Engineering Topological Phases at Interface Between Double Perovskites and Perovskites *:A Materials Perspective*

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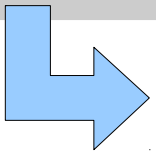
REFS: ***Phys. Rev. B 94, 155405; Phys. Rev. B 92, 161106(R)***

Hall Effects: The big picture

	Induced by B-field	Ferromagnetic Sample
Metal	Ordinary Hall (1879)	Anomalous Hall (1881)
Topological insulator	Quantum Hall (1980)	Quantum Anomalous Hall ?



Chiral edge currents associated with QAHIs in dissipationless electronic circuits is of potential use.

Requisite: *Intrinsic nonzero Berry curvature*

For practical usage one would like to:

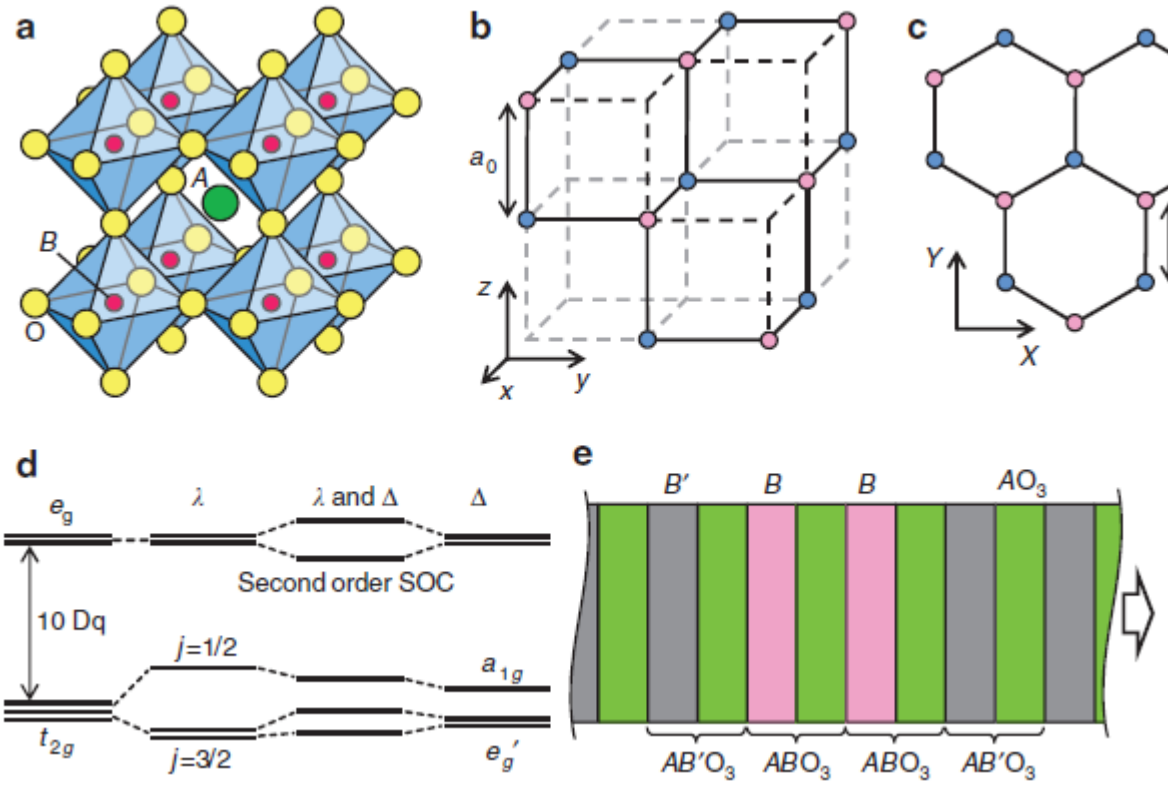
- **Boost the temperature scale for QAH effect**
  [Use d-electron systems rather s or p electron based systems.]

- **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)]

Interface Engineering of QAH effects ?

Bilayers of Perovskites grown along [111]



MOTIVATION

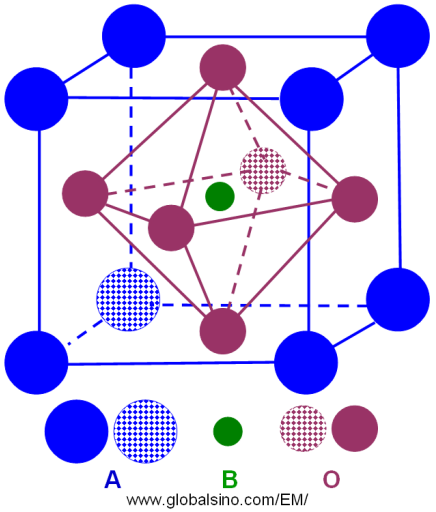
Theoretical Prediction:

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

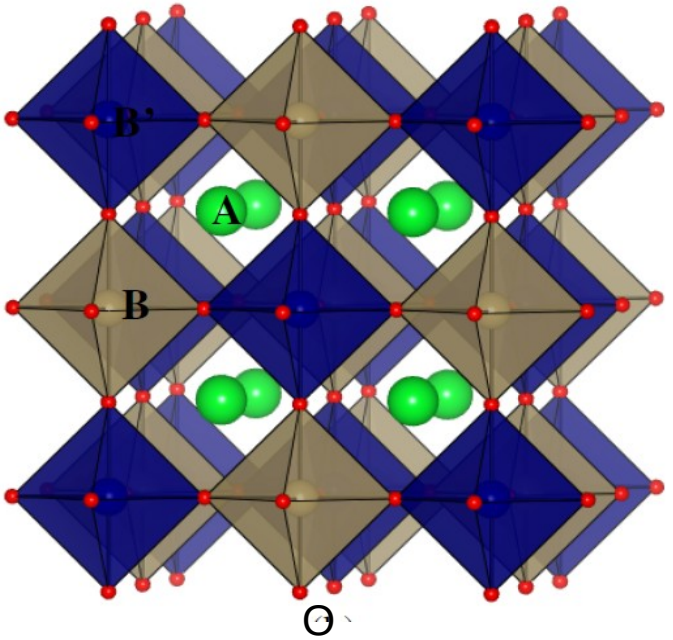
Xia et al, Nature Commun. 2, 596 (2011)

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 Double Perovskites

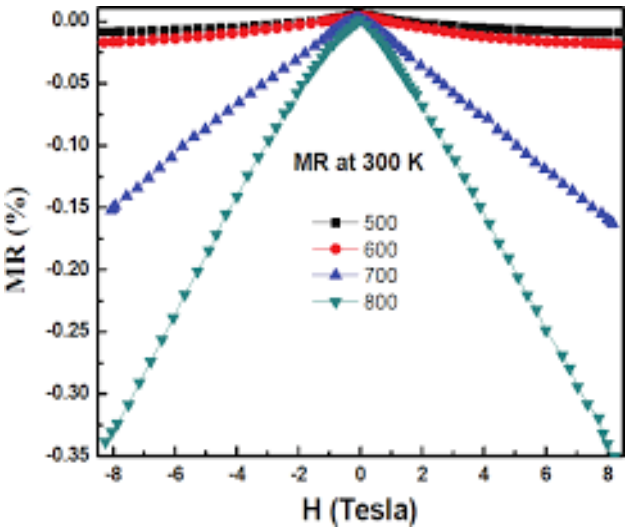
Sr_2FeMoO_6: K-I. Kobayashi, T. Kimura, H. Sawada, K. Terakura and Y. Tokura, Nature 395 677 (1998)

Double Perovskite Sr_2FeMoO_6: A Potential Candidate for Room Temperature Magnetoresistance Device Applications

Nitu Kumar, Geetika Khurana, Ram S. Katiyar, Anurag Gaur and R. K. Kotnala

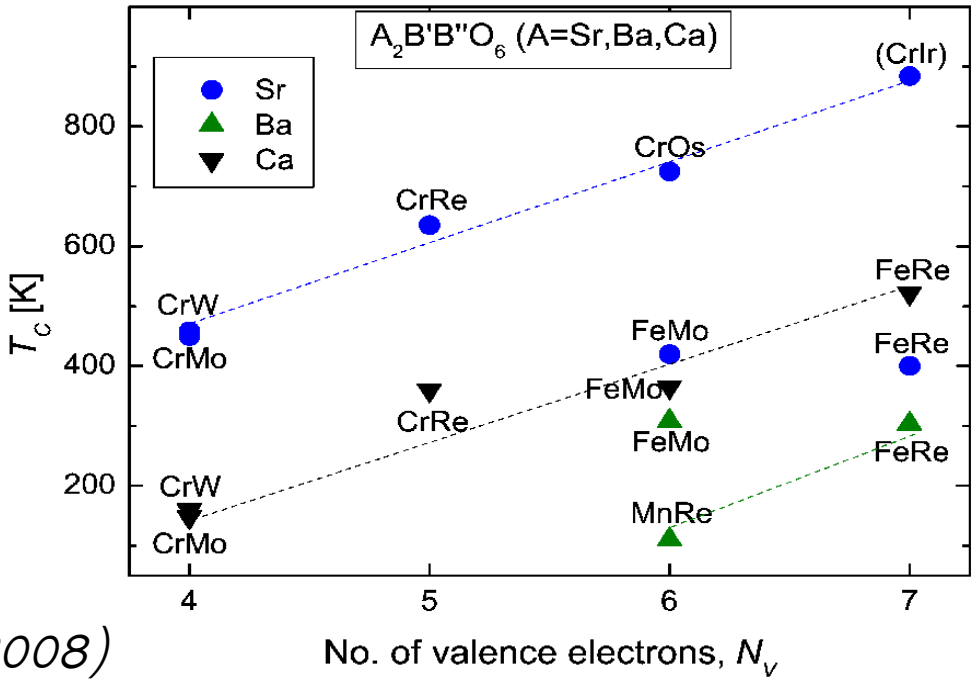
Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/intechopen.70193



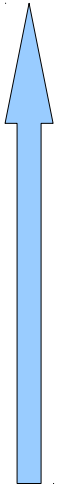
MR behavior of all the SFMO thin films at room temperature.

4 (3d series)	Sc 160	Ti 140	V 135	Cr 140	Mn 140	Fe 140	Co 135	Ni 135	Cu 135	Zn 135
5(4d series)	Y 180	Zr 155	Nb 145	Mo 145	Tc 135	Ru 130	Rh 135	Pd 140	Ag 160	Cd 155
6(5d series)	*	Hf 155	Ta 145	W 135	Re 135	Os 130	Ir 135	Pt 135	Au 135	Hg 150

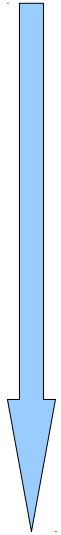


Mandal et. al. PRB 78, 134431 (2008)

Advantages of 3d-4d/5d DPs:



	U (eV)	J_H (eV)	Δ_{CF}	$\zeta \rightarrow Z^4$ $\lambda_{SO} = \zeta/2S$
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



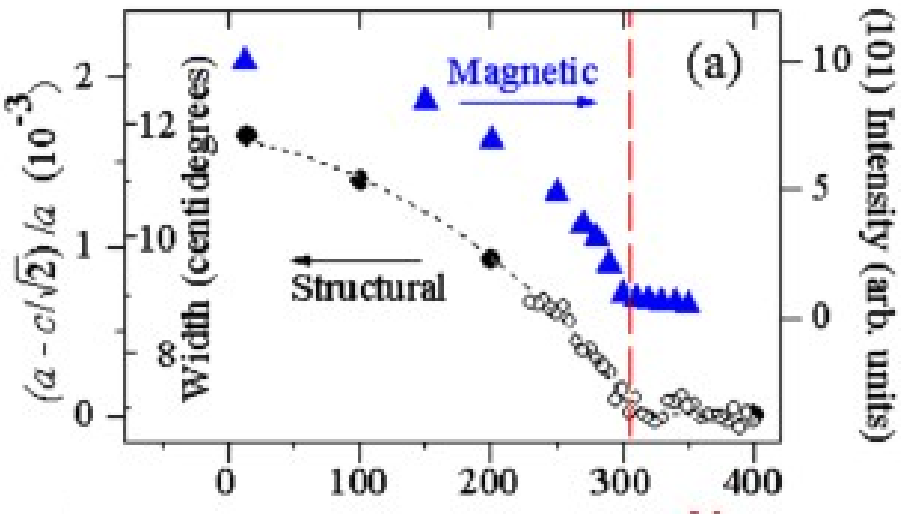
- ***3d*** **TM (B) can allow for a high energy scale for magnetism, while the *4d/5d* TM (B') can feature strong SOC.**

- **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.**

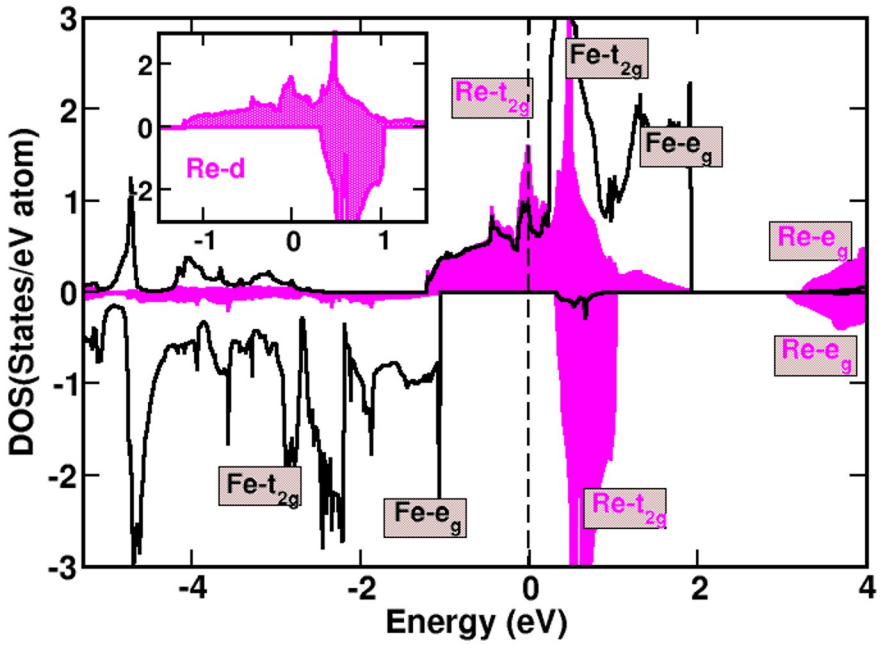
- **Low energy physics is described by t_{2g} bands ⇒ suppresses JT (trivial Ins)**

  [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

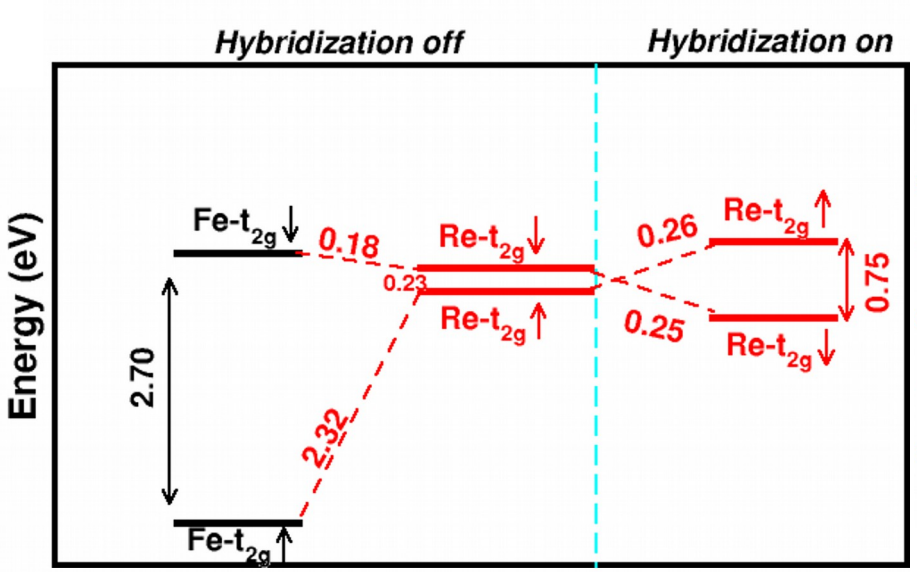


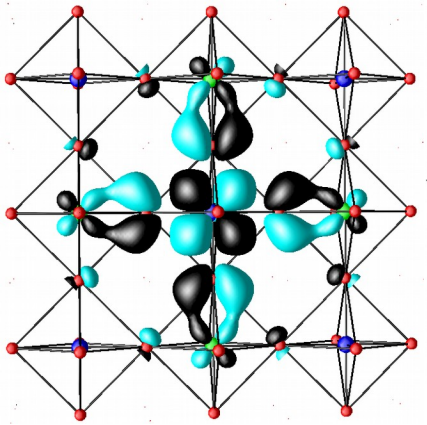
Phys. Rev. Lett. 98, 017204 (2007).

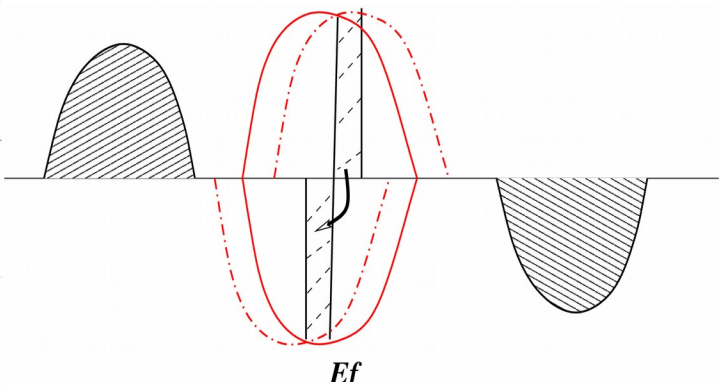


Ferromagnetism is driven by hybridization driven mechanism as found in Sr_2FeMoO_6

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





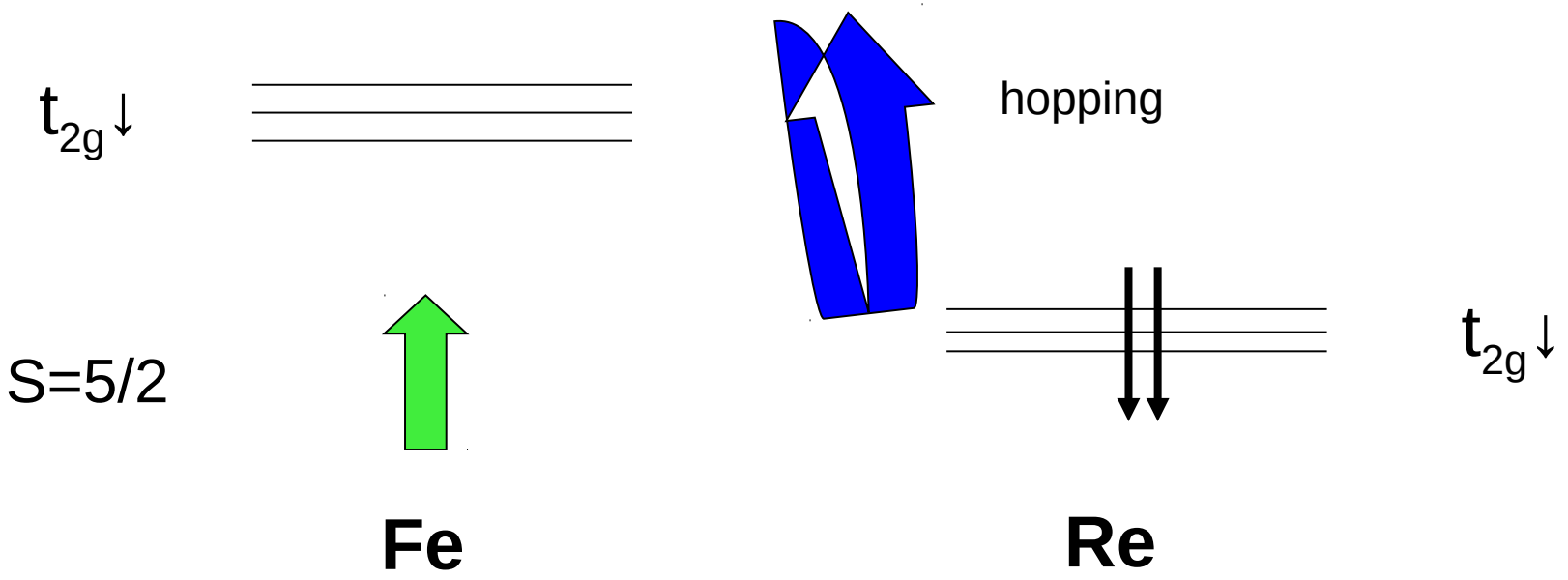


Effective double exchange type model Hamiltonian

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

Re^{5+}**: $4d^2$**: Mobile electron: gives rise to metallic behavior.

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



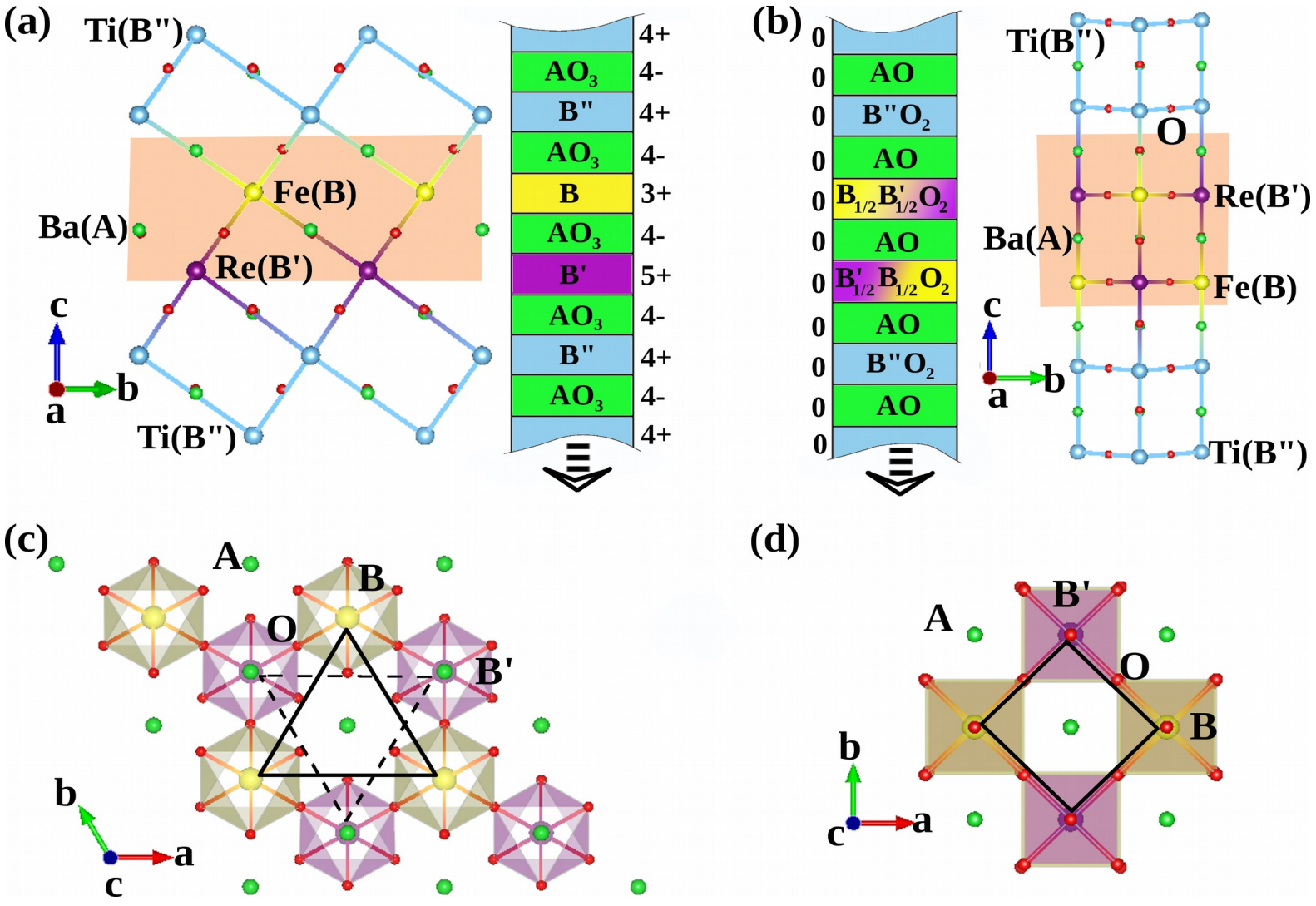
2-sublattice Kondo lattice Hamiltonian : Energy scales: $t_{Fe\,Re}$, $\Delta=\varepsilon_{Re}-\varepsilon_{Fe}$, J

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

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

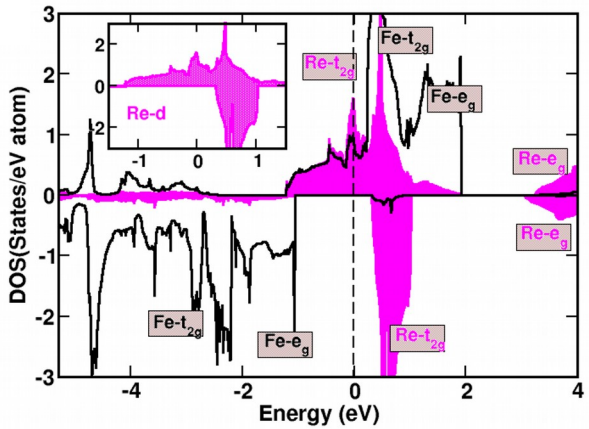
[111] growth direction

[001] growth direction



Electronic Structure of Q.Wells

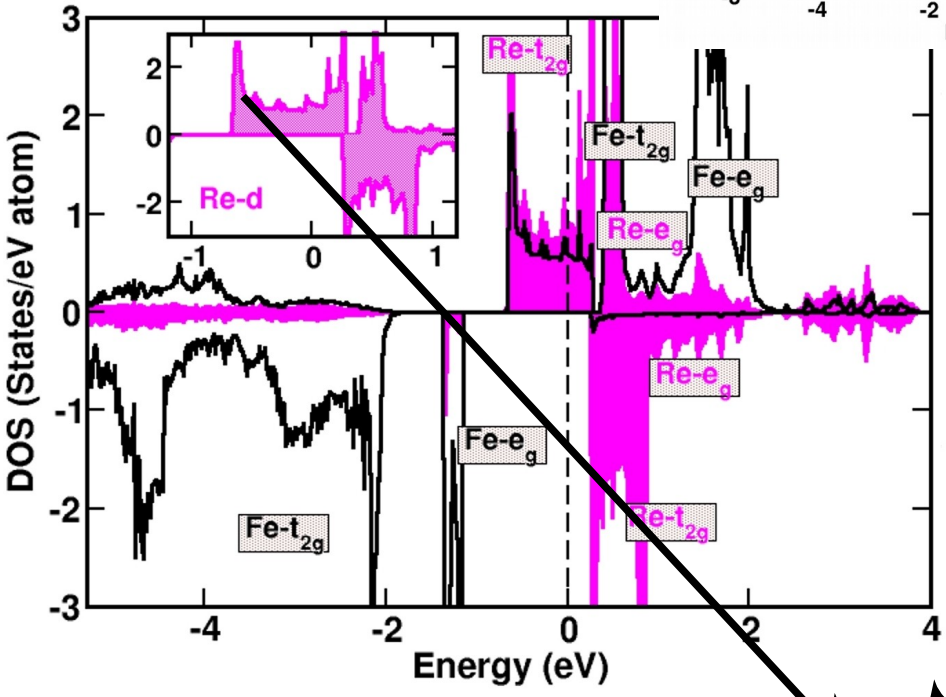
Half-metallicity survives in the heterostructure geometries even for minimum thicknesses!

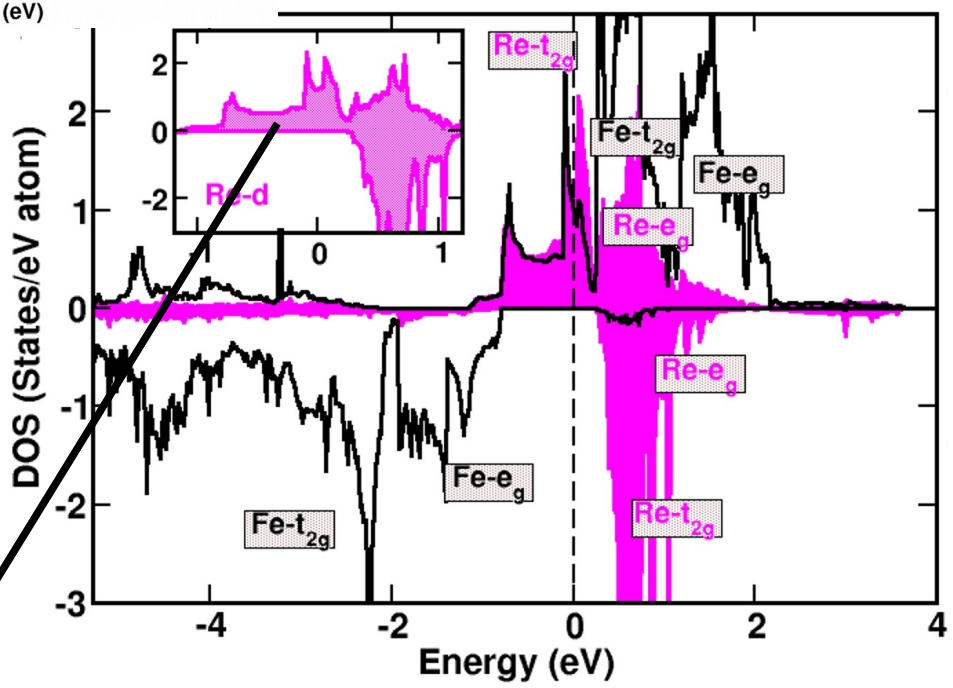


[BULK]

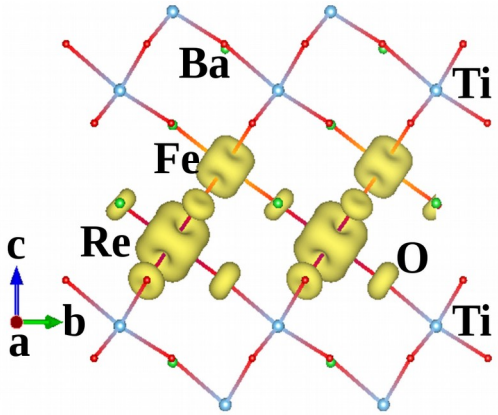
[111]

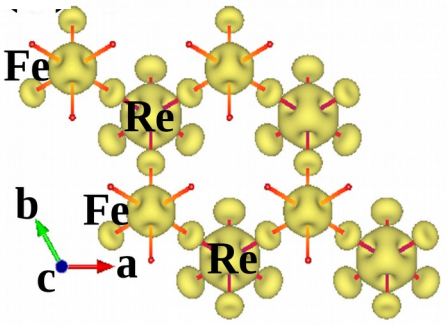
[001]

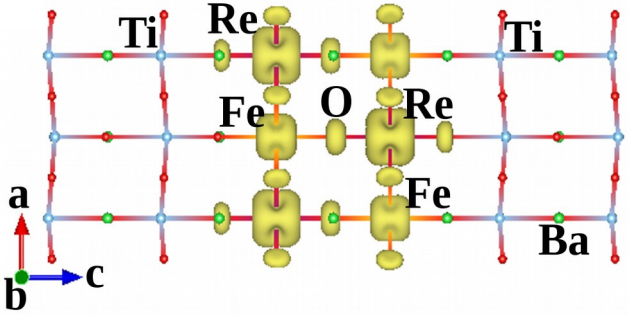


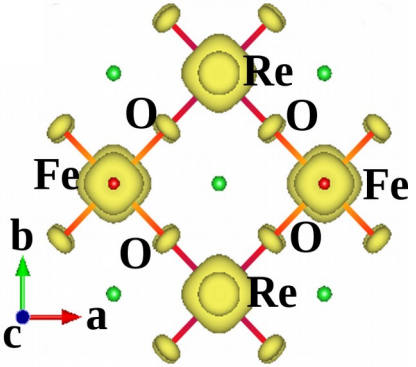


Signature of 1-D features in the density of states → **Reduced dimensionality**

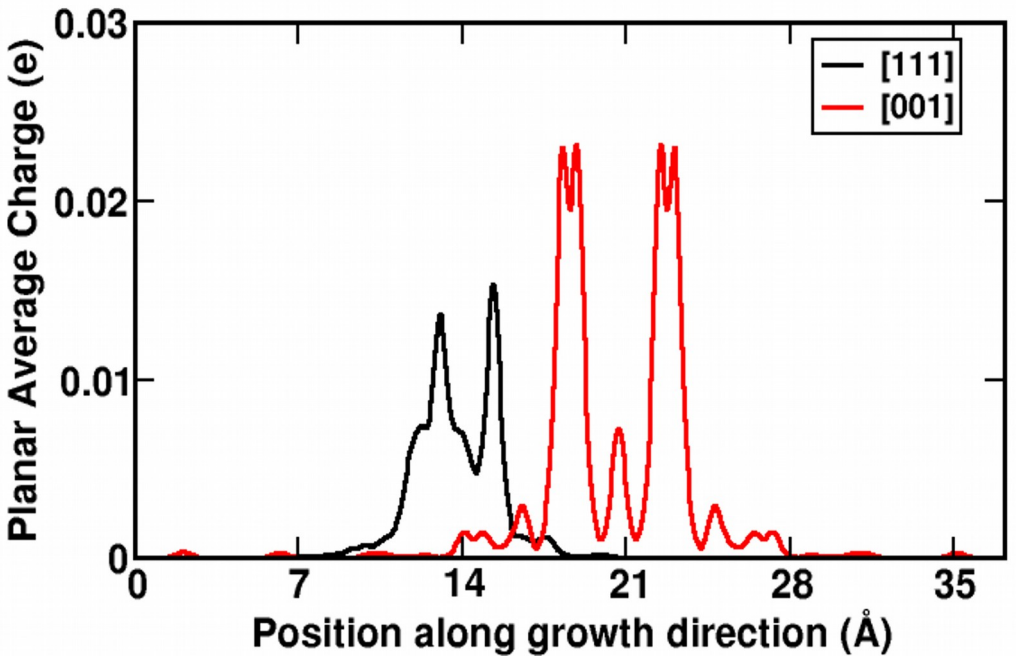








☆ Highly confined 2D electron gas



Band#	$m_{\parallel}^{eff}$	$m_{\perp}^{eff}$		Band#	$m_{\parallel}^{eff}$	$m_{\perp}^{eff}$
3.	1.2 m_0	22 m_0	(001)	3.	2.3 m_0	73 m_0
2.	0.8 m_0	840 m_0		2.	1.0 m_0	73 m_0
1.	3.6 m_0	61 m_0		1.	7.8 m_0	5.6 m_0

Confinement over unit cell thickness (7-14 A^o)

Marked Improvement at the level of confinement!

Complete spin-polarization of 2DEG

Polarity control of 2DEG

PRL 104, 156807 (2010) PHYSICAL REVIEW LETTERS week ending 16 APRIL 2010

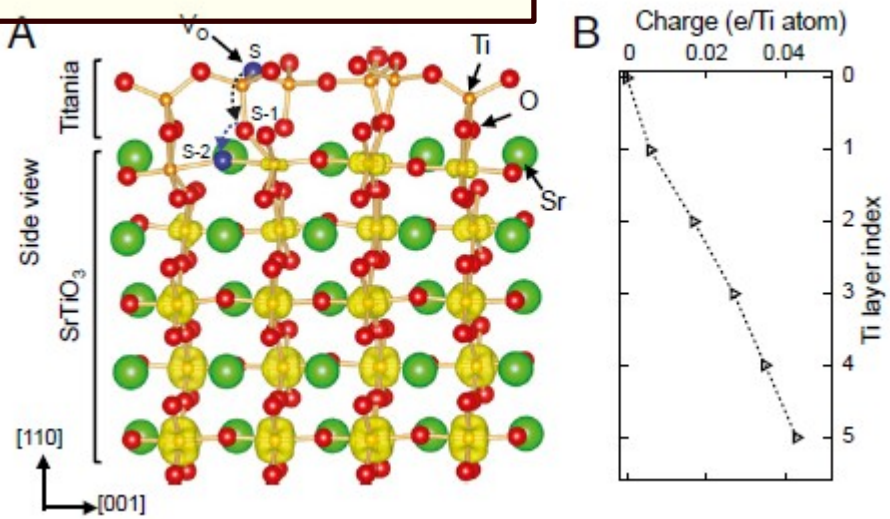
Dynamical Response and Confinement of the Electrons at the $LaAlO_3/SrTiO_3$ Interface

A. Dubroka,[1] M. Rössle,[1] K. W. Kim,[1] V. K. Malik,[1] L. Schultz,[1] S. Thiel,[2] C. W. Schneider,[2,3] J. Mannhart,[2] G. Herranz,[4,*] O. Copie,[4] M. Bibes,[4] A. Barthélémy,[4] and C. Bernhard[1,†]

With infrared ellipsometry and transport measurements we investigated the electrons at the interface between $LaAlO_3$ and $SrTiO_3$. We obtained a sheet carrier concentration of $N_s \approx 5\text{–}9 \times 10^{13}$ cm^{-2}, an effective mass of $m^* = 3.2 \pm 0.4 m_e$, and a strongly frequency dependent mobility. The latter are similar as in bulk $SrTi_{1-x}Nb_xO_3$ and therefore suggestive of polaronic correlations. We also determined the vertical concentration profile which has a strongly asymmetric shape with a rapid initial decay over the first 2 nm and a pronounced tail that extends to about 11 nm.

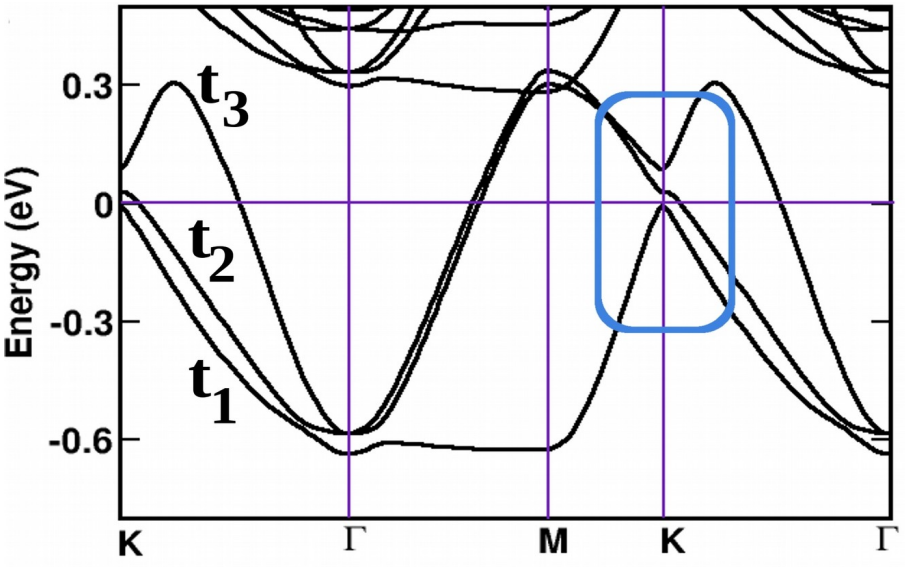
Anisotropic two-dimensional electron gas at $SrTiO_3$(110)

Z. Wang *et al.* PNAS 111, 3933 (2014).



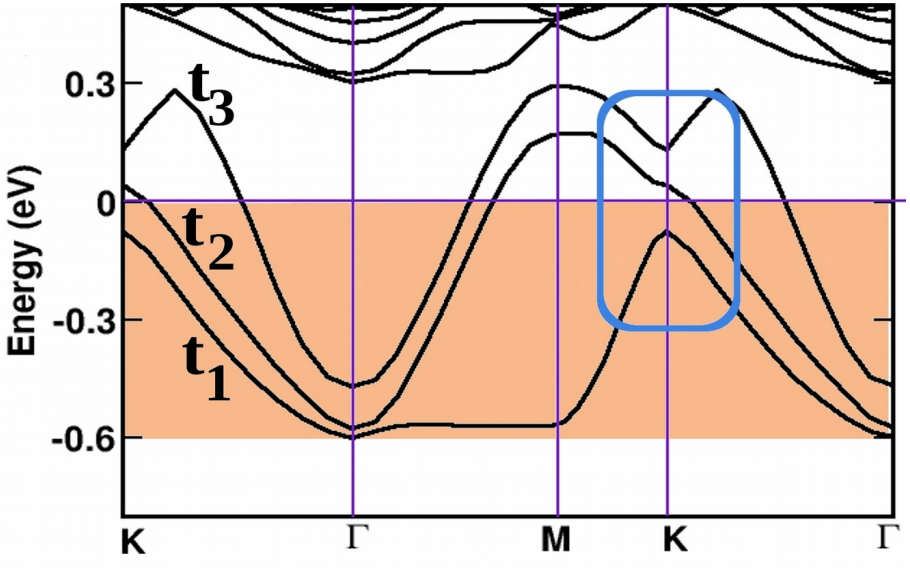
Band structure of [111] heterostructure

GGA



GGA+SO

[Topological HM band structure]

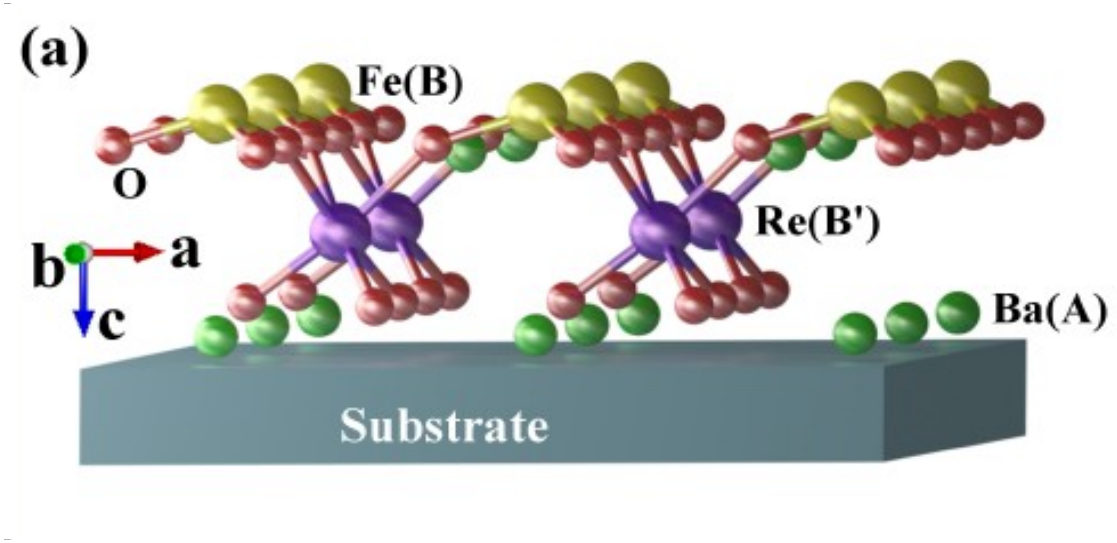


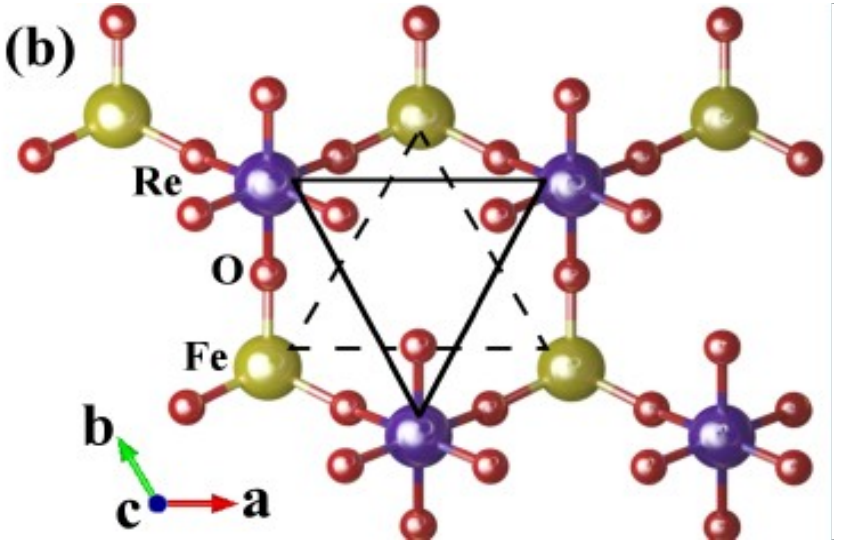
Nontrivial Chern numbers for t_1 and t_2 bands: -2, 2

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

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.

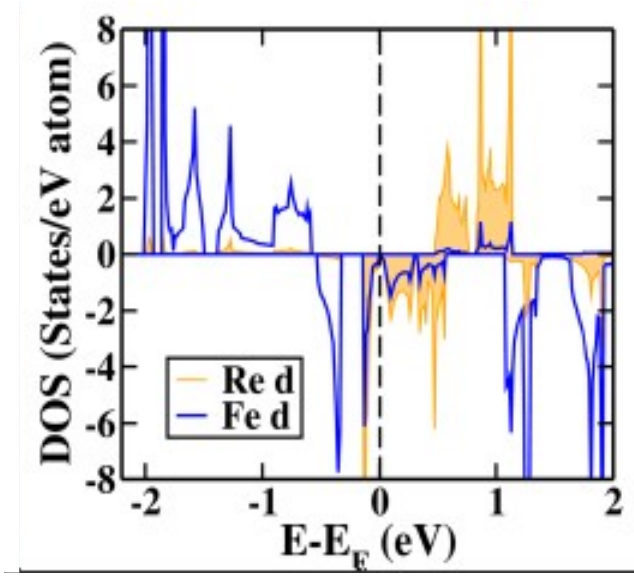
TRY OVERLAYER-SUBSTRATE GEOMETRY

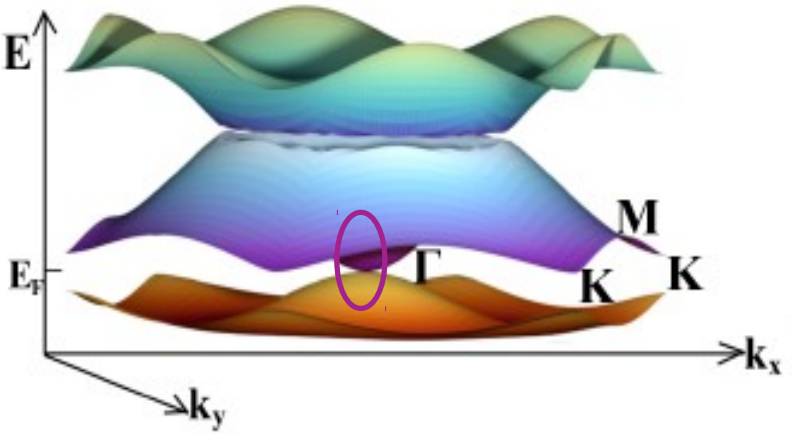


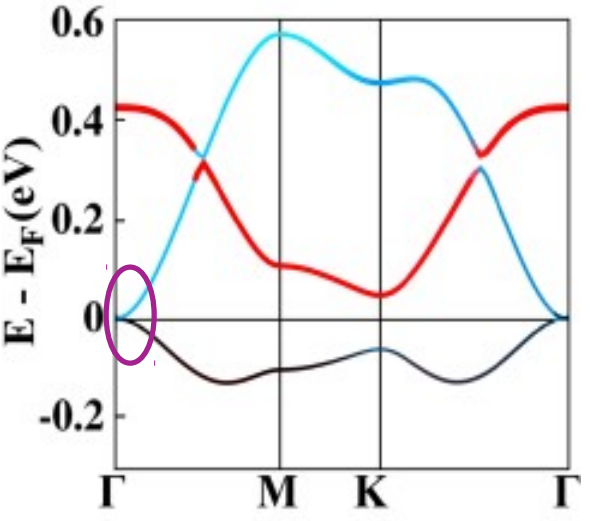


GGA electronic structure:

Band structure in minority spin spin





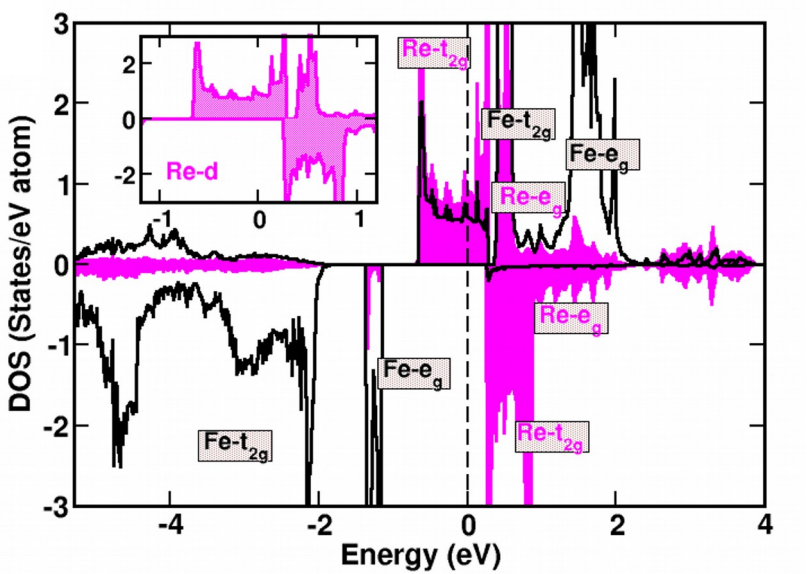


Half-metallic!

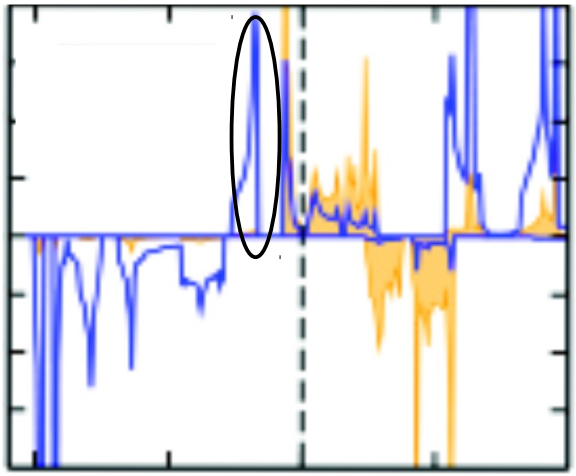
Gapped at every point except Γ (half semi-metal)

Quadratic band touching at Γ !

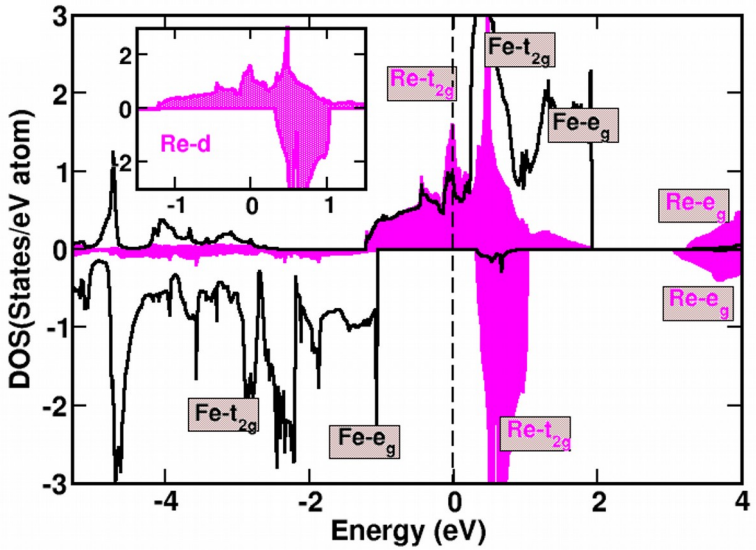
QW Geometry



Overlayer Geometry



BULK



Mag. Mom (μ_B)

	BULK	QW	Overlayer
Fe	3.73	3.68	**2.99**
Re	0.78	0.79	**0.39**
Total	3.00	3.00	3.00

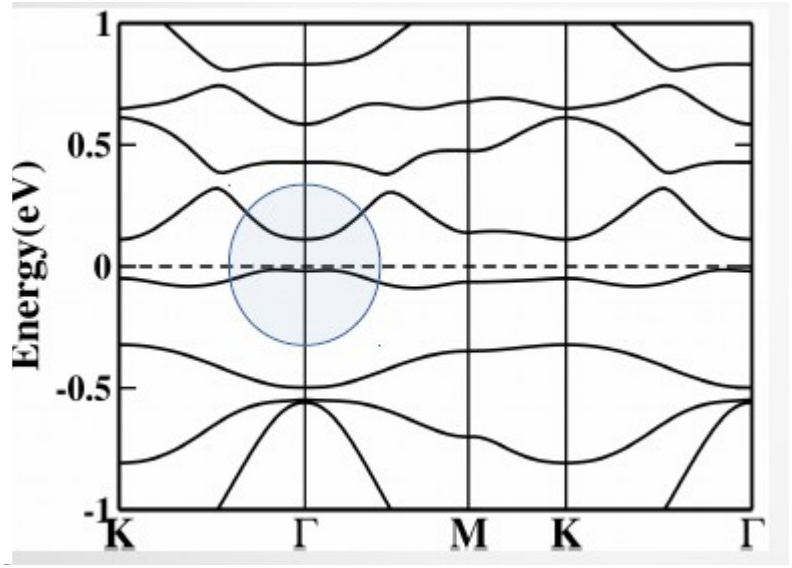
Bulk/QW : $Fe^{3+}(d^5)$-$Re^{5+}(d^2)$

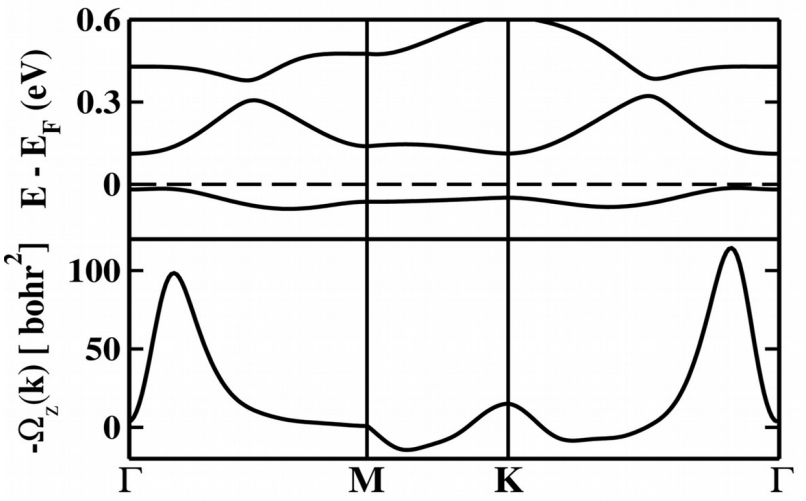
Overlayer: $Fe^{2+}(d^6)$-Re^{6+} (d^1)

Charge Redistribution

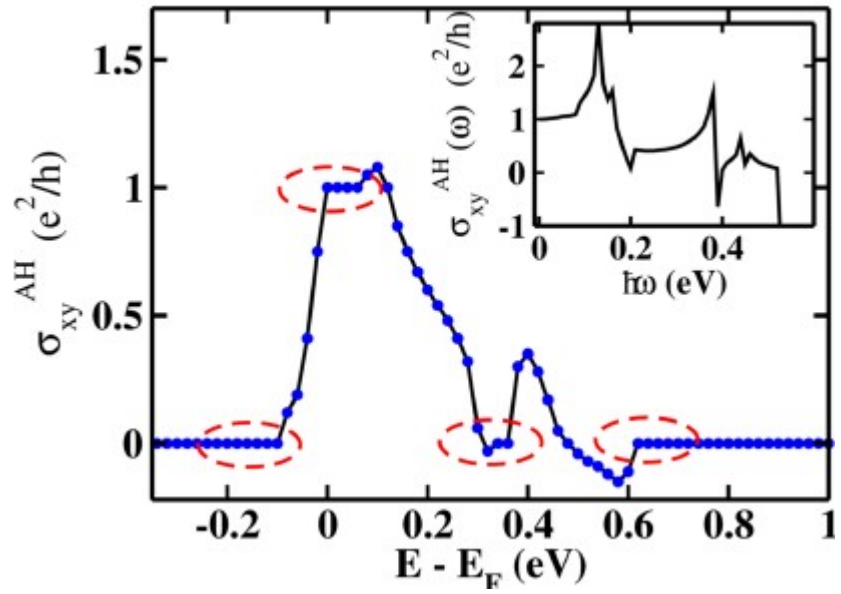
GGA +SOC electronic structure:

Large gap ~ 110 meV

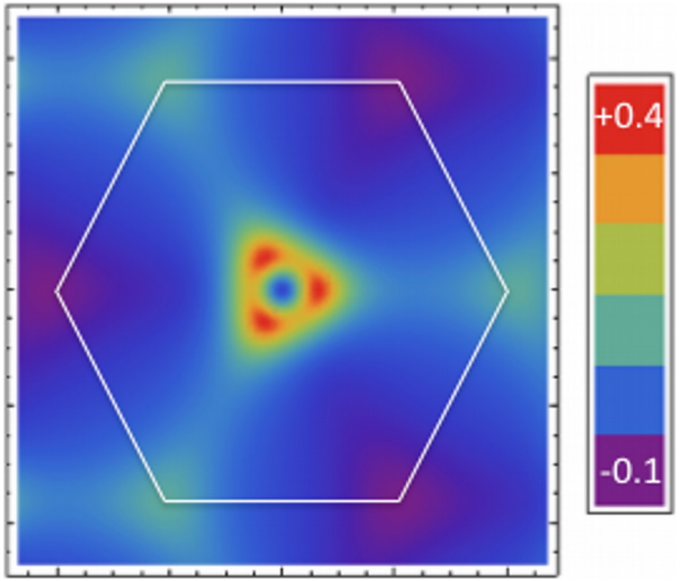




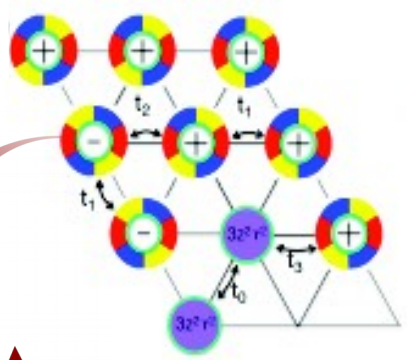
Inclusion of SOC gaps out the QBT

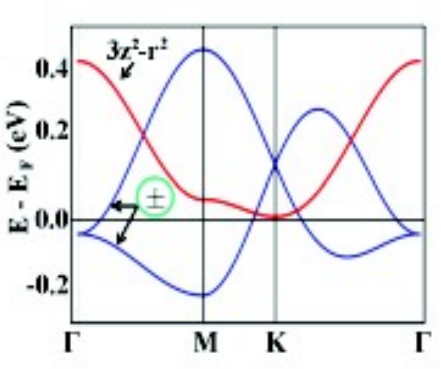


C = 1



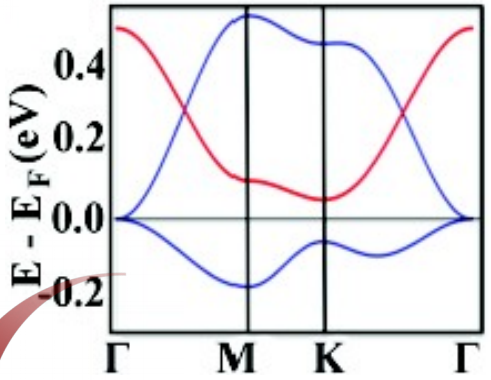
Analysis of band structure: 3 band TB model

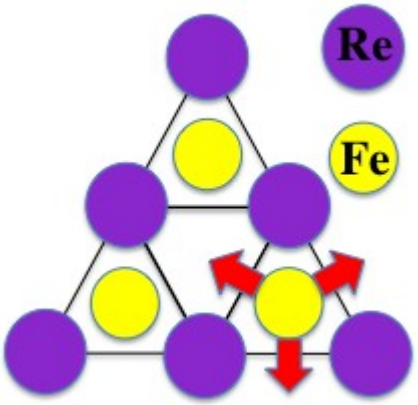




3 band model derived from 5d Re t_{2g} bands in reduced C_3 symmetry

Dirac BT at hexagonal BZ corners and QBT at Γ

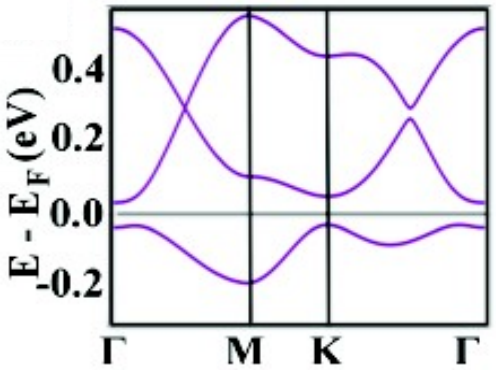




In-plane inversion symmetry breaking by localized 3d Fe generates in-plane electric field that couples with electric dipoles formed by +/- e_g^{π} doublets

Gaps out the Dirac points at BZ corners.

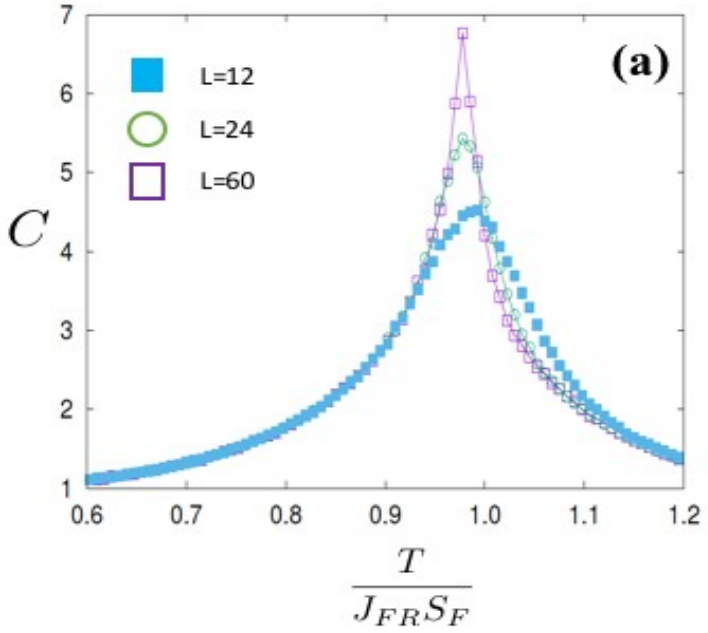
► ***Orbital Rashba-type effect (PRL 2011)***

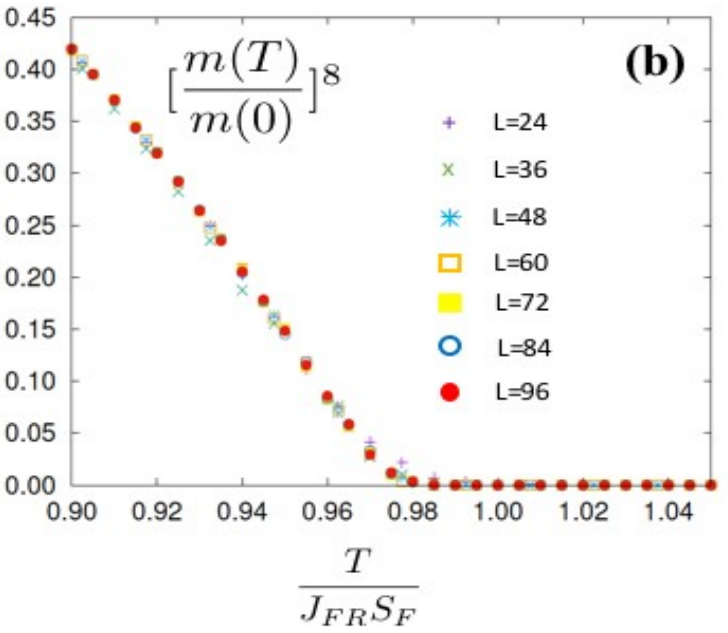


Introduction of SOC term
gaps out the QBT.

►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!)**

Conclusions & outlook

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)]

Thank You