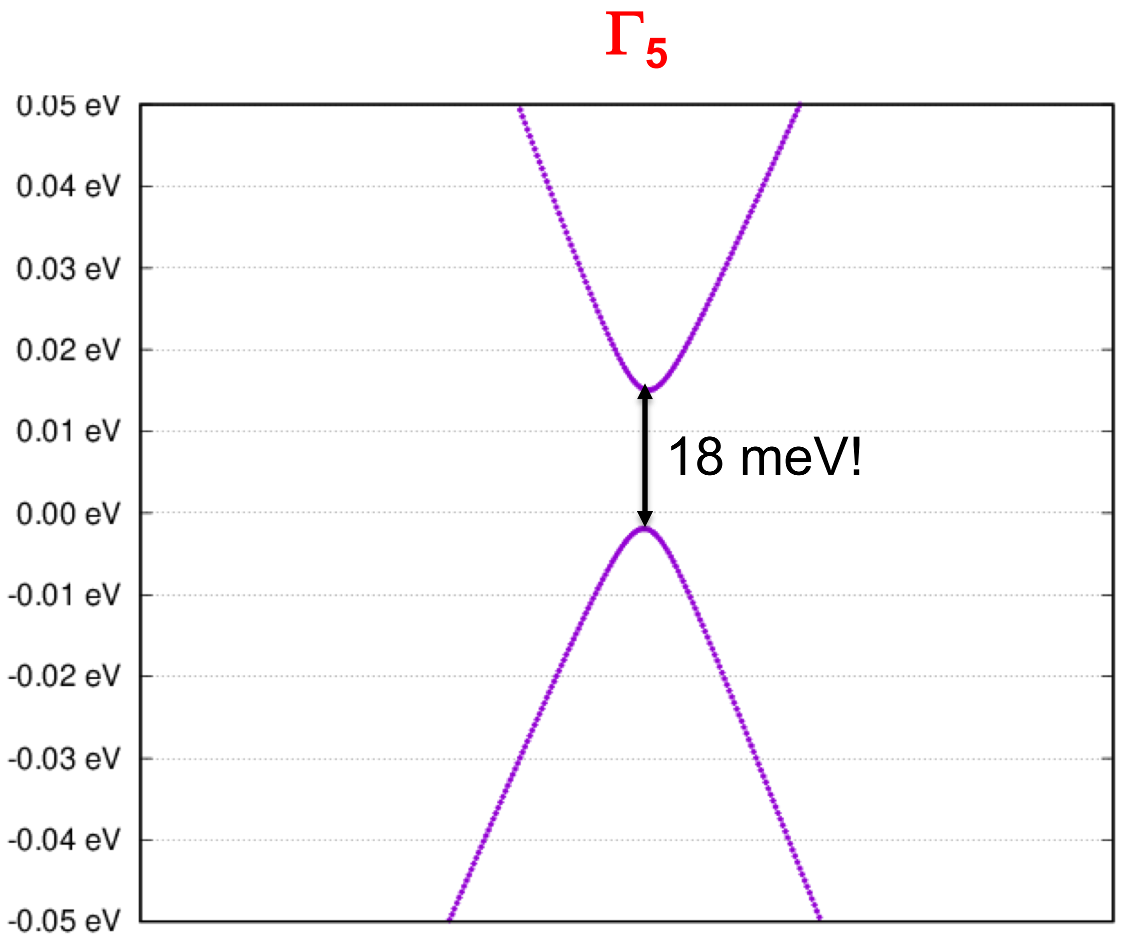
Dirac cones with SOC?



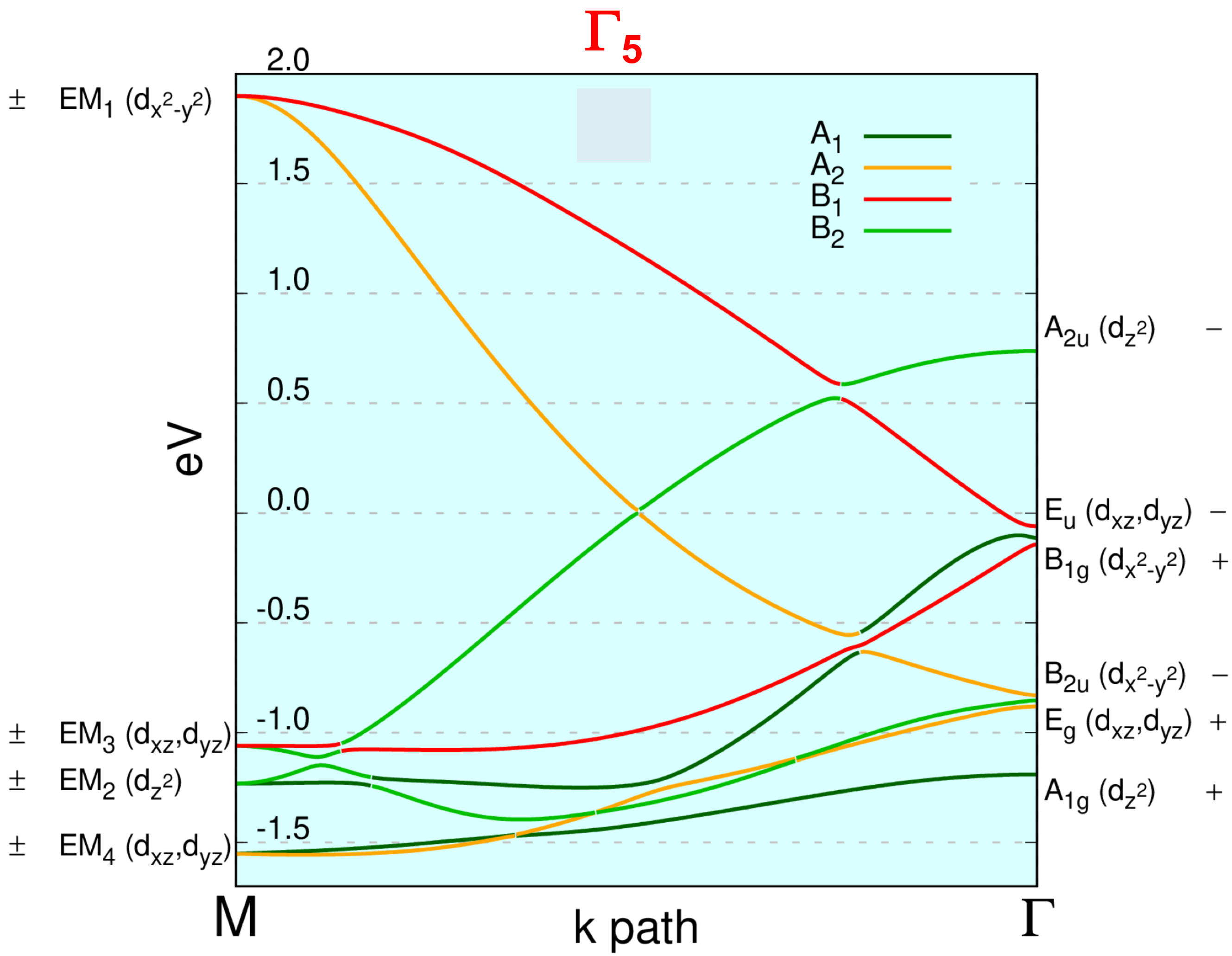
Massive Dirac cones



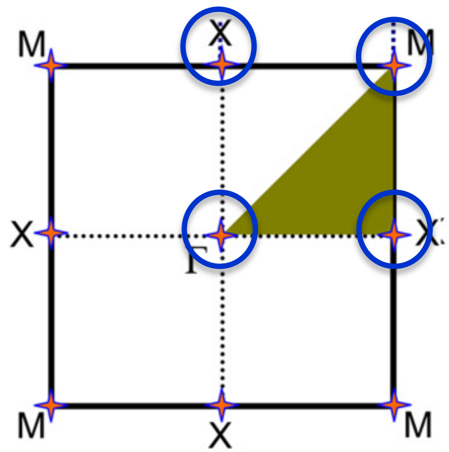
Massive Dirac cones



Parity analysis



Parity analysis



Fu Kane PRB **76** (2007)

Inversion symmetry
+ time reversal

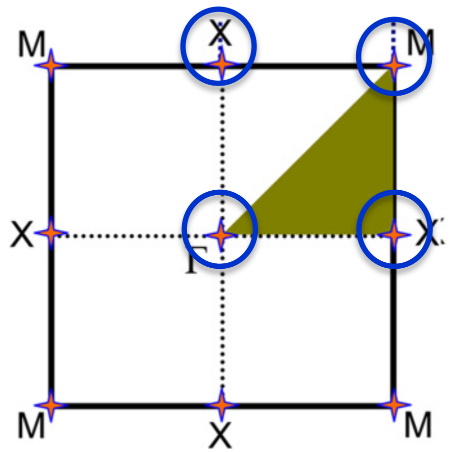
$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i)$$

$$(-1)^{\nu} = \prod_i \delta_i$$

Product over the time reversal invariant momenta

Parity analysis

Inversion symmetry
+ time reversal

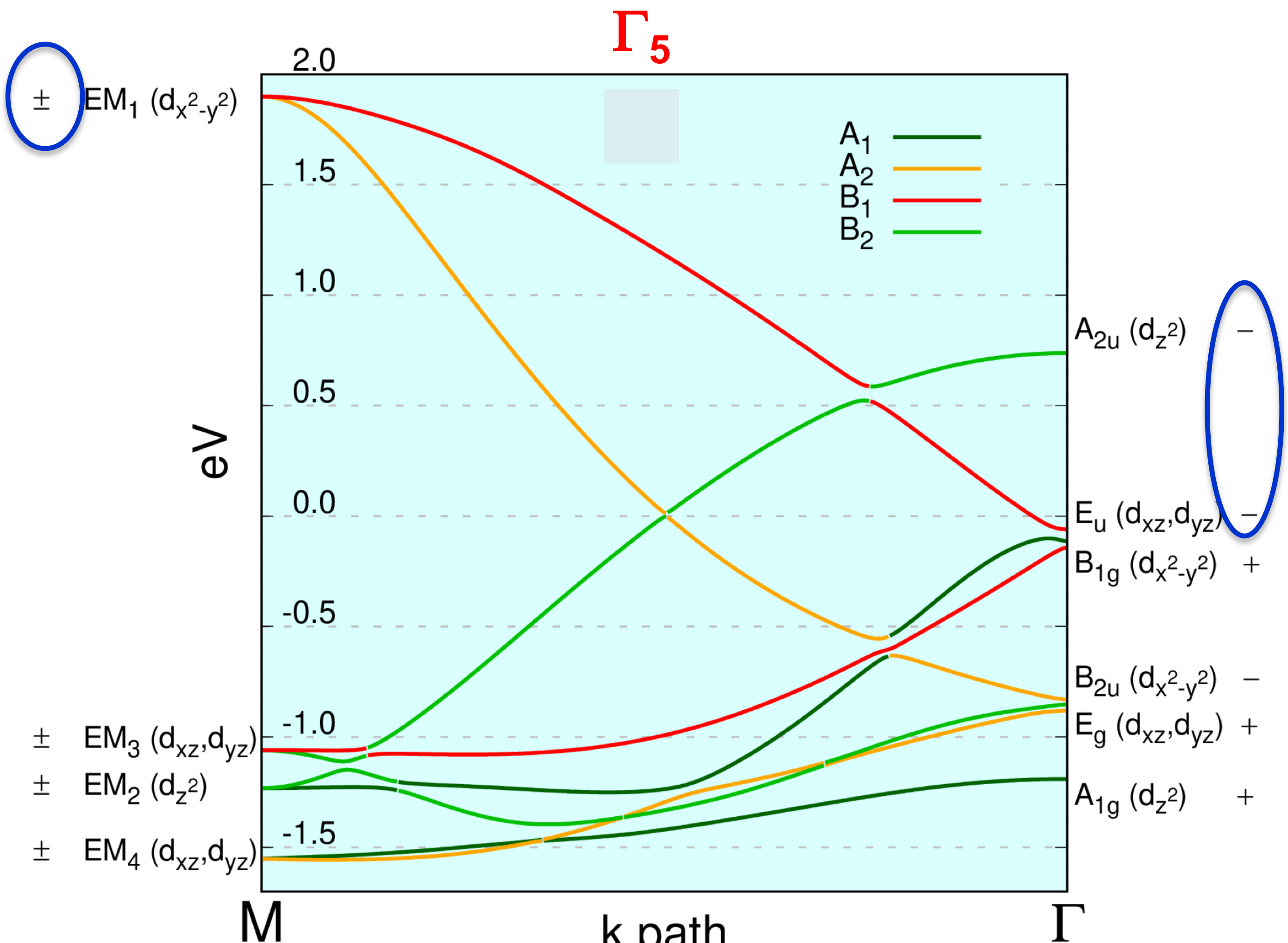


Fu Kane PRB **76** (2007)

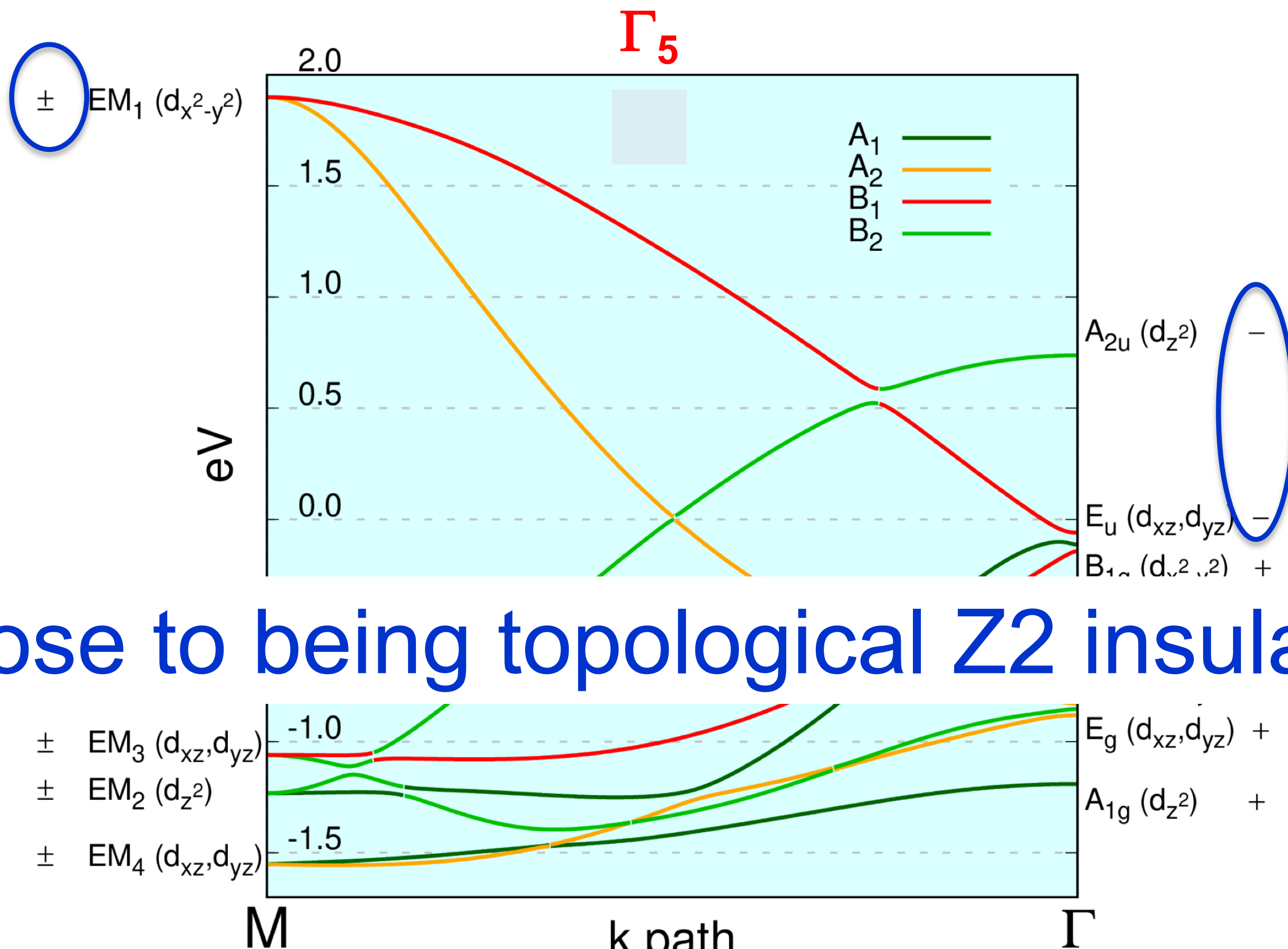
$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) \qquad (-1)^{\nu} = \prod_i \delta_i$$

If ν=1 → Z2 topological insulator

Parity analysis



Parity analysis



Close to being topological Z2 insulator!

Conclusions

- Presence of Dirac cones made of d orbitals lying at the Fermi level
- Very large Rashba splitting
- Monolayer can become a Z2 topological insulator for some value of the lattice parameter

PERSPECTIVES

- Feasibility study
- Interplay between correlation, topology and spin properties
- Other ways to open the gap?

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