Engineering Topological Phases
:A Materials Perspective

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Season's Greetings
Season's Greetings
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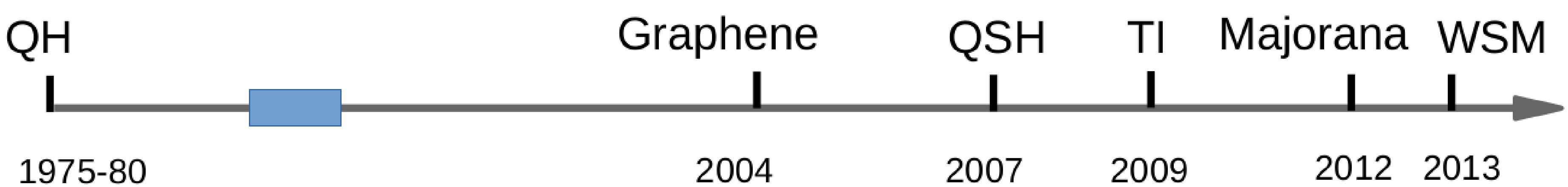
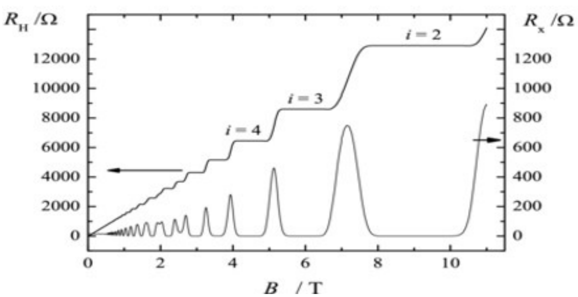
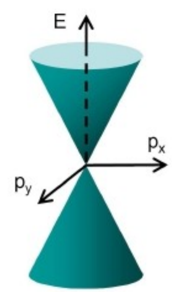
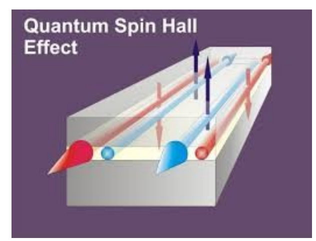
POCO
SHOT ON POCO F1

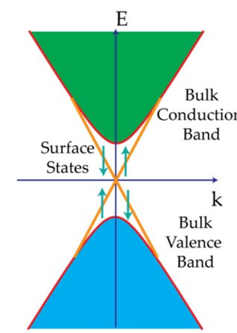
Topology "ZOO"

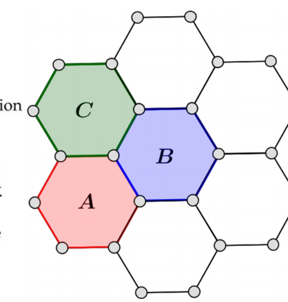


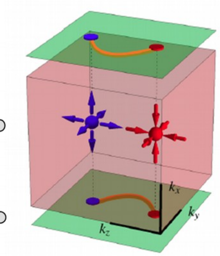






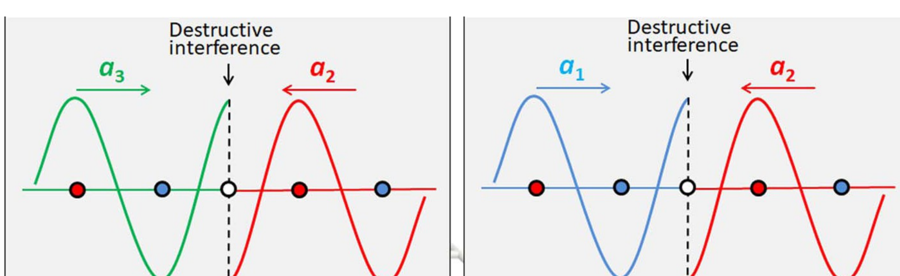


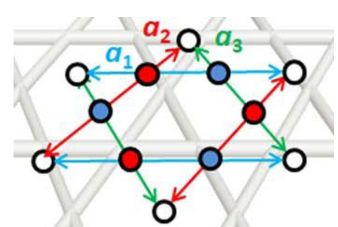


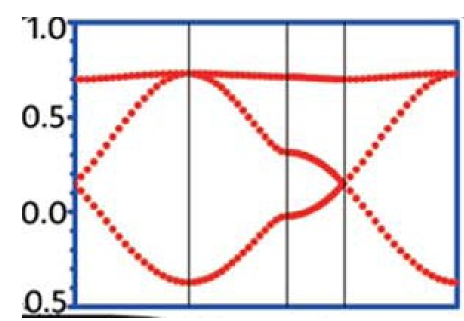


Topological phases from gapped matter (insulator) to gap-less systems (metals)

Topologically non-trivial Flat bands : Fractional QHE
(site of "instability")



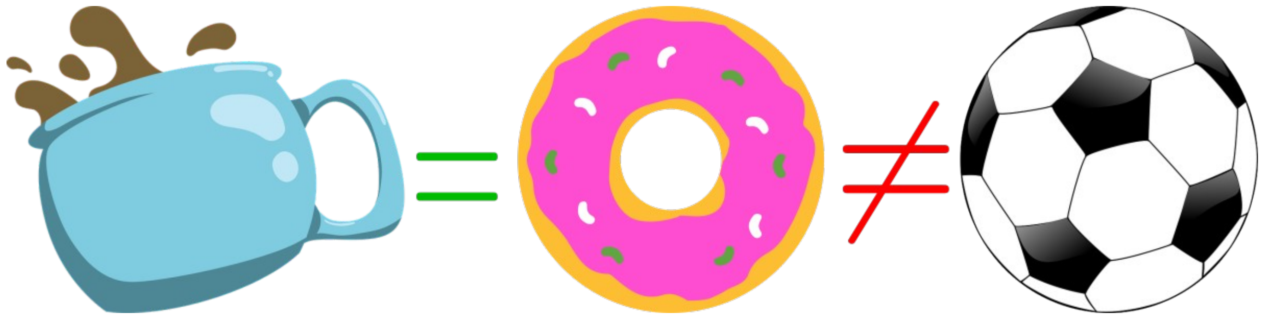




Li et al Sci Adv 2018

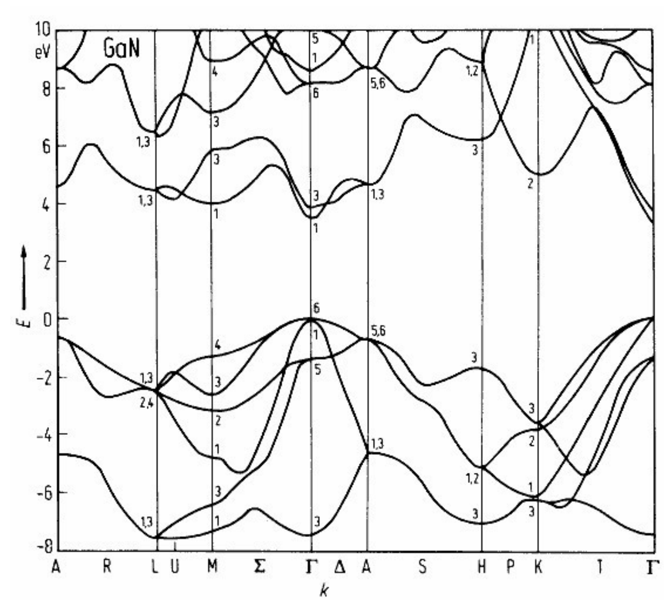
Topology (2016 Nobel prize)

Geometrical Topology:



“Same” if can be deformed without singularity. The value of an orientable surface's genus is equal to the number of holes!   **Topological Invariant:** Quantity that does not change under continuous deformation

Band Structure Topology:

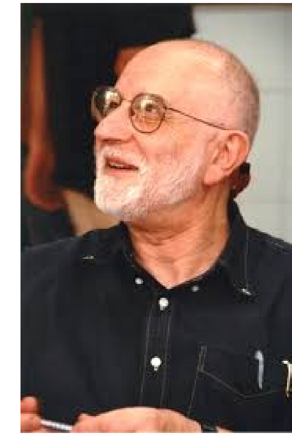


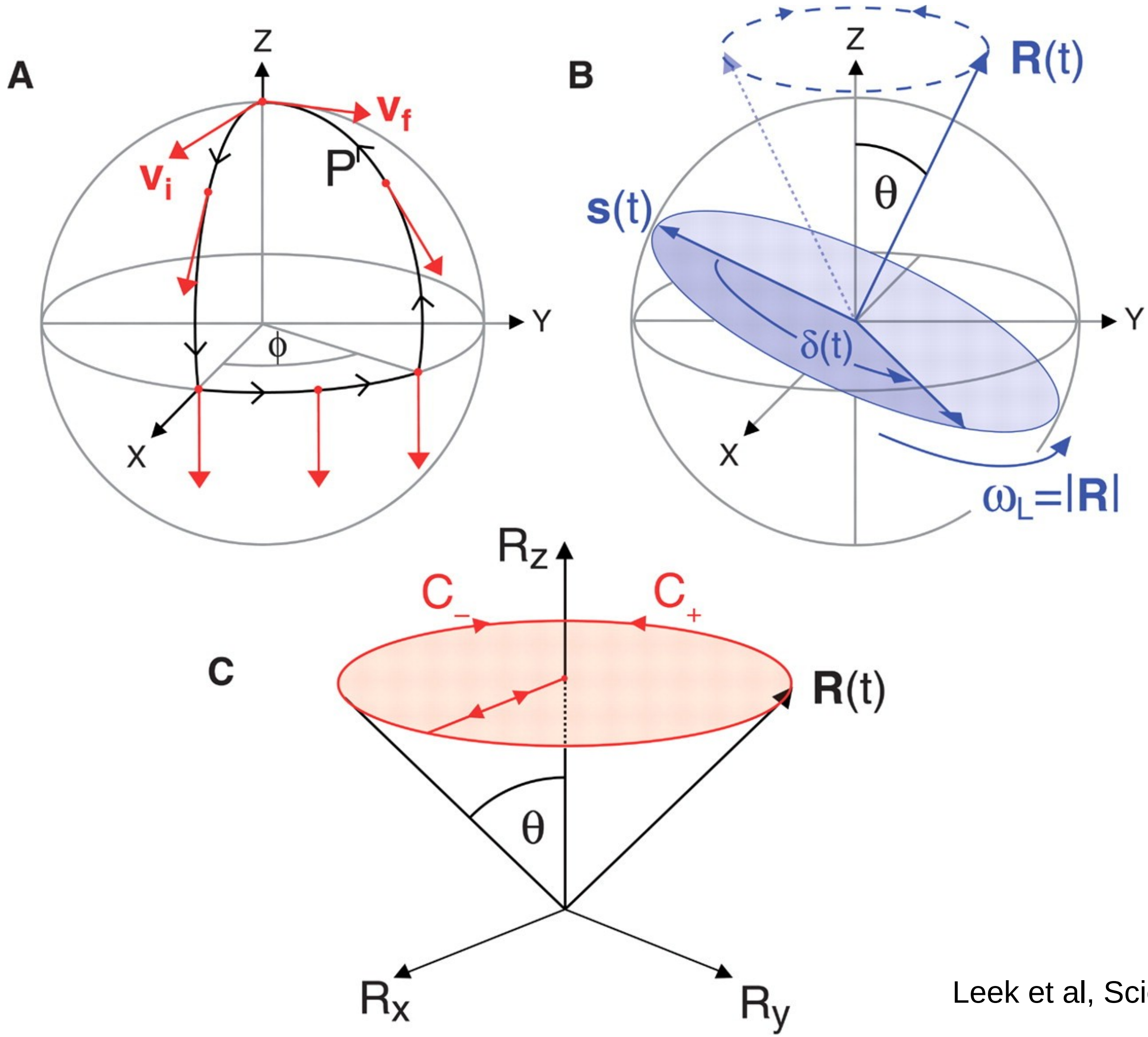
“Same” if can be adiabatically perturbed without gap closure.

Topological Invariant: Cannot change unless the energy gap between bands closes and reopens

Pancharatnam Berry Phase

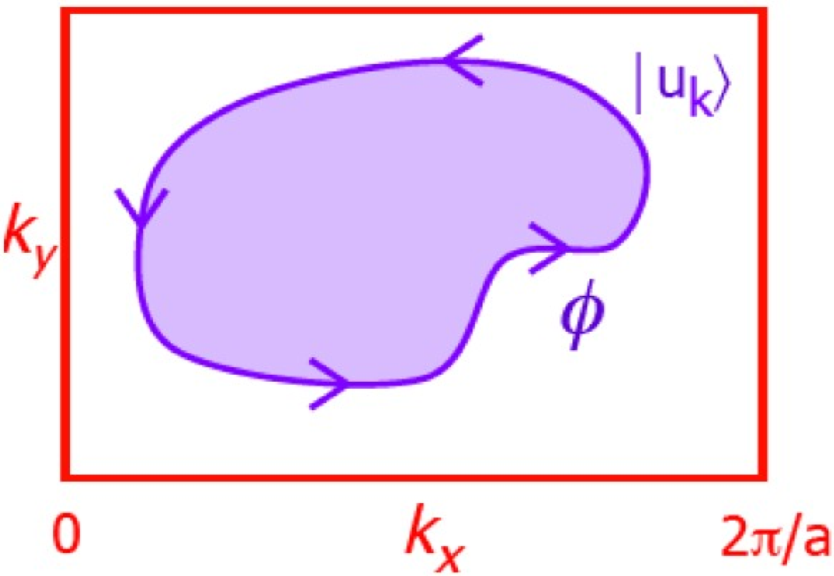
Geometrical Phase





Leek et al, Science 21 Dec 2007

Berry Phase and Curvature in the BZ



$$u_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\underbrace{\psi_{\mathbf{k}}(\mathbf{r})}$$

Bloch function

$$A_n^a(\boldsymbol{k}) = -i\langle\Psi_n(\boldsymbol{k})|\frac{\partial}{\partial k_a}\Psi_n(\boldsymbol{k})\rangle$$

"Berry connection": k-space analog of the magnetic vector potential.

$$F_n^{ab}(\boldsymbol{k}) = \frac{\partial}{\partial k_a}A_n^b(\boldsymbol{k}) - \frac{\partial}{\partial k_b}A_n^a.$$

"Berry curvature": k-space analog of magnetic flux density (gauge invariant)

the integer quantum Hall effect in a 2D crystal

$$n = \sum_{bands}\frac{i}{2\pi}\int d^2k\left(\left\langle\frac{\partial u}{\partial k_1}\Big|\frac{\partial u}{\partial k_2}\right\rangle - \left\langle\frac{\partial u}{\partial k_2}\Big|\frac{\partial u}{\partial k_1}\right\rangle\right) \qquad \mathcal{F} = \nabla\times\mathcal{A}$$

$$\sigma_{xy} = n\frac{e^2}{h}$$

TKNN, 1982 "first Chern number"

"Chern number" classifies Bloch bands with broken time-reversal symmetry

Chern I ⇦

Gapless chiral edge states → potential use in dissipationless electronic circuits

T-invariant systems

"spin Chern number"

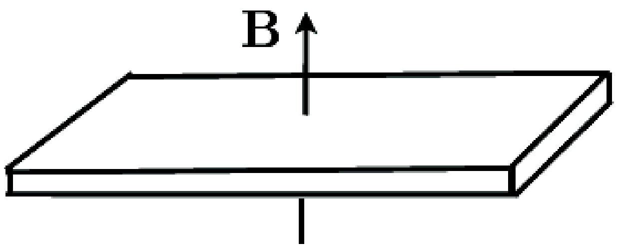
Each pair of spin-orbit-coupled bands in 2D has a Z_2 invariant, essentially integral over half the BZ

$$Z_2 = \sum_n^{occ.}\frac{1}{2\pi}\left(\oint_{\text{Half BZ}}\mathbf{A}_n\cdot d\mathbf{k} - \int_{\text{Half BZ}}dk_x dk_y F_n\right) = 0 \text{ or } 1 (\text{mod } 2)$$

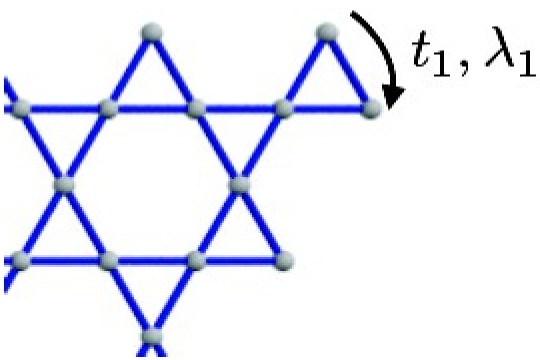
⇨ TI

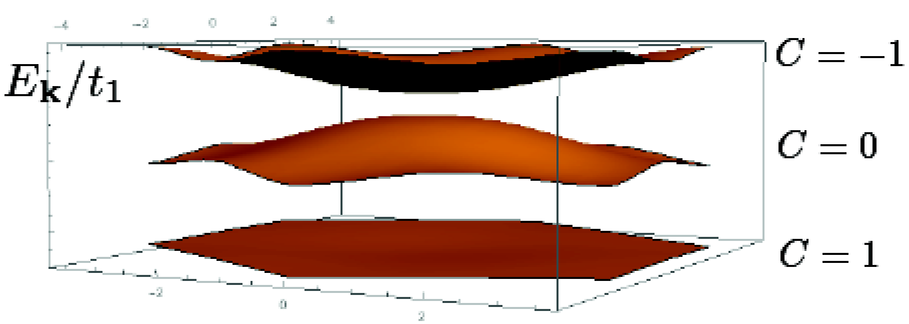
Topological Flat Bands, Landau Levels

- Lattice models with complex hopping parameters (SOC)
  - ⇨ Analogues of Landau Levels
- Almost flat, topological bands with any Chern number, C= N, possible
- Time-reversal broken spontaneously - No need for strong magnetic field
- Partial filling may give rise to Fractional QH state.
- High temperature scale may be achievable



- Cold 2D electrons in a strong magnetic field
- Flat Landau bands with C=1
- Interaction scale set by magnetic length ~ 1 K

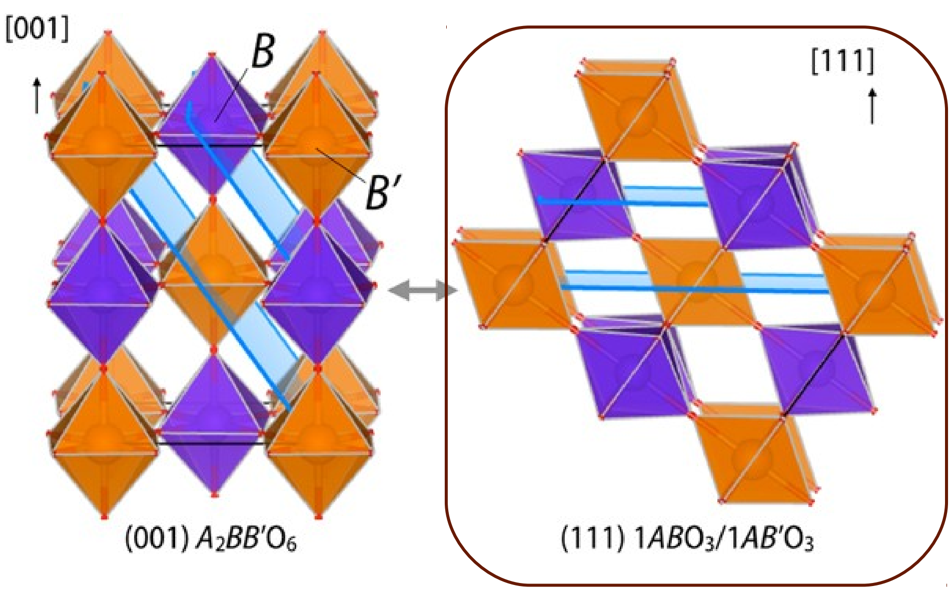




PRL 106, 236802; PRB 99, 165141

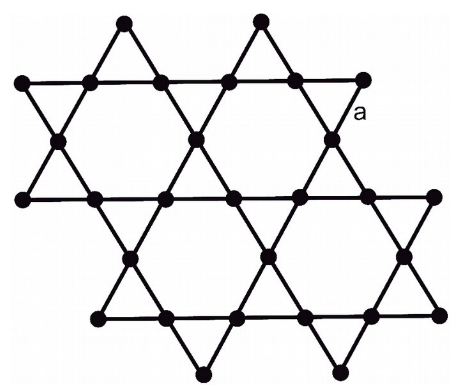
Search for Materials Candidates

Bilayer Double Perovskite



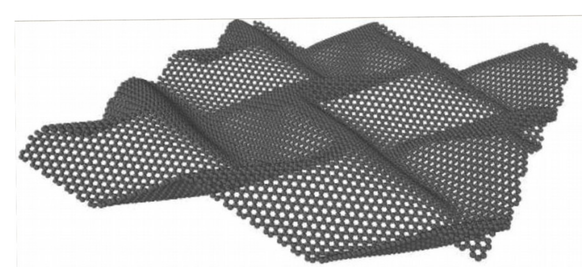
Candidate for RT QAH ?!

Binary Intermetallics in kagome lattice



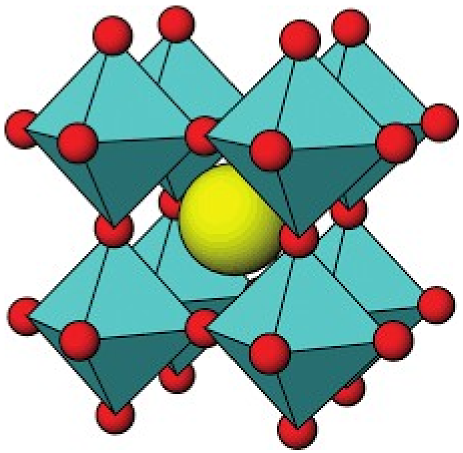
Possible Host for Chern metal, Topological SC ?!

Graphene under Deformation - “Ripplocation”



Topological Flat band ?!

OXIDE MATERIALS



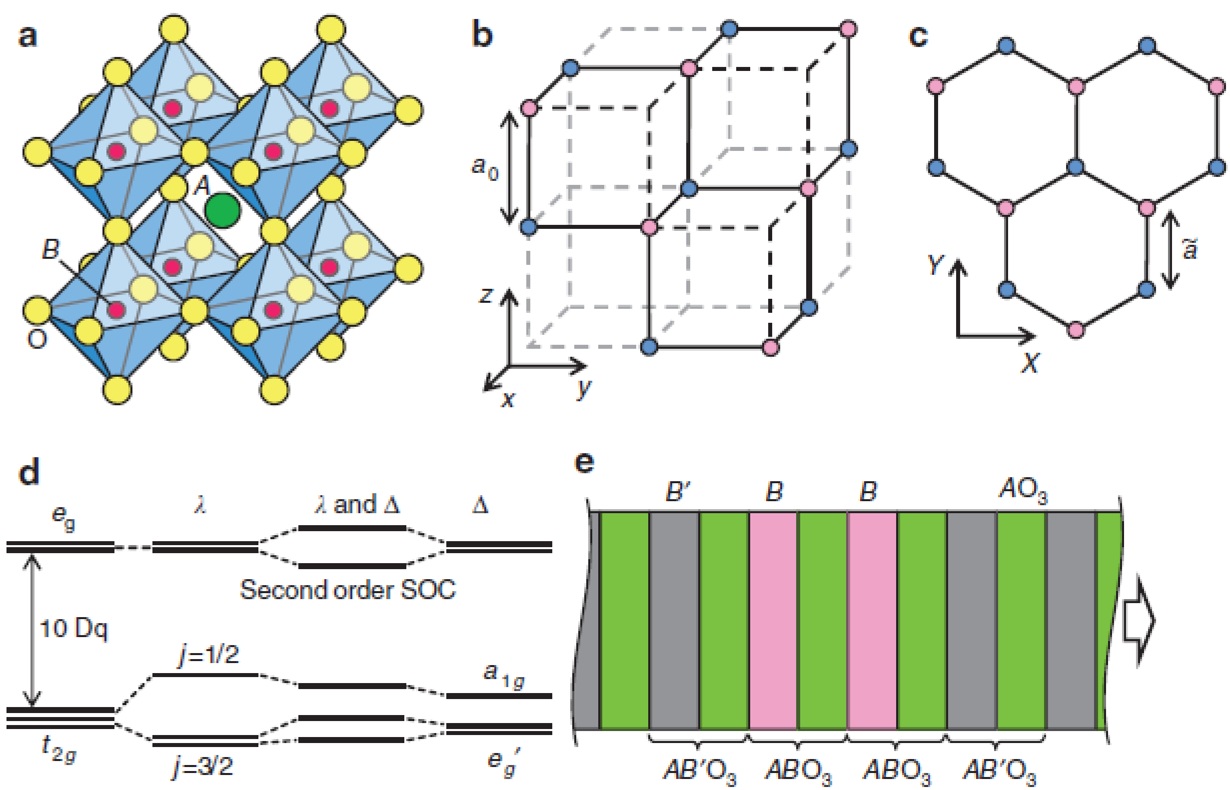
Santu Baidya
(SNBNCBS-> Duisburg-Essen
-> SNU-> Rutgers)

Arun Paramekanti
(U. Toronto)

Umesh Waghmare
(JNCASR, Bangalore)

Interface Engineering of QAH effects ?

Bilayers of Perovskites grown along [111]



Theoretical Prediction:

Combination of buckled honeycomb structure together with SOC can give rise to 2D time reversal Invariant TI.

Xia et al, Nature Commun. 2, 596 (2011)

QAH: MOTIVATION

For practical usage one would like to:

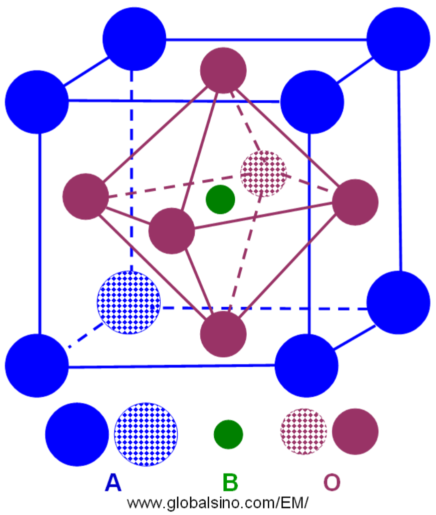
- **Boost the temperature scale for QAH effect**
  [Use d-electron systems rather s or p electron based systems.]

- **Engineer a large topological band gap**

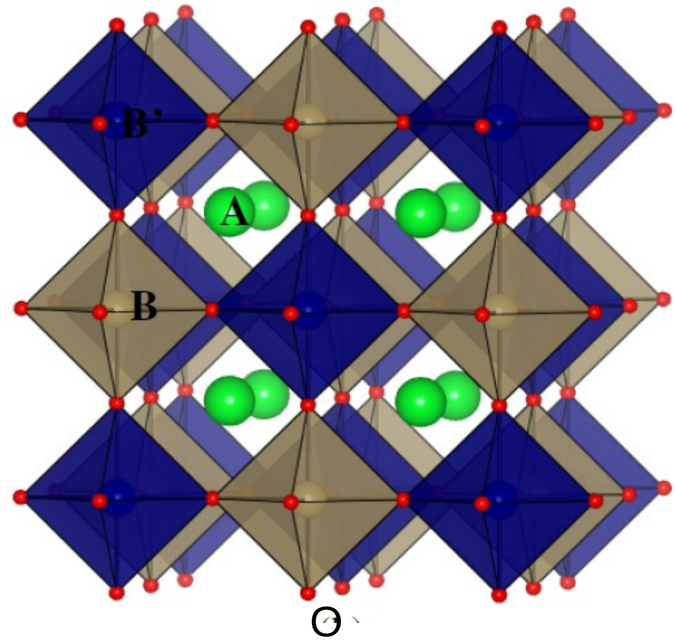
- **Avoid possible dopant or adatom-induced inhomogeneities by considering stoichiometric composition**
  [Doping TR-invariant TIs with magnetic atoms (Chang et al, Science 2013), Magnetic atoms on graphene (Qiao et al, PRB 2010), heavy atoms with large SOC on magnetic substrates (Garrity, PRL 2013)]

Double Perovskites : $A_2BB'O_6$

Perovskite: ABO_3



Doubling of unit cell
($A_2B_2O_6$)
Replacing one of B by B'
Ordering of B/B'



Diversity of Applications:

Spintronics: Sr_2FeMoO_6 (Nature, 1998; PRL 2000)

Multiferroicity: Bi_2NiMnO_6 (JACS, 2005)

Magnetodielectric: La_2NiMnO_6, La_2CoMnO_6 (Adv Mater 2005; PRL 2008; PRB 2008)

Magneto-optic Devices:
Sr_2CrWO_6, Sr_2CrReO_6, Sr_2CrOsO_6 (APL, 2008)

3d-4d/5d DPs:

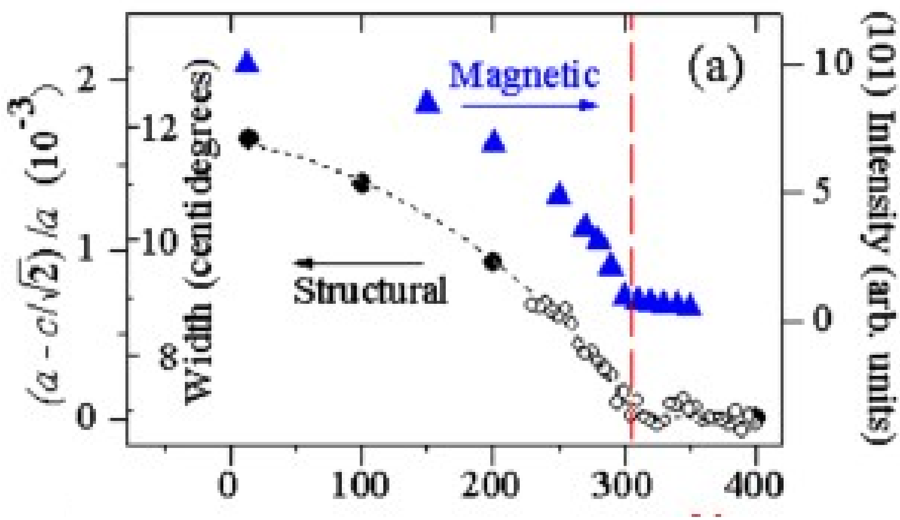
	U (eV)	J_H (eV)	Δ_{CF}	$\zeta \to Z^4$ $\lambda_{SO} = \zeta/2S$
3d	3 – 7	0.8 -0.9	$\Delta \sim J_H < U$	0.01 – 0.1
4d	2 – 3	0.5 – 0.7	$\Delta \sim U > J_H$	0.1 – 0.4
5d	1 – 2	0.4 – 0.5	$\Delta > U > J_H$	0.4 - 1

- ***3d*** **TM (B) can allow for a high energy scale for magnetism, while the** ***4d/5d*** **TM (B') can feature strong SOC.**

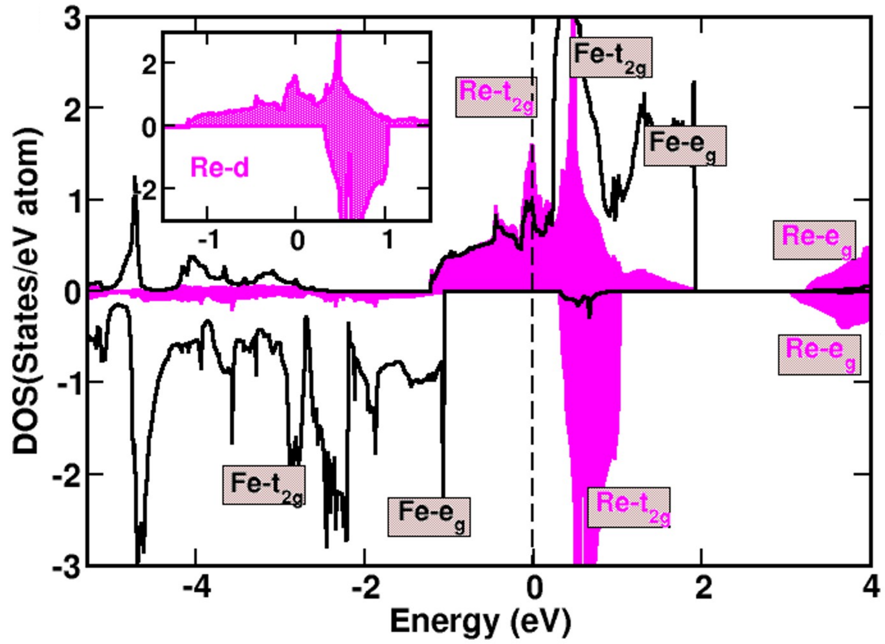
- **Physical separation of ions hosting magnetism from those hosting strong SOC, avoids the issue related to interplay of correlation effect and SOC at the same site.**

- **Low energy physics is described by t_{2g} bands ⇨ suppresses JT (trivial Ins)**
  [Doennig et al, PRB 2016, $(LaXO_3)_2/(LaAlO_3)_4$ X = Ti-Cu]

Ba_2FeReO_6 (BFRO) : Half-metallic (HM) ferromagnet with transition temperature of 304 K

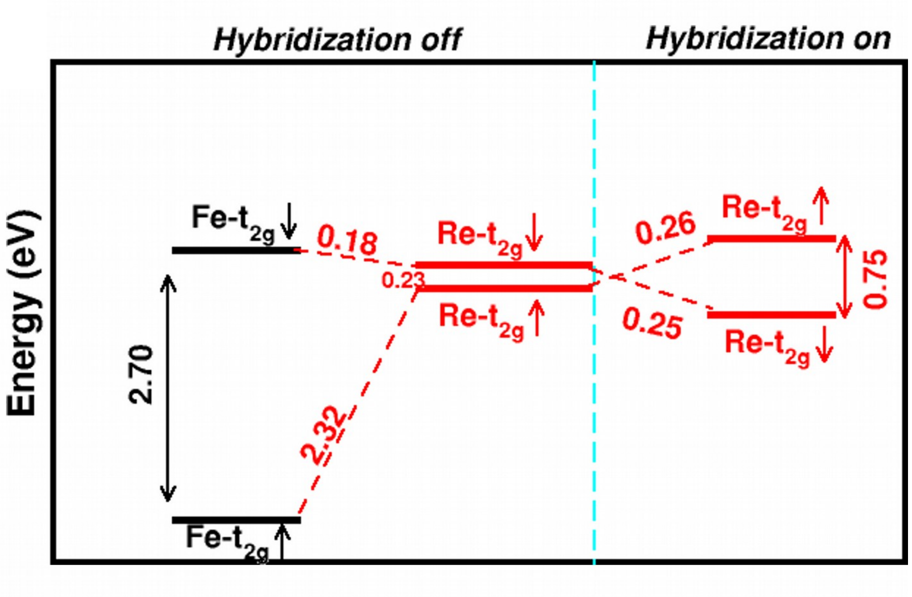


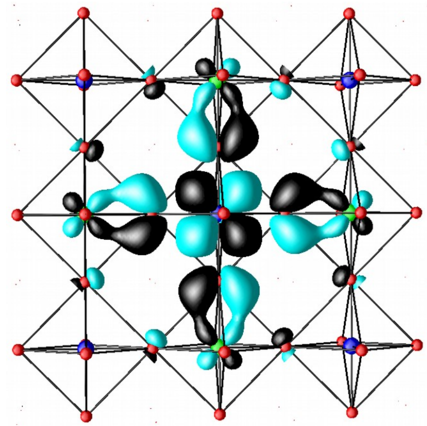
Phys. Rev. Lett. 98, 017204 (2007).

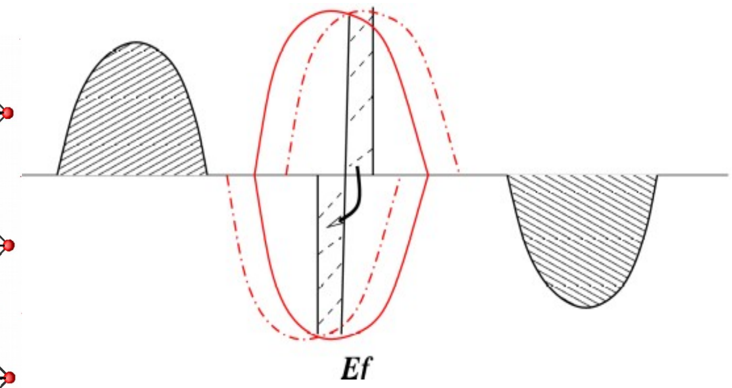


Ferromagnetism is driven by hybridization driven mechanism as found in Sr_2FeMoO_6

Sarma, Mahadevan, TSD, et al, Phys. Rev. Lett. 85, 2549 (2000)







Effective double exchange type model Hamiltonian

Fe^{3+}**: 3d⁵**: Hund's rule: Large (classical) spin **S=5/2** : Site-localized.

Re^{5+}**: 4d²**: Mobile electron: gives rise to metallic behavior.

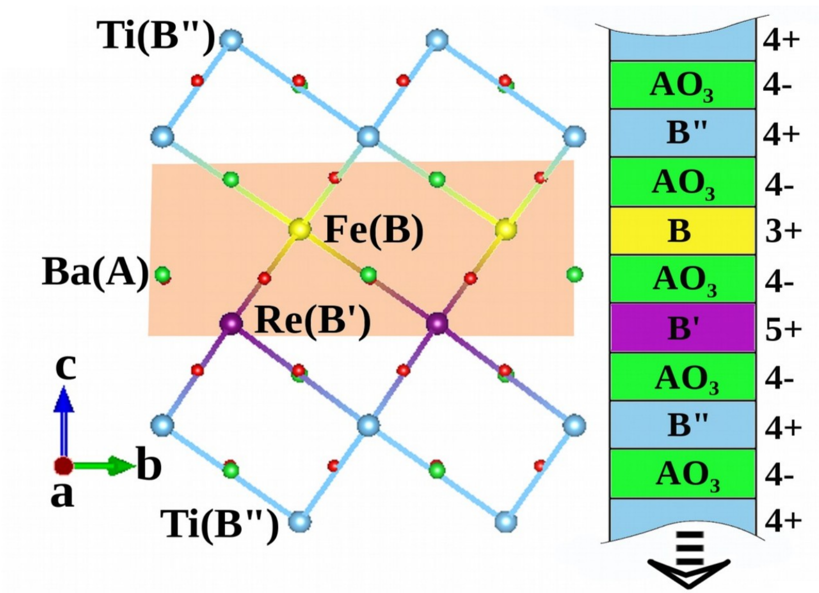
Ferromagnet: **S_{total}= 3/2**

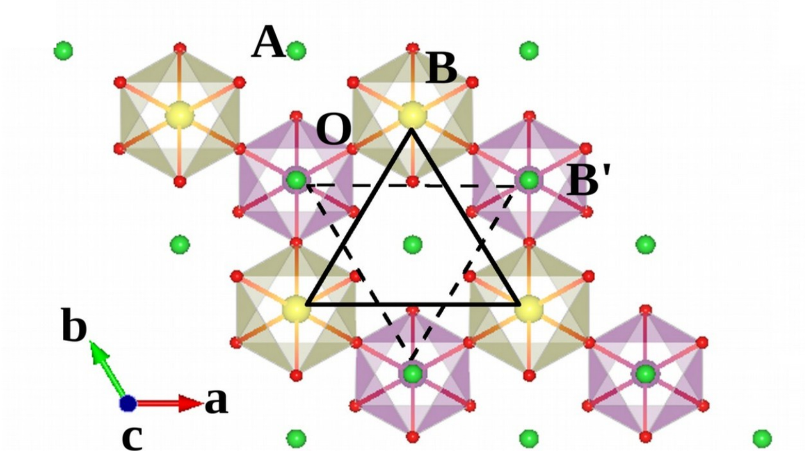
2-sublattice Kondo lattice Hamiltonian : Energy scales: t_{FeRe}, $\Delta=\varepsilon_{Re}-\varepsilon_{Fe}$, J

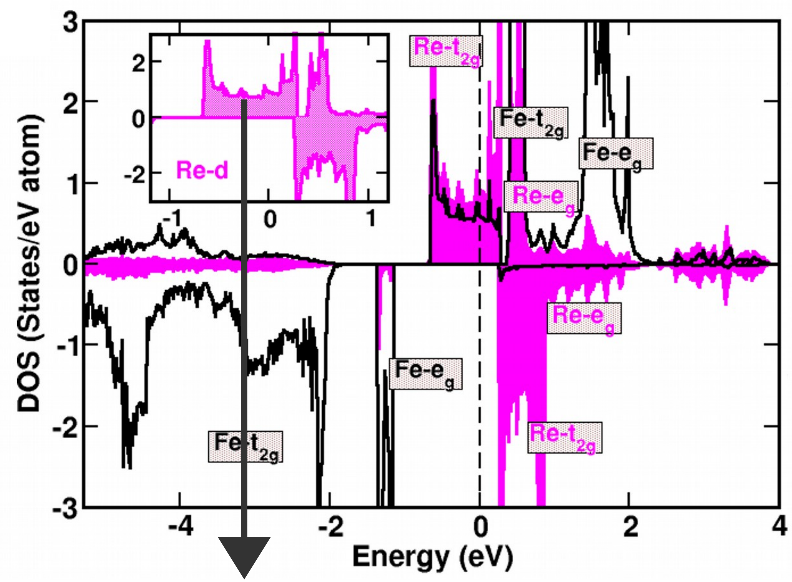
$$H = \varepsilon_{Fe} \sum_{i \in B} f^{+}_{i\sigma,\alpha} f_{i\sigma,\alpha} + \varepsilon_{Re} \sum_{i \in B'} m^{+}_{i\sigma,\alpha} m_{i\sigma,\alpha} + t_{FM} \sum_{<ij>\sigma,\alpha} (f^{+}_{i\sigma,\alpha} m_{j\sigma,\alpha} + h.c.) + J \sum_{i \in B} S_i \cdot f^{+}_{i\alpha} \sigma_{\alpha\beta} f_{i\beta}$$

Consider quantum wells of a double perovskite (Ba_2FeReO_6) embedded in a wide band gap insulating oxide ($BaTiO_3$)

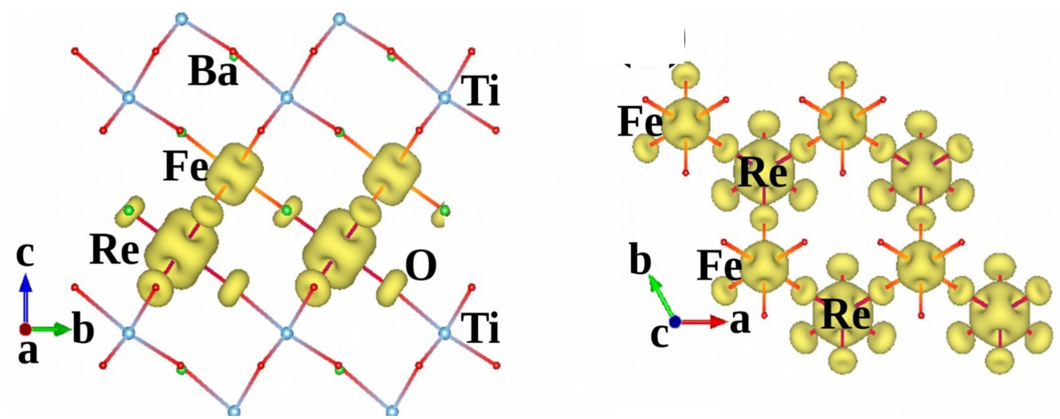
[111] growth direction







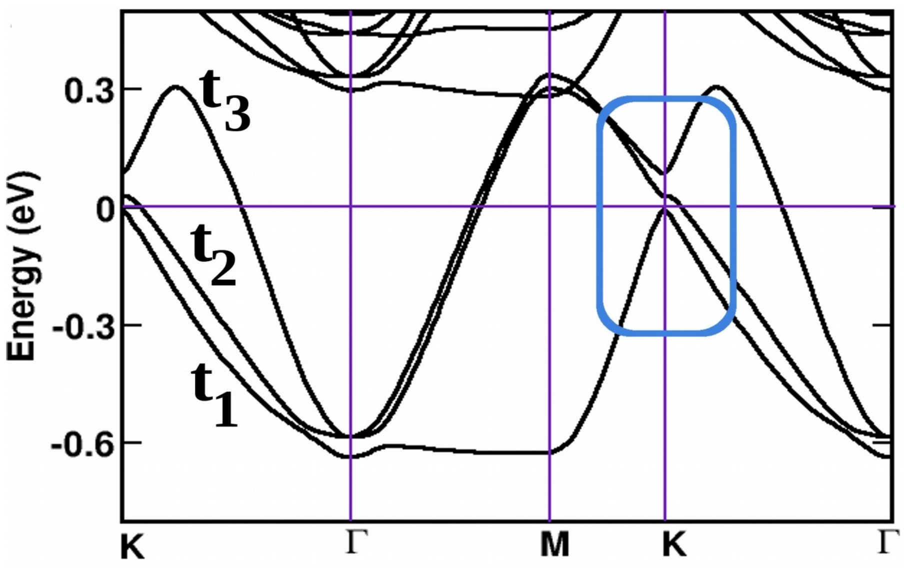
Signature of 1-D features ➡ Reduced dimensionality



☆ **Highly confined 2D electron gas**

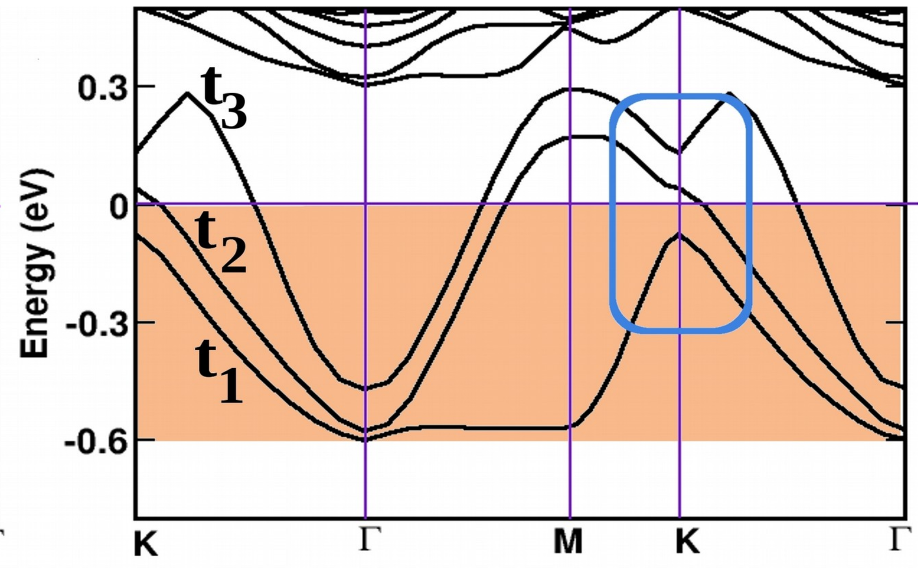
Band structure of [111] heterostructure

GGA



GGA+SO

[Topological HM band structure]



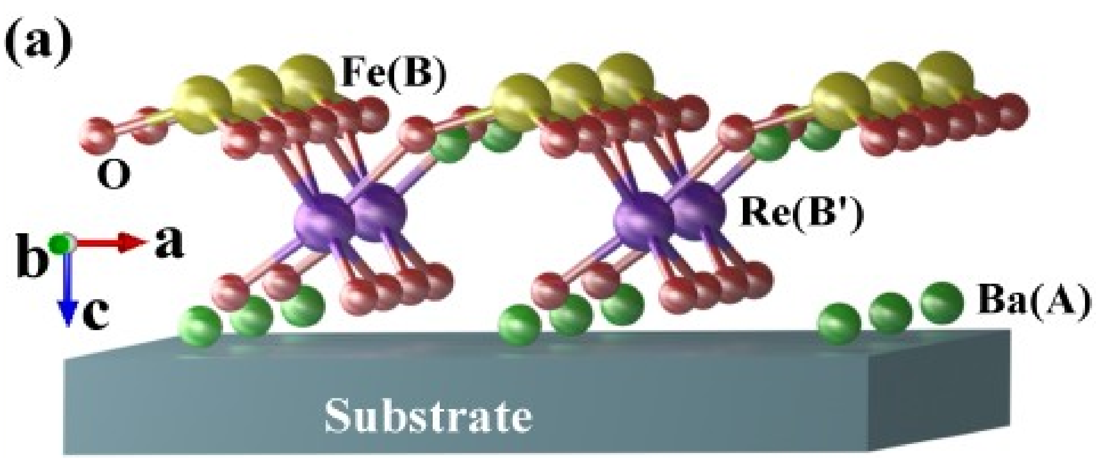
Nontrivial Chern numbers for t_1 and t_2 bands: -2, 2

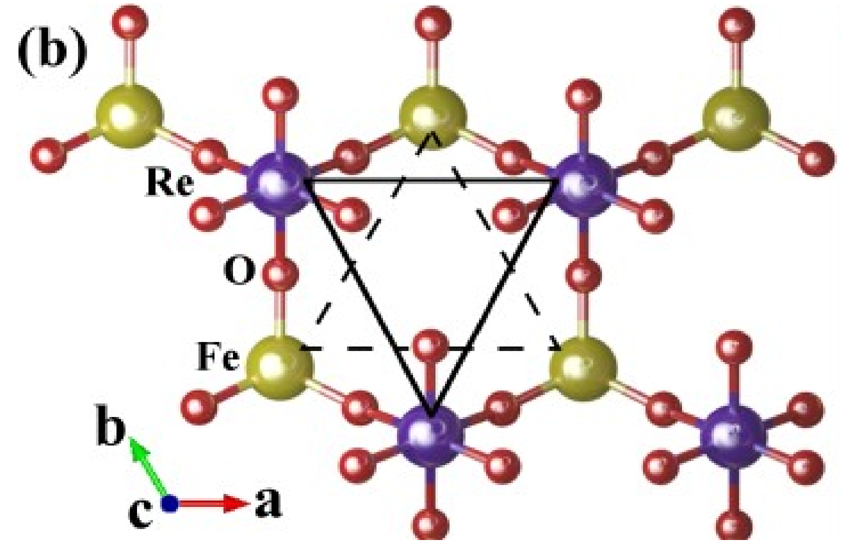
$$C_n = \sum_{n' \neq n} \int \frac{d^2\mathbf{k}}{2\pi} \, \mathrm{Im} \frac{\langle n\mathbf{k}|v_x(\mathbf{k})|n'\mathbf{k}\rangle\langle n'\mathbf{k}|v_y(\mathbf{k})|n\mathbf{k}\rangle}{(E_n(\mathbf{k}) - E_{n'}(\mathbf{k}))^2}$$

The (111) bilayer thus can be a quantum anomalous Hall insulator, if t1 and t2 bands can be prevented from spanning a common energy window.

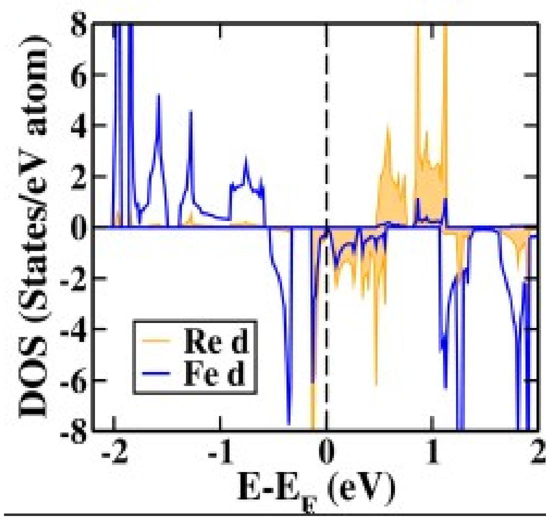
Santu Baidya, Umesh Waghmare, Arun Paramekanti, TSD Phys. Rev. B 92, 161106(R) (2015)

TRY OVERLAYER-SUBSTRATE GEOMETRY

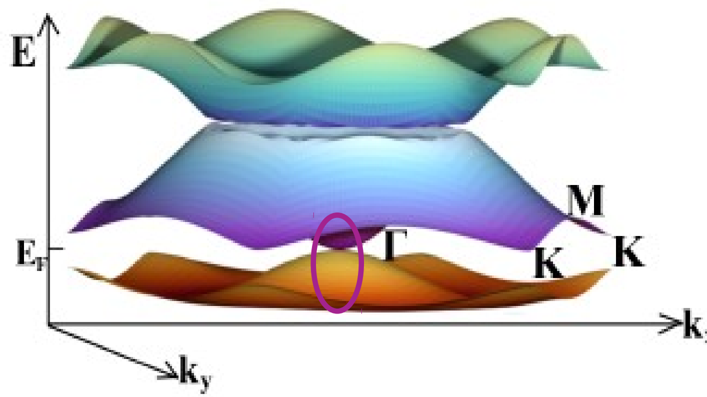


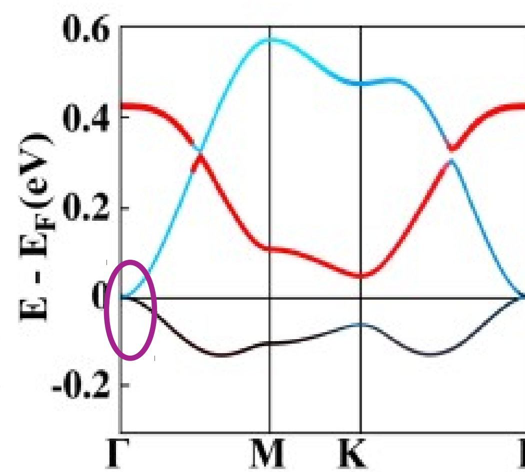


GGA electronic structure:



Band structure in minority spin spin





Half-metallic!

Overlayer: $Fe^{2+}(d^6)$-Re^{6+} (d^1)

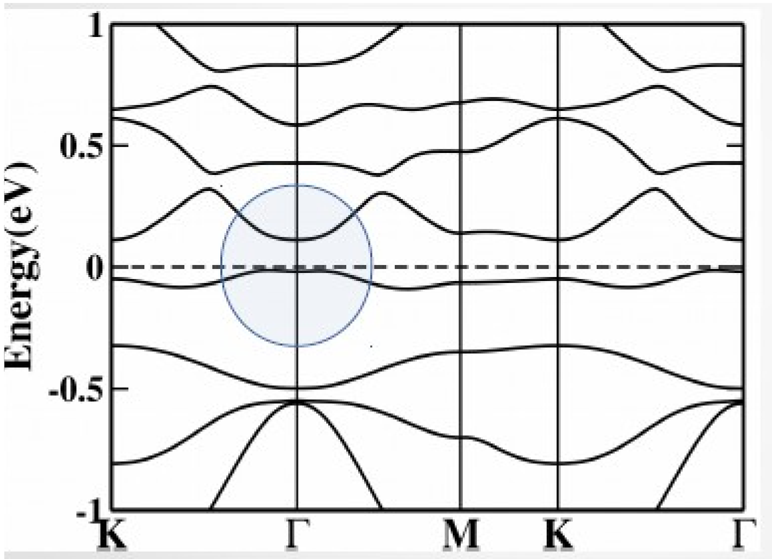
Bulk/QW : $Fe^{3+}(d^5)$-$Re^{5+}(d^2)$

Gapped at every point except Γ (half semi-metal)

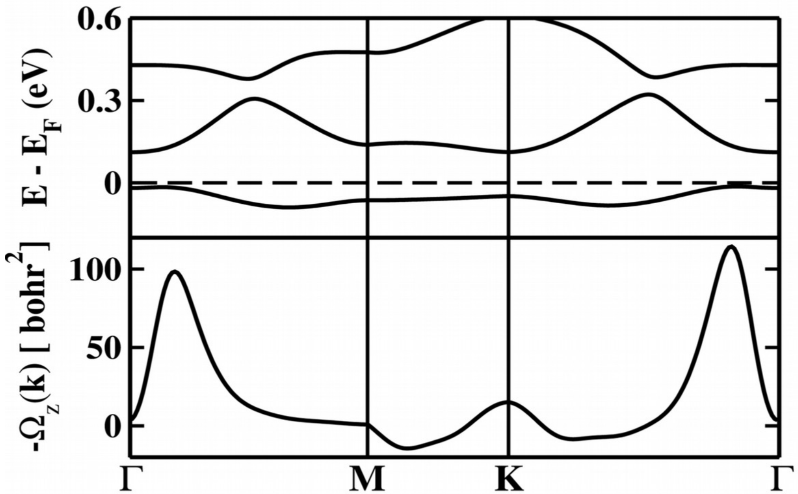
Charge Redistribution

Quadratic band touching at Γ

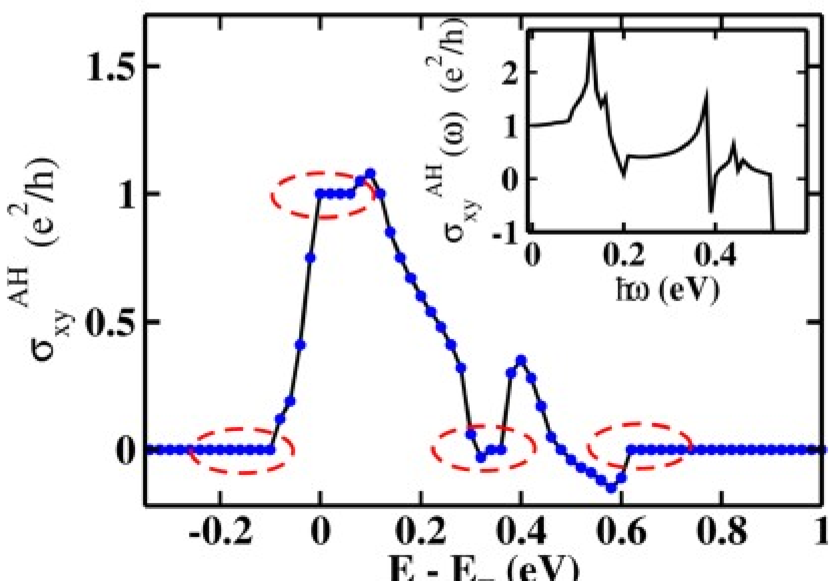
Effect of SOC: GGA +SOC electronic structure



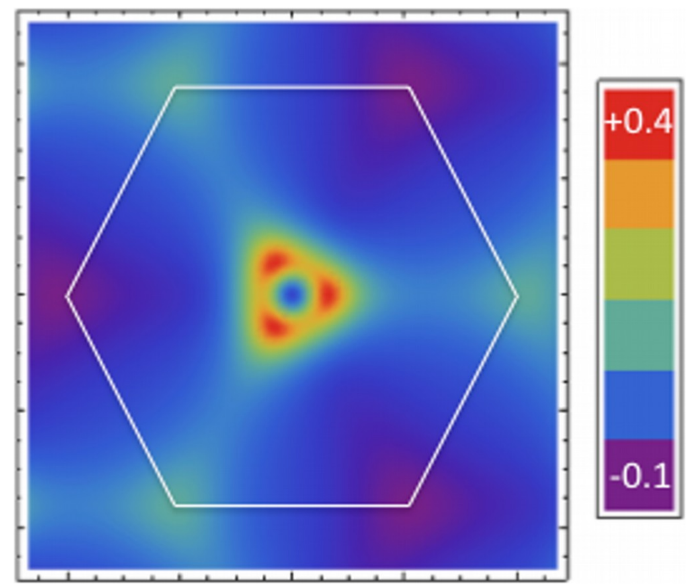
Large gap ~ 110 meV



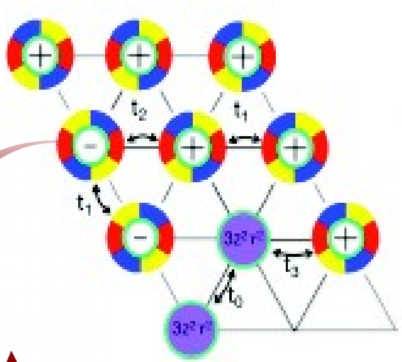
Inclusion of SOC gaps out the QBT

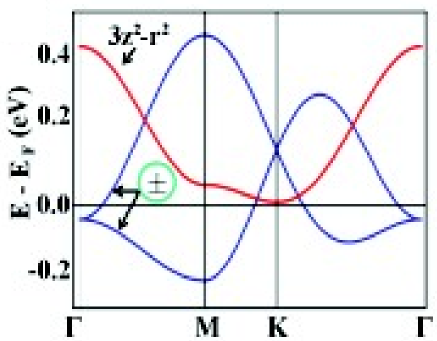


C = 1



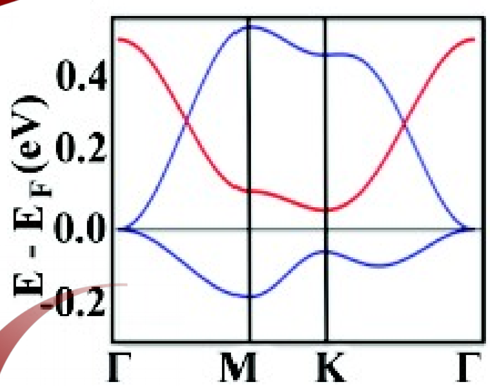
Analysis of band structure: 3 band TB model

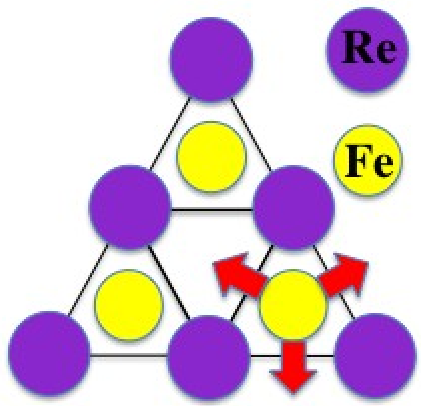




3 band model derived from 5d Re t_{2g} bands in reduced C_3 symmetry

Dirac BT at hexagonal BZ corners and QBT at Γ

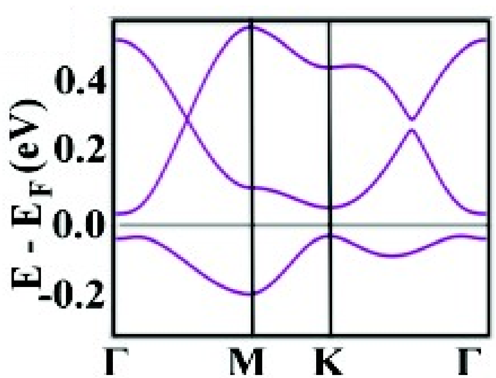




In-plane inversion symmetry breaking by localized 3d Fe generates in-plane electric field that couples with electric dipoles formed by +/- e_g^{π} doublets

Gaps out the Dirac points at BZ corners.

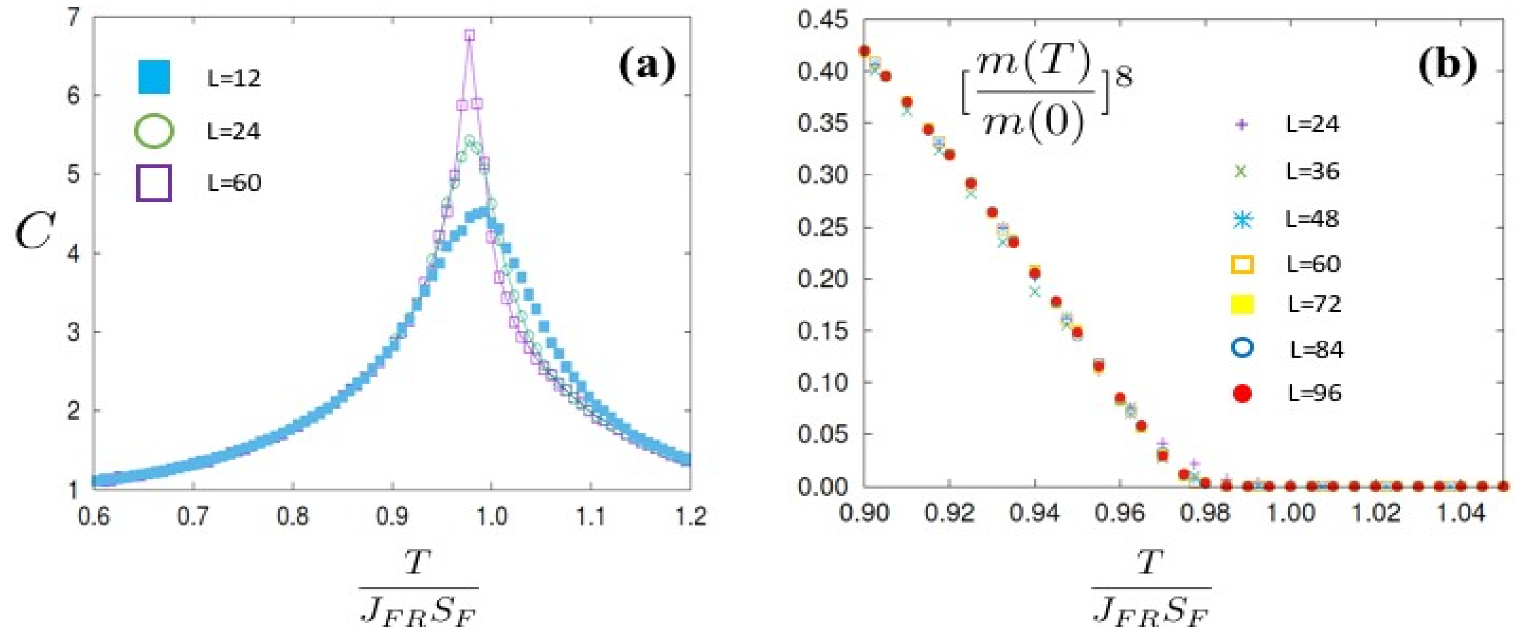
► ***Orbital Rashba-type effect (PRL 2011)***



Introduction of SOC term gaps out the QBT.

►For **right filling** (*d^1* of Re), this leads to QAHI

Strong SOC and trigonal distortion conspire to pin the Re moments to be perpendicular to the plane, leading to high FM T_c



DFT: **$J_{Fe\text{-}Fe}$ (bulk) ~ 1 meV** [agrees well INS Phys. Rev. B 87, 184412 (2013)],

$J_{Fe\text{-}Fe}$ (bilayer) ~ 3.5 meV

$$H_{Fe-Re} = J_{F\text{-}R} \Sigma_{i \in Fe,\delta} S_i^z \sigma_{i+\delta}$$

Monte Carlo

(mixed Heisenberg-Ising): **T_c ~ 315K** **(even slightly higher than bulk!)**

Three Key Ingredients

1. [111] Bilayers of half-metallic 3d-4d/5d DPs show a strong **trigonal** distortion, favoring a non-Kramers doublet from t_{2g} states of 4d/5d TM in reduced C_3 symmetry → bands in conducting spin channel features **Dirac band touching at +/- K, and a QBT at Γ.**

2. Breaking of in-plane inversion symmetry by 3d TM ions gaps out Dirac points BZ corners (**orbital Rashba effect**) → for appropriate filling of 4d/5d this leads **half semi-metal**.

3. Strong SOC of 4d/5d TM ions gaps out QBT. *Strong SOC and trigonal distortion also conspire to pin 4d/5d moments perpendicular to the plane, maintaining high FM T_c even for bilayer.*

Should be general [DPs like Sr_2FeMoO_6 (T_c – 420 K), Sr_2CrWO_6(T_c – 458 K)]

Santu Baidya, Umesh Waghmare, Arun Paramekanti, TSD Phys. Rev. B 94, 155405 (2016)

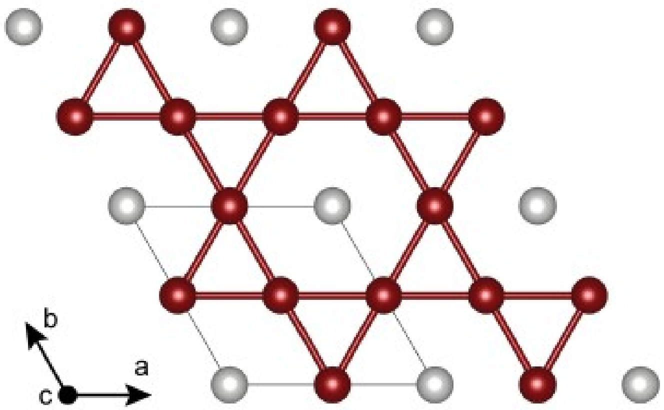
KAGOME INTERMETALLICS

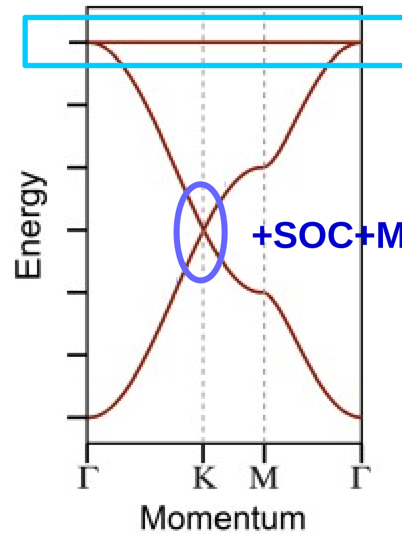
Santu Baidya
(SNBNCBS-> Duisburg-Essen -> SNU-> Rutgers)

Aabhaas Mallik
(ICTS, Bangalore)

Subhro Bhattacharya
(ICTS, Bangalore)

Isolated Kagome' Layer





Phenomenology of Landau levels without external magn field

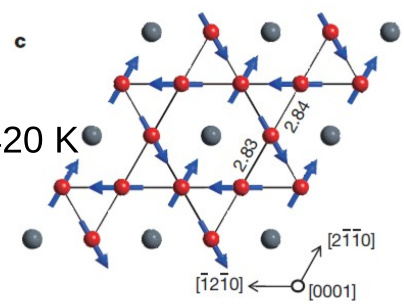
+SOC+Magn

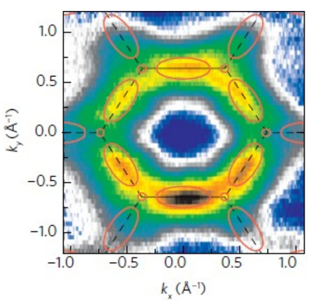
2D Chern Insulator (QAH)

Binary intermetallic T_mX_n Kagome series (T = Mn/Fe/Co, X = Sn/Ge, $m{:}n$ = 3:1,3:2,1:1)

Mn_3Sn

AFM, T_N ~ 420 K



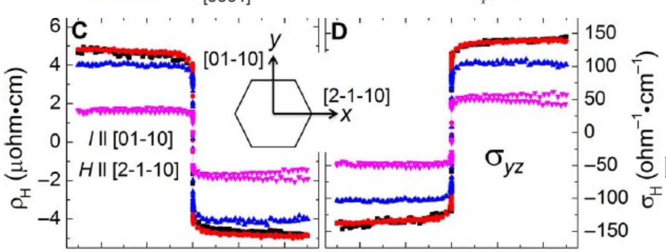


Large Anomalous Hall at RT (Nature, 2015)

Magnetic Weyl points (Nature Mater, 2017)

Mn_3Ge

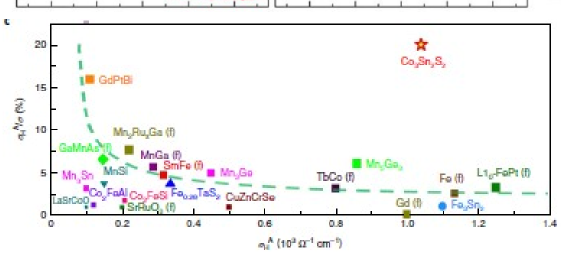
AFM, T_N ~ 365 K



Large Anomalous Hall (Sci Adv, 2016)

$Co_3Sn_2S_2$

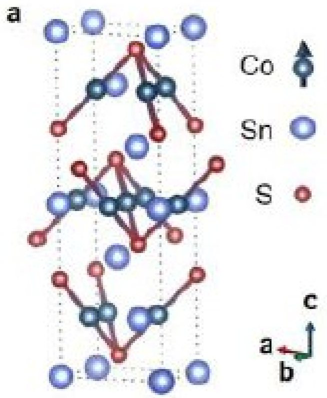
FM, T_c ~ 170 K

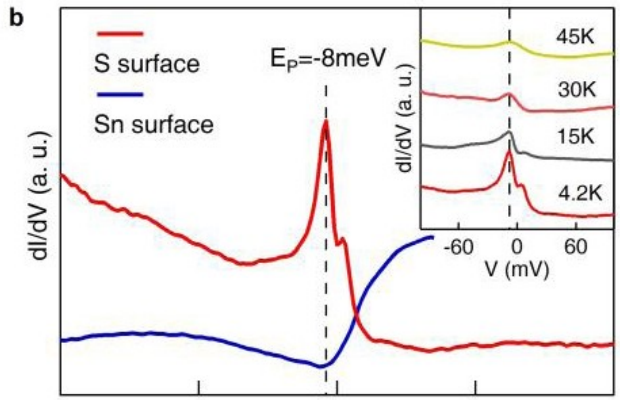


Giant Anomalous Hall (Nat Phys, 2018)

Search for Flat Bands

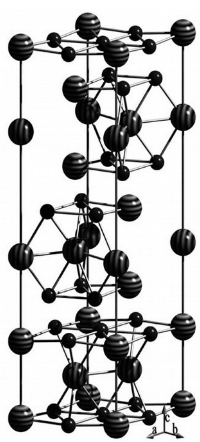
$Co_3Sn_2S_2$

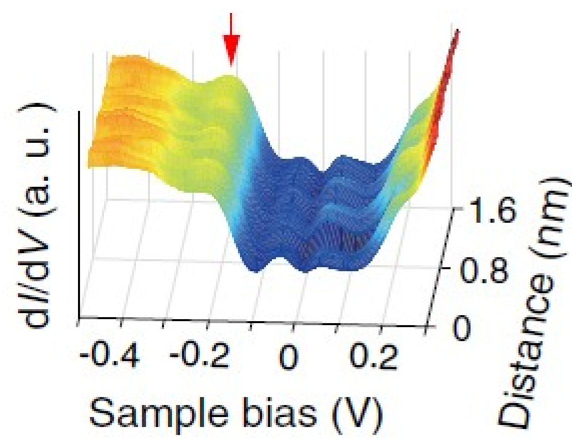




Nat Phy 15, 443 (2019)

Fe_3Sn_2

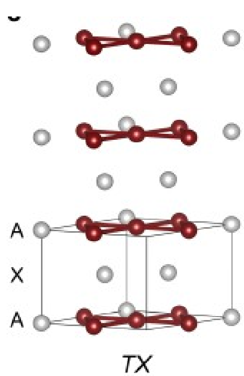


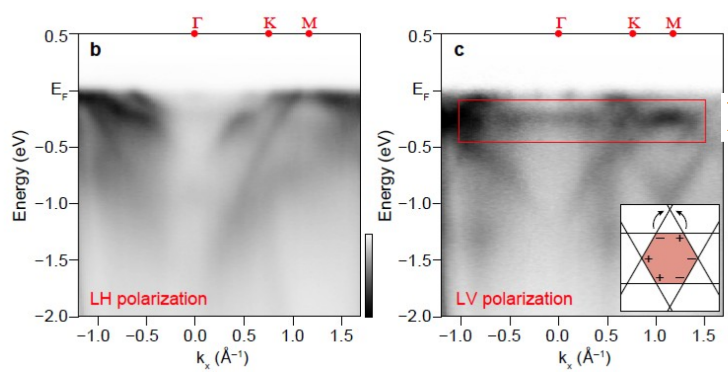


PRL 121, 96401 (2018)

Direct Signatures remain elusive

FeSn
(A-type AFM
FM Kagome layers
coupled AF)



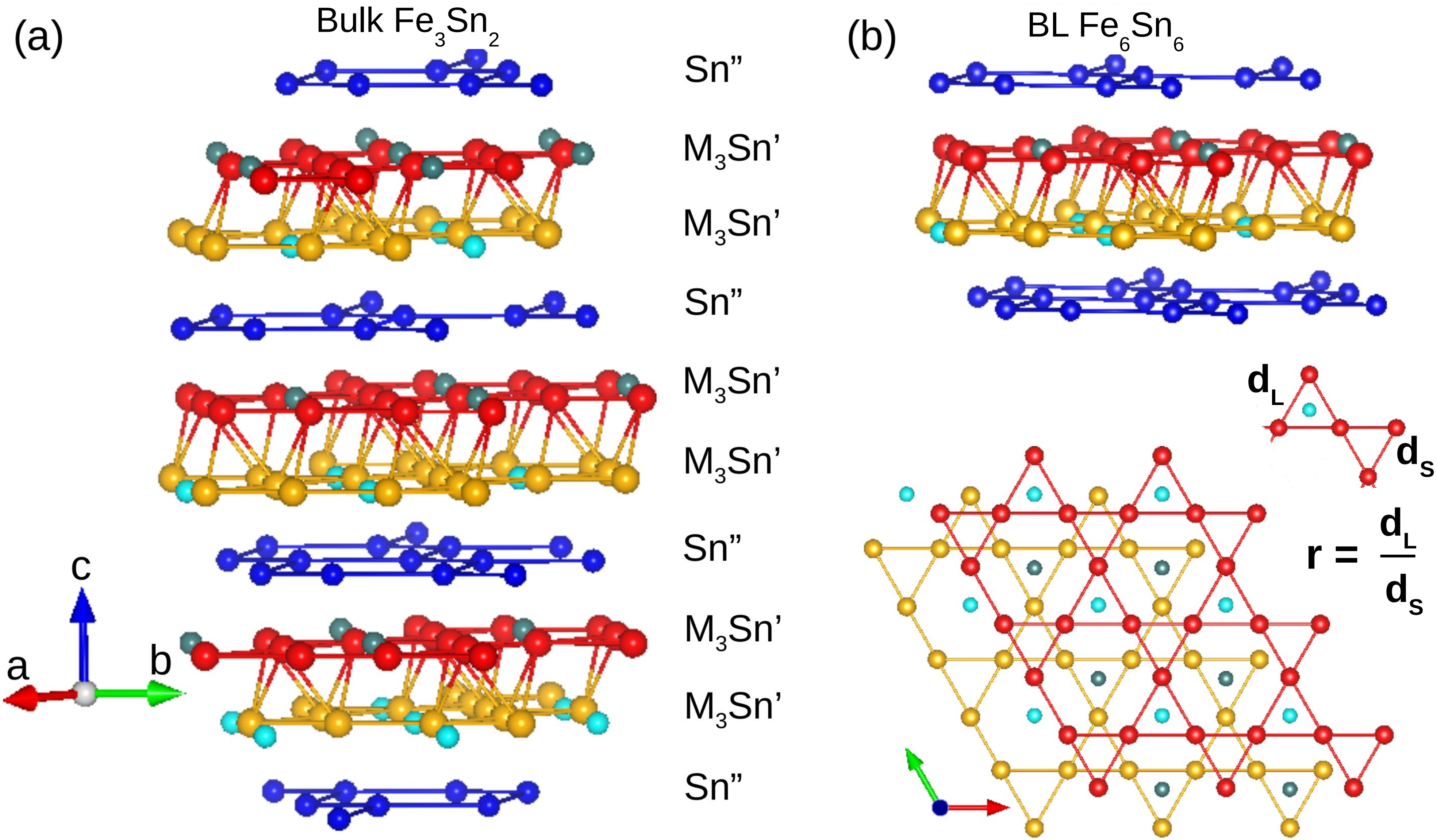


$E_{flat} = -0.23$ eV

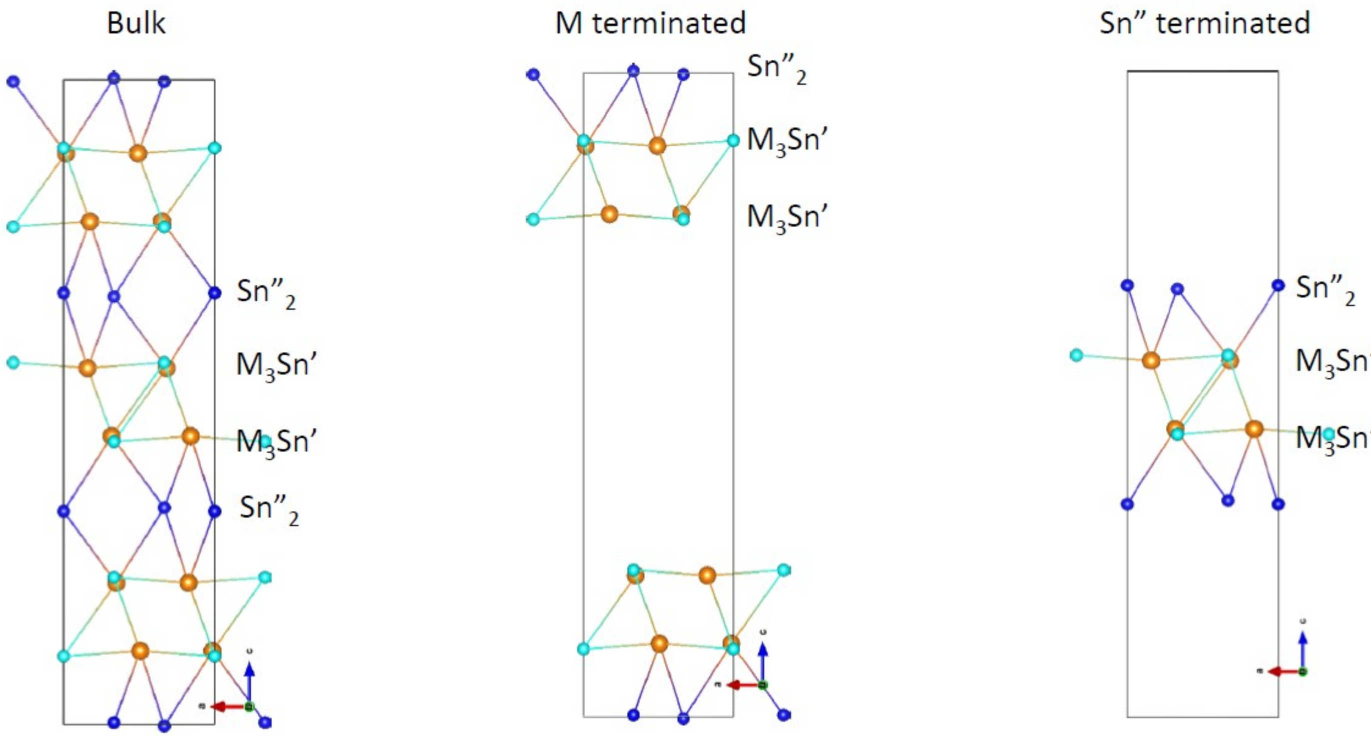
Kang et al, arXiv:1906.02167

Can it be made better ?

How about creating 2D (quasi-2D) compounds ?



CLEAVAGE ENERGY

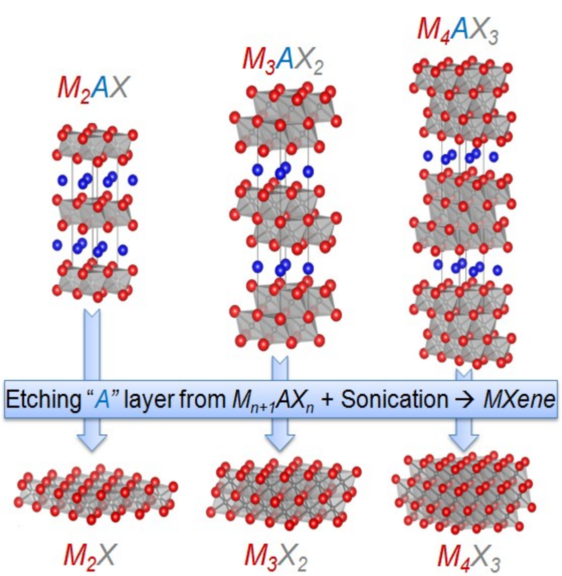


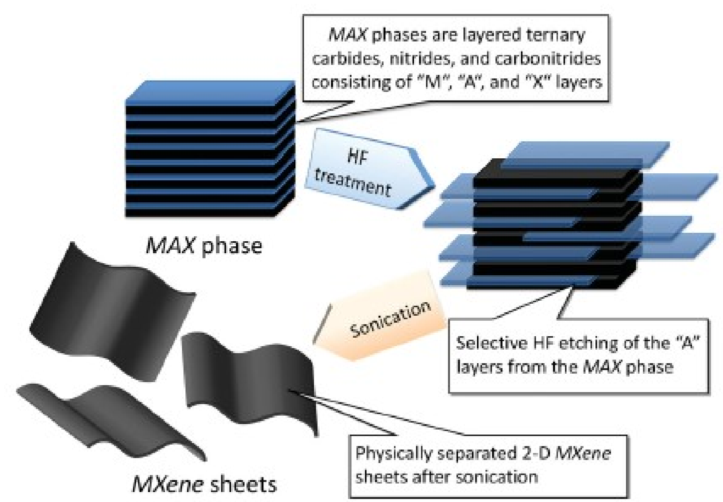
1.762

(J/m^2)

Cleave Energy = (Energy$^{\text{M-term}}$ + Energy$^{\text{Sn''term}}$ - Energy$^{\text{Bulk}}$) / (2 * Area of surface of the slab)

Employ *chemical etching* route

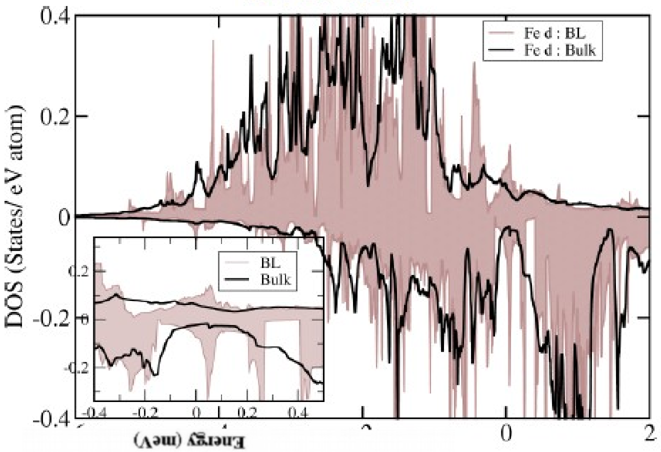




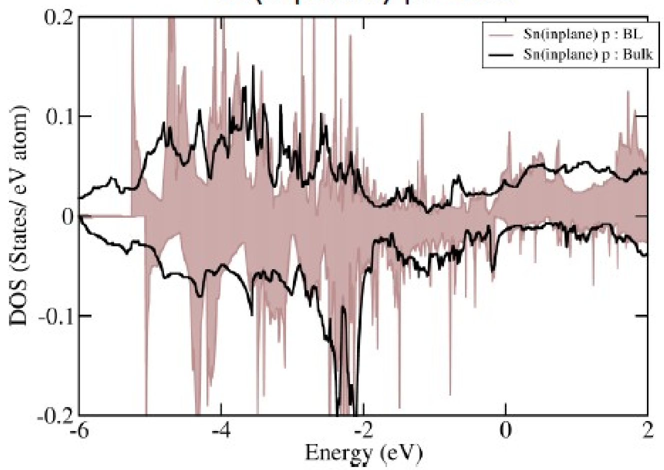
Adv.Mater.2014,26,992-1005

Electronic Structure – Bulk vs BL

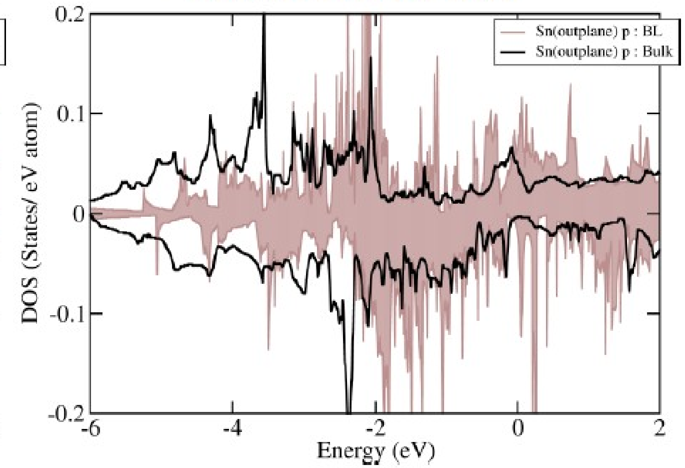
Fe d PDOS

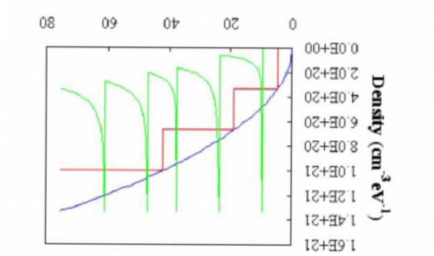


Sn(inplane) p PDOS



Sn(outplane) p PDOS





Effective mass at “K” in the BZ

band	$m_{[100]}$	$m_{[010]}$	$m_{[001]}$
1	-3.50	-0.46	2041
2	-2.50	11.3	-2176
3	-5.43	0.33	16297

Spin moment in μ_B

	Bulk(Rhomb)	Bilayer
Fe :	2.2	2.0
Sn’ :	-0.2	-0.2
Sn”:	-0.13	-0.1

Total moment:

	Bulk(Rhomb)	Bilayer
	12.3217	11.5432

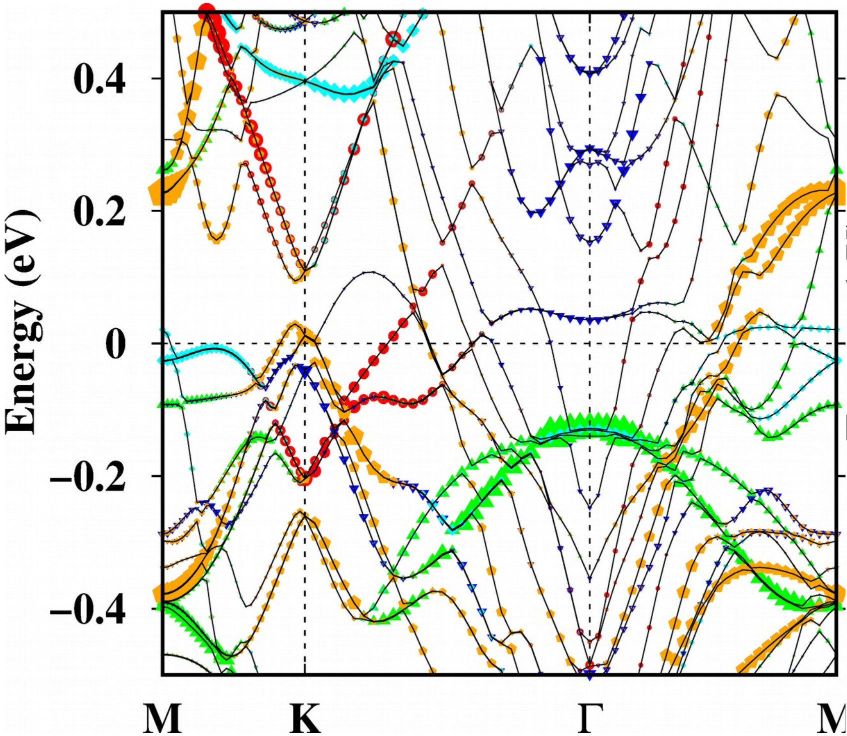
Magnetic exchanges:

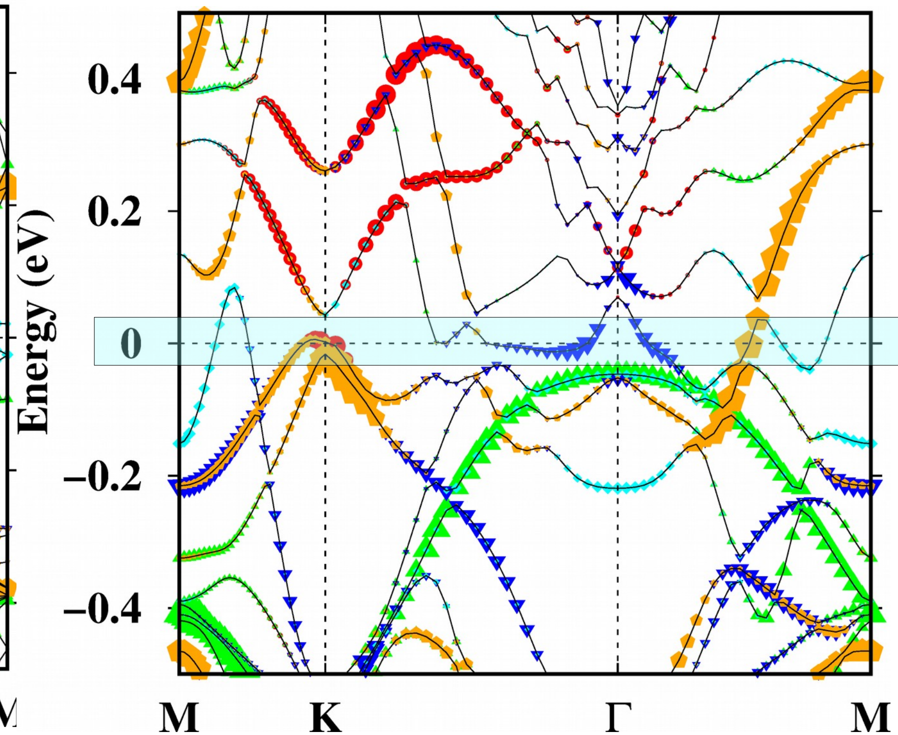
$J_{||}$ ~ 10 meV

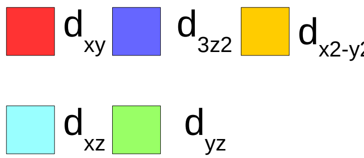
$J_{\perp}$ ~ 0.3 meV

FM correlation survives down to BL

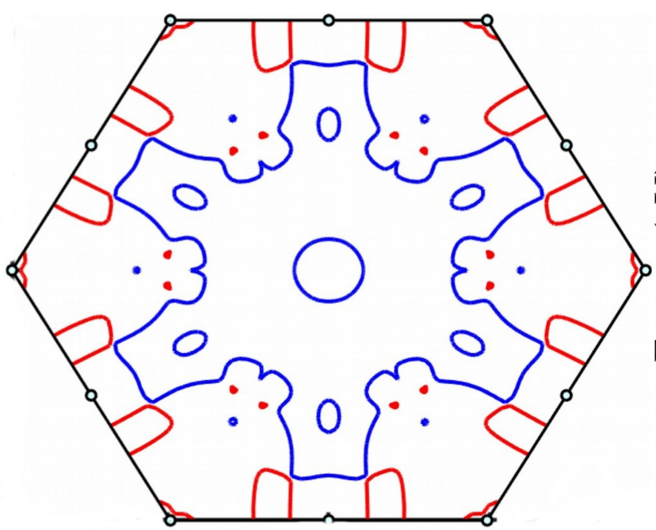
Electronic Structure – Bulk vs BL

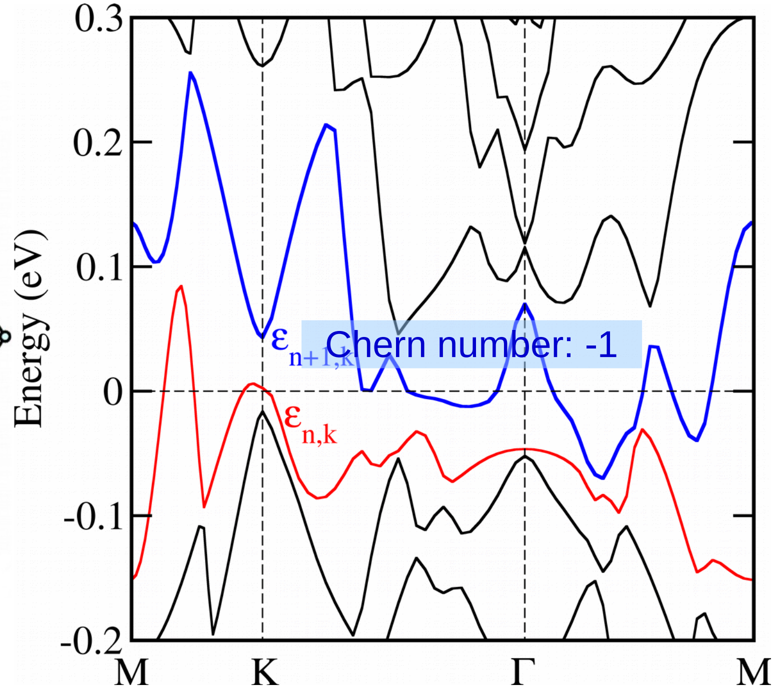


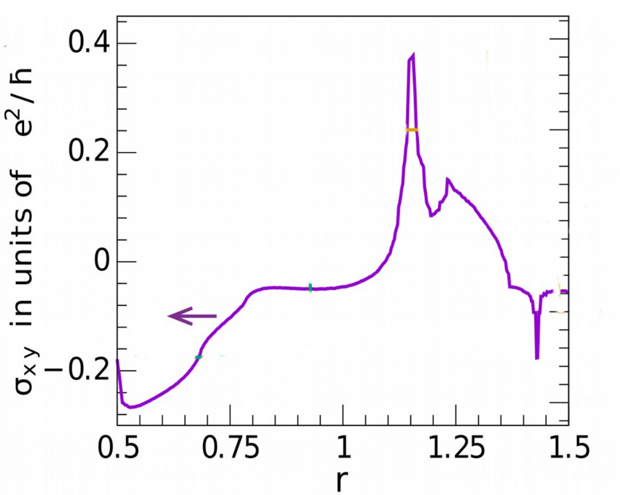




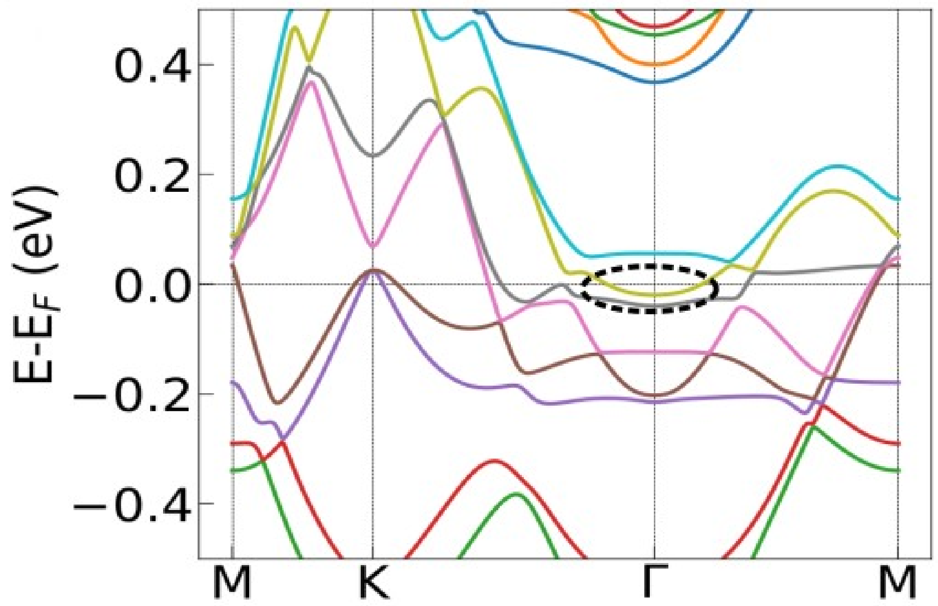
Signature of "*flat bands*" within 10 meV of E_f

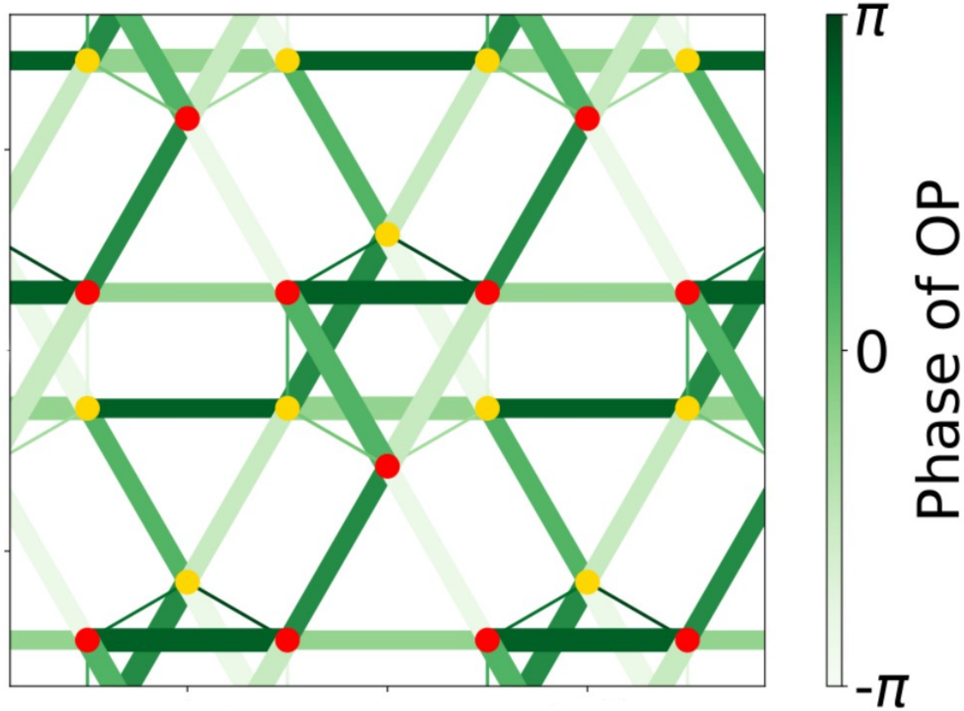


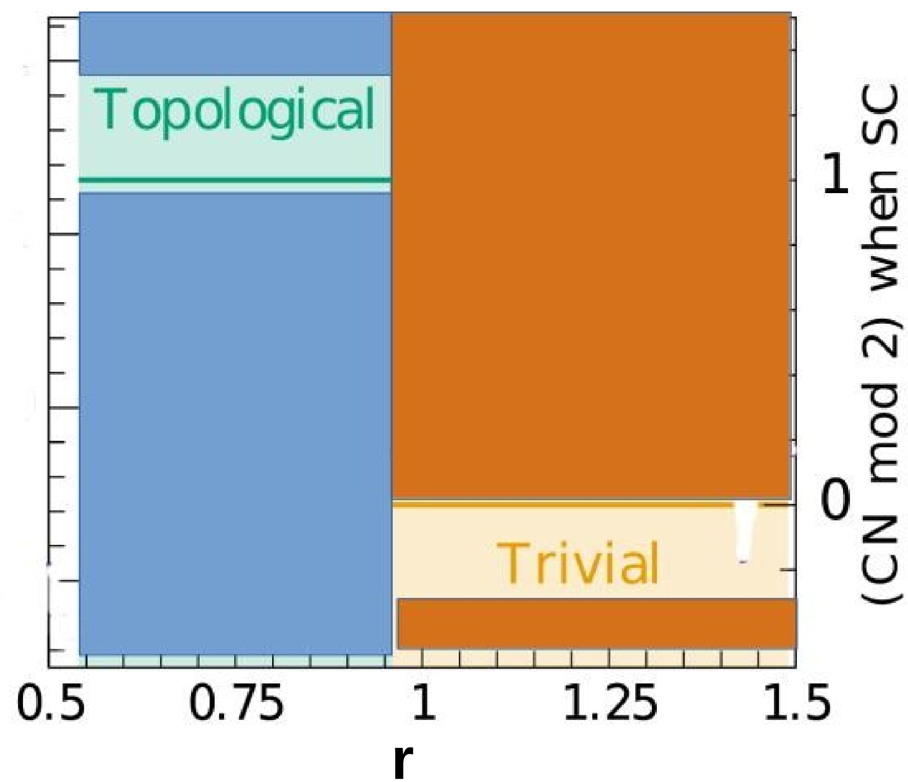




Unconventional Superconductivity







Conclusions

1. Geometric confinement to bilayer, results in (a) **quasi-2D or 2D** electronic structure, (b) survival of **ferromagnetic correlation**, and (c) realization of low-energy bands with suppressed band width – almost **flat bands.**

2. Finite AHC response for a wide range of asymmetry parameter, r. → Robust feature of a possible **Chern metal** phase in bilayer FeSn and allied materials.

3. Destruction of magnetic long-range order due to enhanced quantum fluctuations in low dimension can lead to **exotic superconductivity** (or fractional Chern insulating phase).

Santu Baidya, Aabhaas Vineet Mallik, Subhro Bhattacharjee, TSD, under preparation

GRAPHENE UNDER DEFORMATION

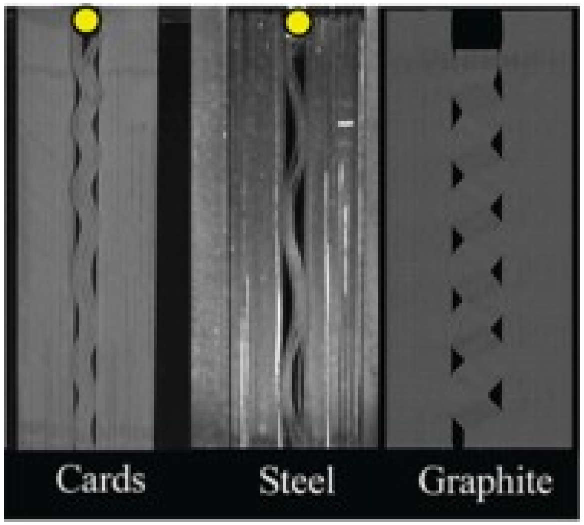
Santu Baidya
(SNBNCBS-> Duisburg-Essen -> SNU-> Rutgers)

Surajit Sengupta
(TIFR, Hyderabad)

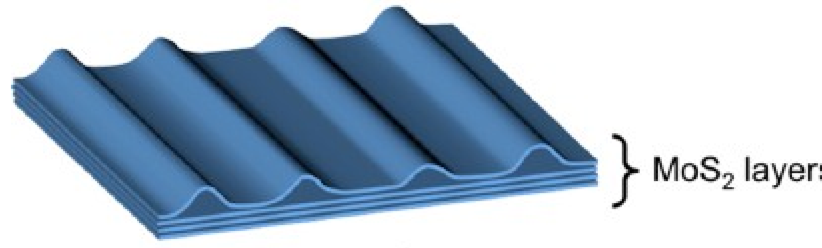
Debankur Das
(TIFR, Hyderabad)

C. Sandhya
(TIFR, Hyderabad)

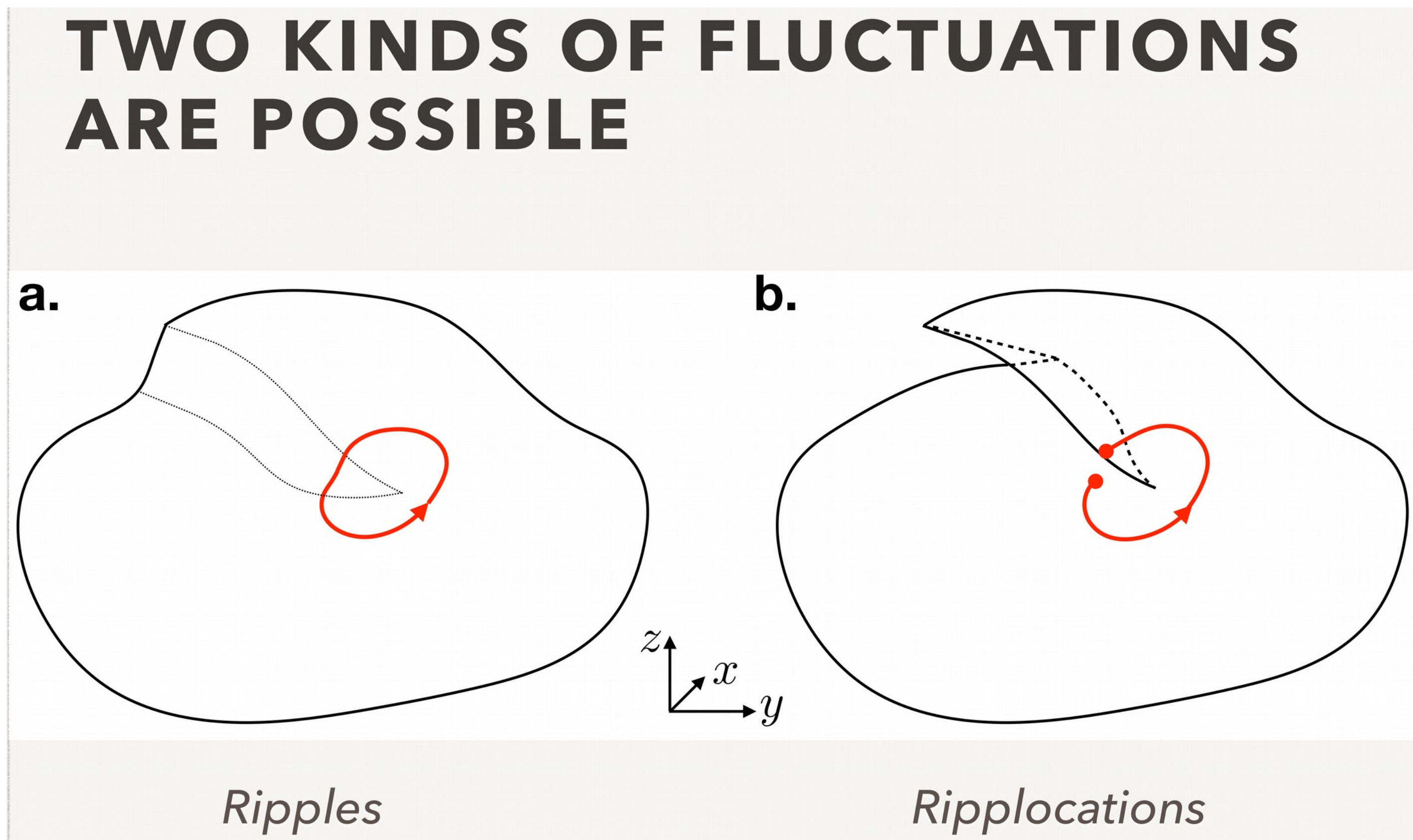
Deformation Mechanism in Layered Solids



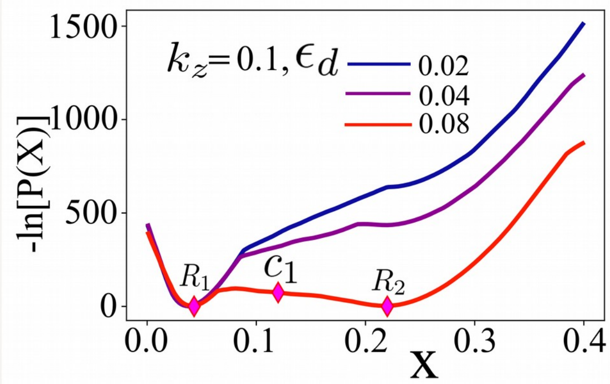
Phys. Rev. Materials 3, 013602 (2019)



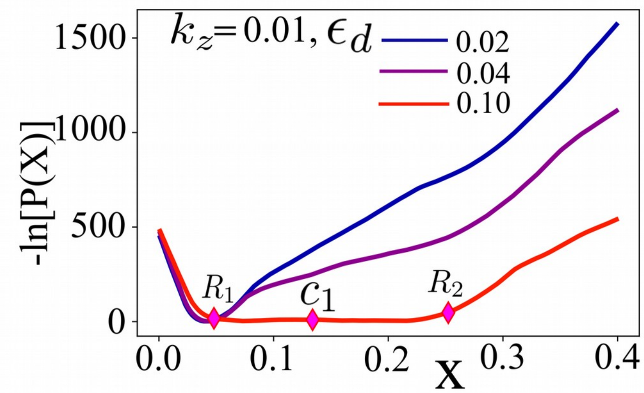
Nano Lett. 2015, 15, 1302−1308



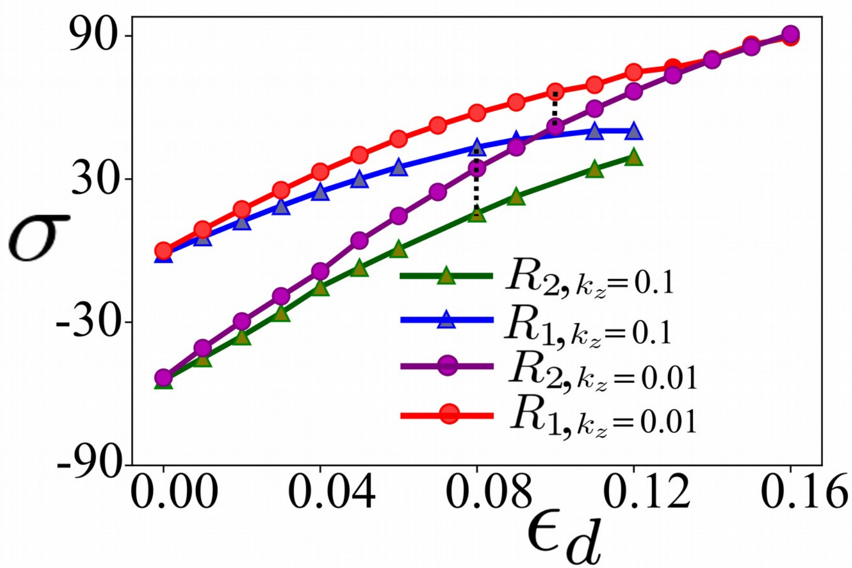
STRONG CONFINEMENT FAVOURS RIPPLOCATIONS

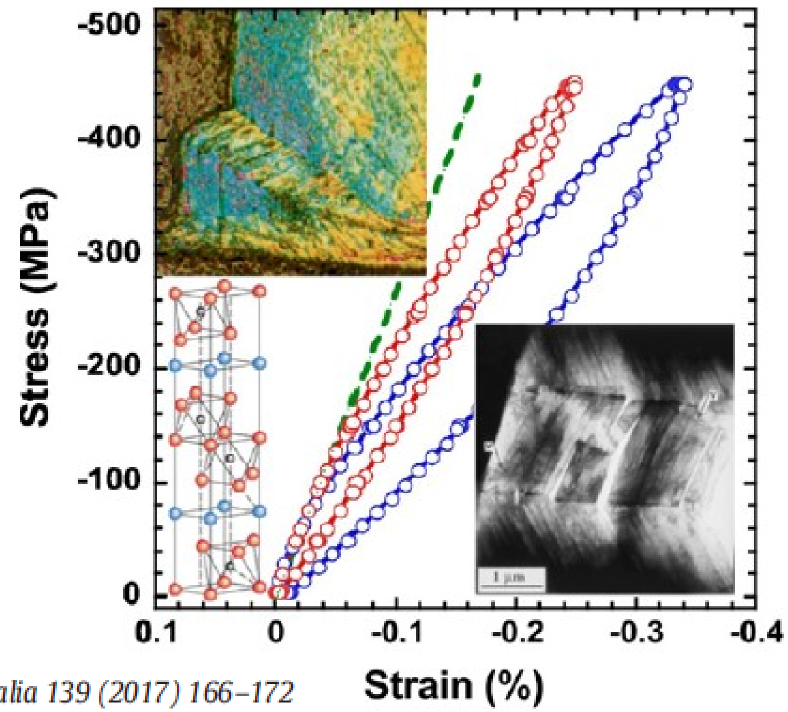


Ripplocations



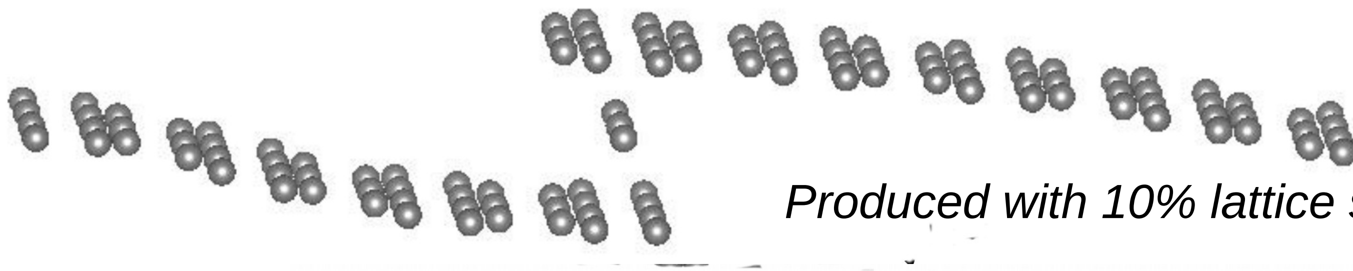
Ripples



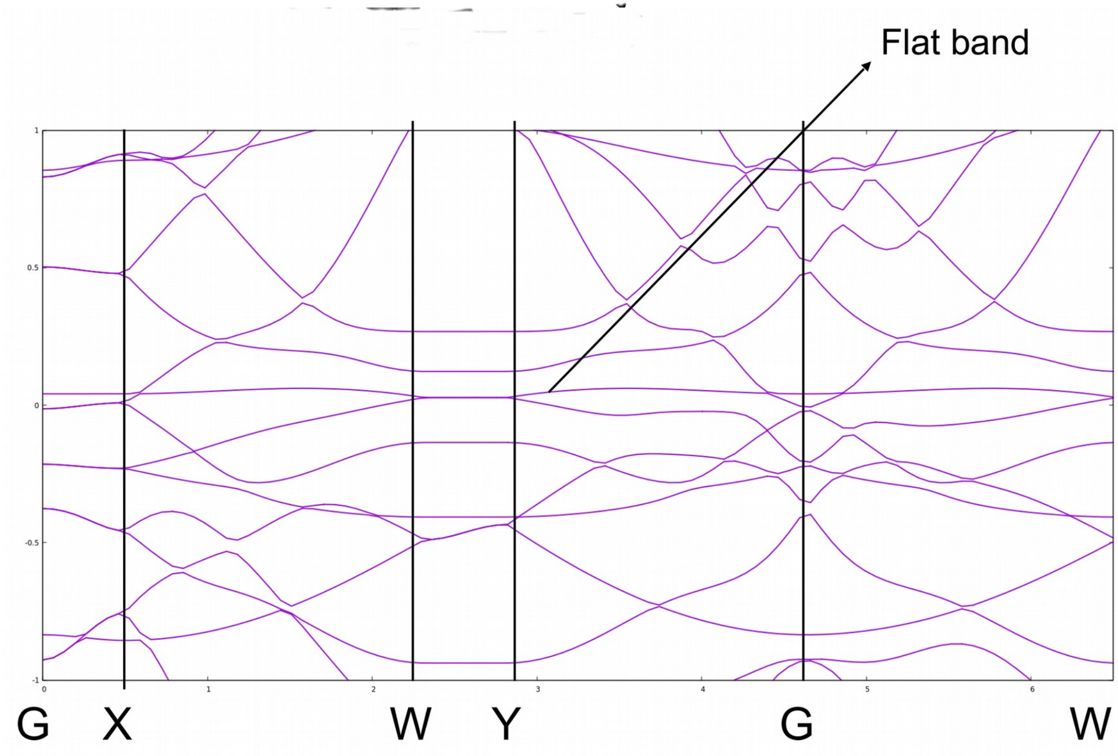


M.W. Barsoum, G.J. Tucker / Scripta Materialia 139 (2017) 166–172

ELECTRONIC STRUCTURE OF PLEATED GRAPHENE

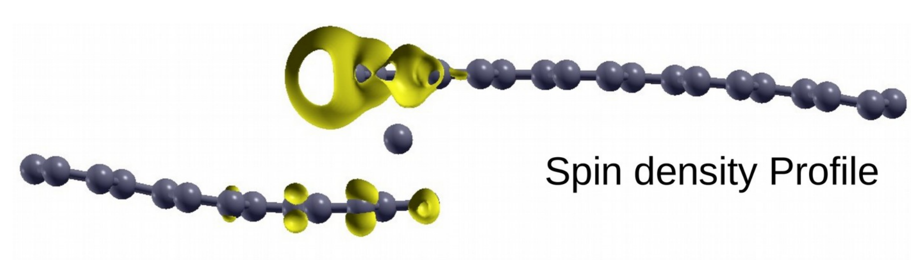


Produced with 10% lattice strain



Calculated Chern Number turned out to be non trivial (-2)

Deformed graphene under strain may be source of **magnetic flat** Bands with **non trivial topological characters.**



Spin density Profile

Thank You