Title: Topological states in honeycomb materials

Date: May 25, 2017 02:30 PM

URL: http://pirsa.org/17050088

Abstract: The topological Haldane model (THM) on a honeycomb lattice is a prototype of systems hosting topological phases of matter without external fields. It is the simplest model exhibiting the quantum Hall effect without Landau levels, which motivated theoretical and experimental explorations of topological insulators and superconductors. Despite its simplicity, its realization in condensed matter systems has been elusive due to a seemingly difficult condition of spinless fermions with sublattice-dependent magnetic flux terms. While there have been theoretical proposals including elaborate atomic-scale engineering, identifying candidate THM materials has not been successful, and the first experimental realization was recently made in ultracold atoms. Here we suggest that a series of Fe-based honeycomb ferromagnetic insulators, AFe2(PO4)2 (A=Ba,Cs,K,La) possess Chern bands described by the THM.

Searching for Haldane Chern Insulator in Honeycomb Materials

Hae-Young Kee

University of Toronto

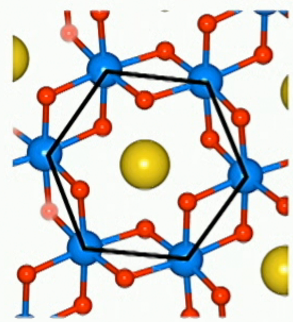
4 corner symposium, Perimeter Institute, May 25, 2017

Correlated Honey Materials

1 H																		2 He
3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Uun	111 Uuu	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

* candidates for Kitaev spin liquid



Iridates (5d): Na_2IrO_3, Li_2IrO_3

Ruthenates (4d): $RuCl_3$

* candidates for Haldane Chern insulator

Fe oxides (3d): $AFe_2(PO_4)_2$

Haldane model:
Fe honeycomb oxides

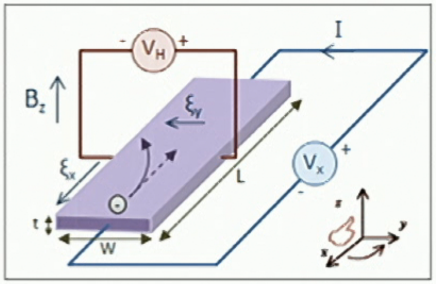
Univ. of Toronto

⟶ Rutgers Univ.

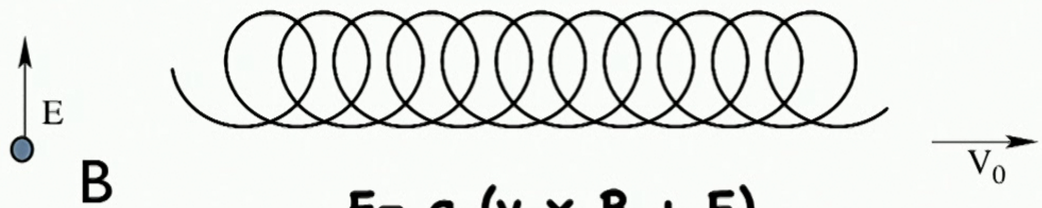
H.-S. Kim & HYK, npj Quantum Materials (2017)2:20

charged particle in a magnetic field

Classical vs. Quantum



Hall effect; Edwin H. Hall (1879)



F= q (v x B + E)

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{xx} \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix}$$

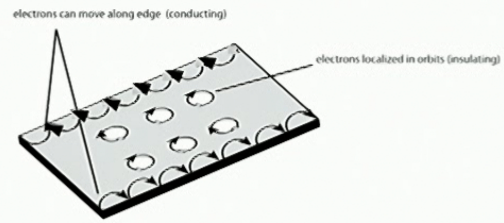
$$\rho_{xy} = \frac{B}{ne}$$

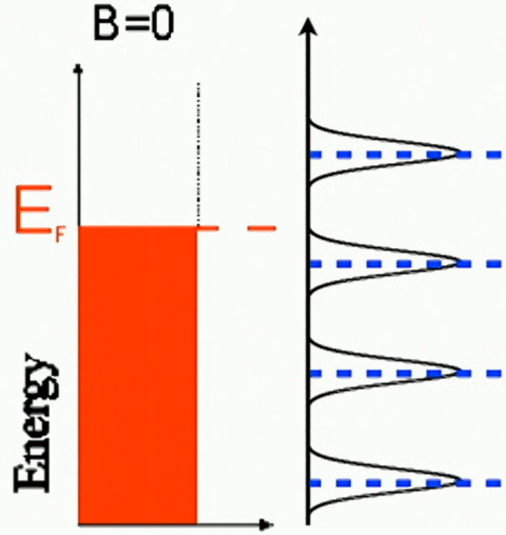
Quantum formulation

vector potential $\mathbf{A}(\mathbf{r})$ for the magnetic field: $B = \partial_x A_y - \partial_y A_x$

$$H_0 = \frac{1}{2m}\left(\mathbf{p} + e\mathbf{A}\right)^2 \quad \text{(set c=1)}$$

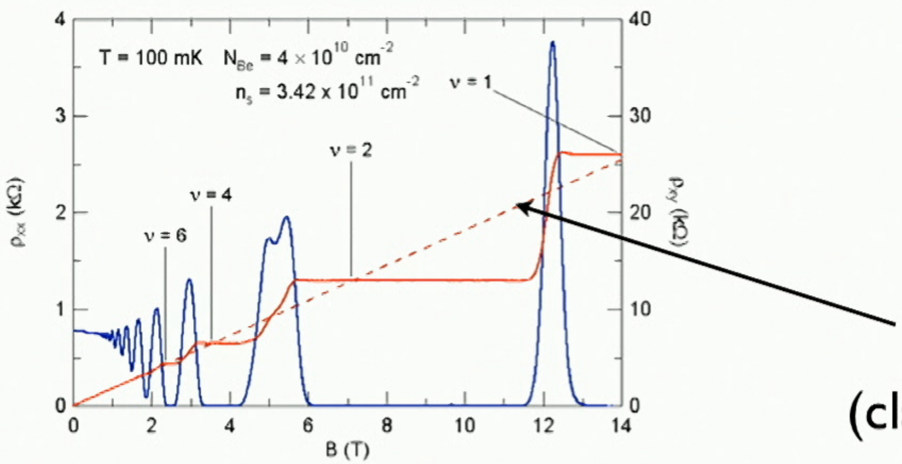
$$E_n = \hbar\omega(n + \frac{1}{2}),$$





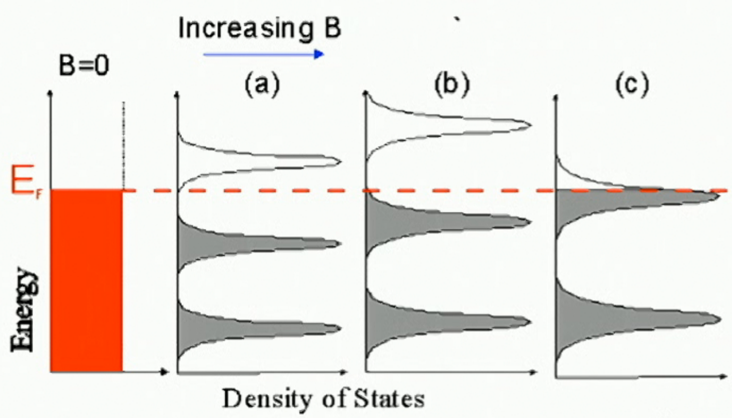
ν : filling factor
= total electron N/degeneracy

Integer Quantum Hall Effect (IQHE):



$\rho_{xy} \propto B$

(classical limit)



$\sigma_{xx} = 0$ σ_{xy}?

$$\rho_{xy} = \frac{1}{\nu}\frac{h}{e^2}$$

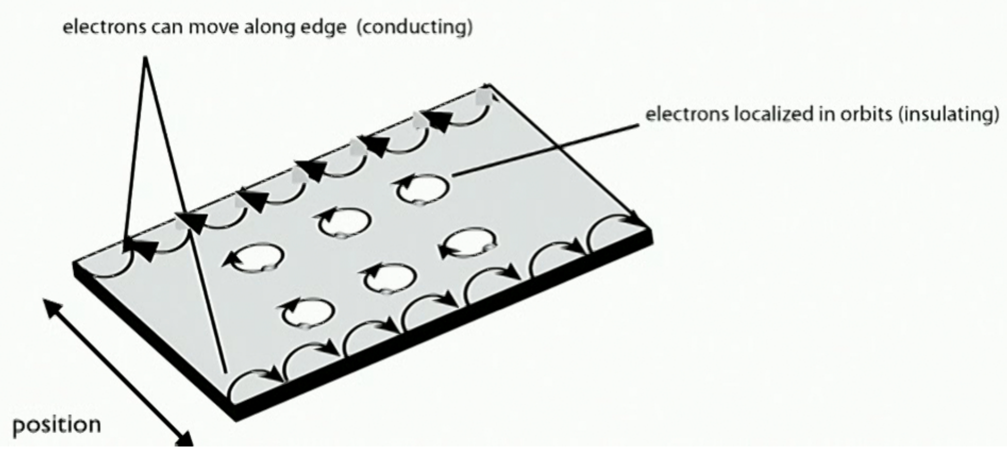
$$\sigma_{xy} = \nu \frac{e^2}{h}$$

not only finite, it is quantized (integers of e^2/h)

⟶ Berry phase & Chern number

$$\sigma_{xy} = \frac{\gamma}{2\pi}\frac{e^2}{h} = n_c \frac{e^2}{h}$$

In case of IQHE $n_c = \nu$



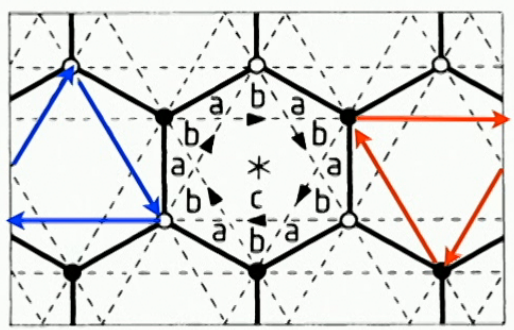
Haldane model, PRL (1988)

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"

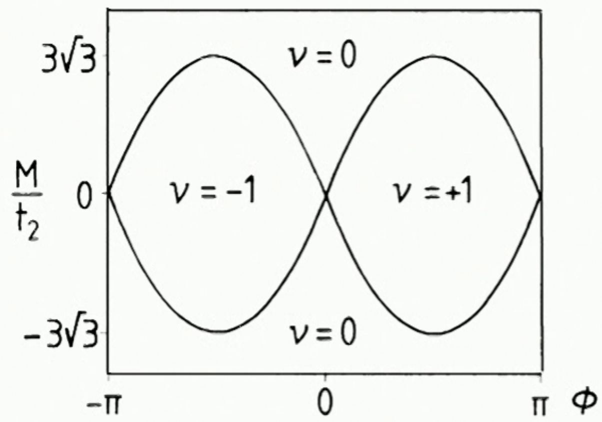
F. D. M. Haldane
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 16 September 1987)

$$\mathbf{H}(\mathbf{k}) = 2t_2\cos\phi\left[\sum_i \cos(\mathbf{k}\cdot\mathbf{b}_i)\right]\mathbf{I} + t_1\left[\sum_i [\cos(\mathbf{k}\cdot\mathbf{a}_i)\sigma^1 + \sin(\mathbf{k}\cdot\mathbf{a}_i)\sigma^2]\right] + \left[M - 2t_2\sin\phi\left[\sum_i \sin(\mathbf{k}\cdot\mathbf{b}_i)\right]\right]\sigma^3$$



spinless fermion
TRS broken
sublattice dependent flux

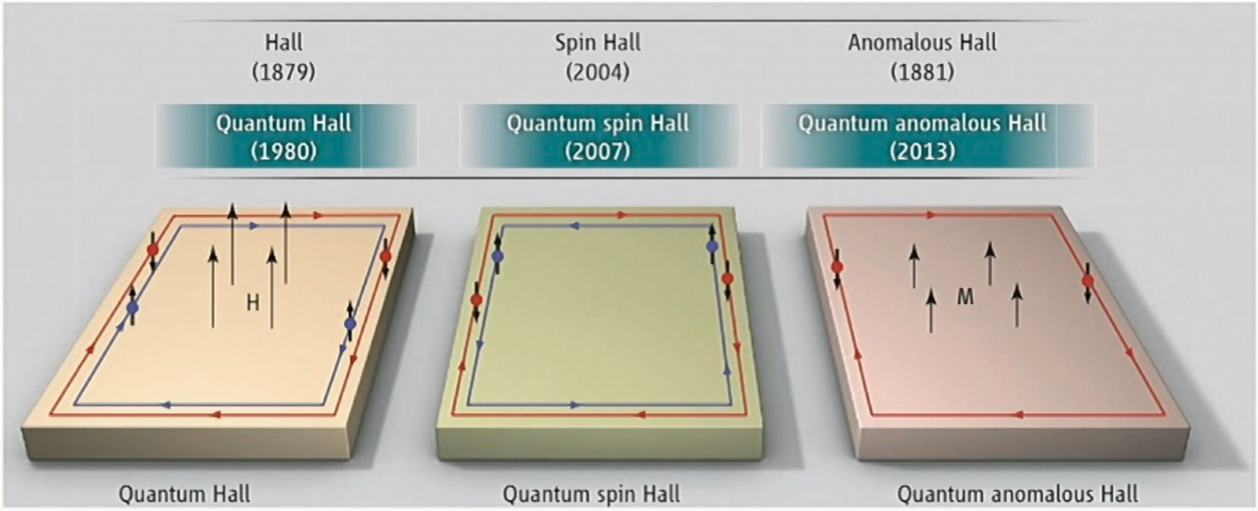
Topological Phase Transition

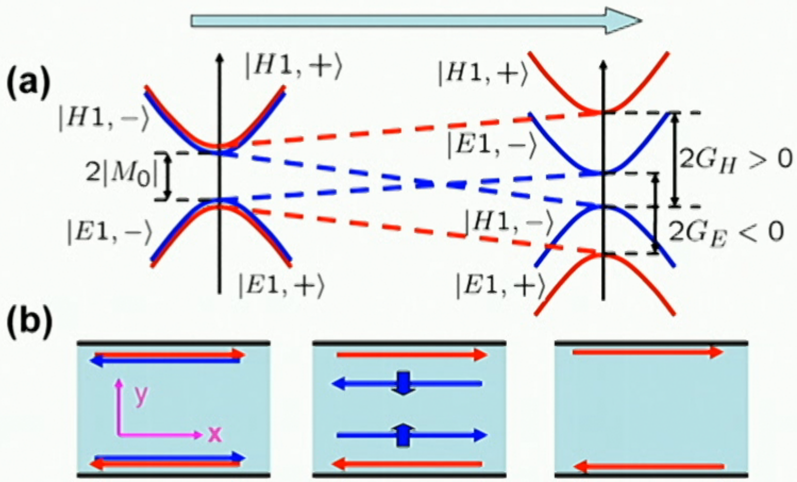


While the particular model presented here is unlikely to be directly physically realizable, it indicates that, at least in principle, the QHE can be placed in the wider context of phenomena associated with broken time-reversal invariance, and does not necessarily require external magnetic fields, but could occur as a consequence of magnetic ordering in a quasi-two-dimensional system.

: motivate to explore new topological phases

Magnetic Topological insulators



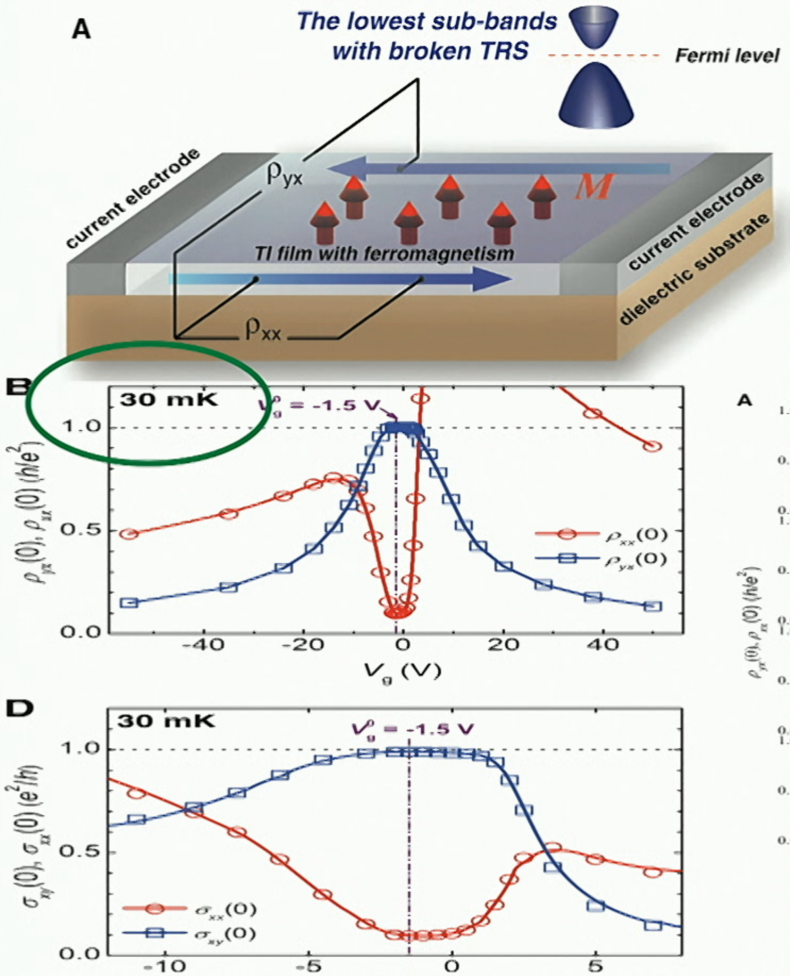


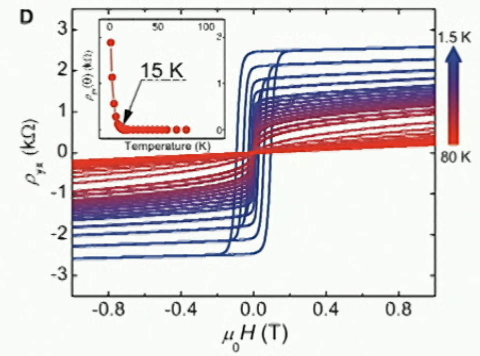
Proposal:
HgTe (TI) doped with Mn magnetic atoms
Liu et al, PRL (2008).

Exp: $\mathrm{Cr}_{0.15}(\mathrm{Bi}_{0.1}\mathrm{Sb}_{0.9})_{1.85}\mathrm{Te}_3$
Chang et al, Science (2013)

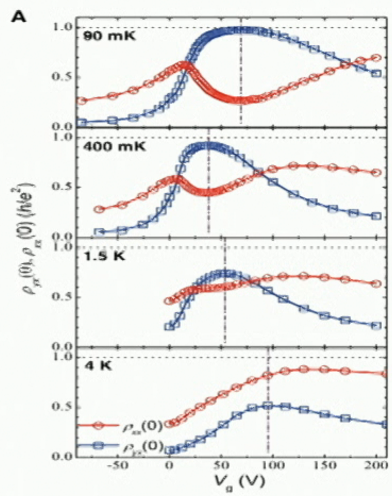
$Cr_{0.15}(Bi_{0.1}Sb_{0.9})_{1.85}Te_3$

thickness of 5 quintuple layers grown on SrTiO3 (111) substrates





ferromagnet below 15K



Chang et al, Science, 340, 167 (2013)

How to achieve Haldane Chern (QAH) insulator?

Why difficult?

Two conditions

Broken TRS:

Ferromagnetic insulator : spinless fermion

2nd n.n. complex hopping integrals :

relevant orbitals?

electronic correlation (ferromagnetic order)
+ crystal-field splitting
+ spin-orbit coupling

Fe-based ferromagnetic honeycomb oxides are described by Haldane model:

$$AFe_2(PO_4)_2,\ A = Ba, La, Cs, K$$

Magnetic Materials

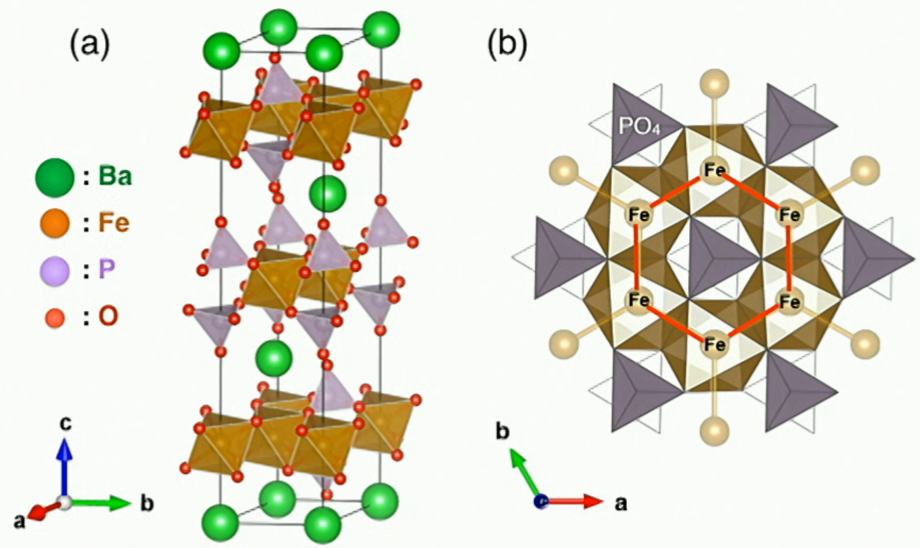
DOI: 10.1002/ange.201205843

A Genuine Two-Dimensional Ising Ferromagnet with Magnetically Driven Re-entrant Transition**

*Houria Kabbour, Rénald David, Alain Pautrat, Hyun-Joo Koo, Myung-Hwan Whangbo, Gilles André, and Olivier Mentré**

$BaFe_2(PO_4)_2$

$Fe^{2+}: 3d^6$



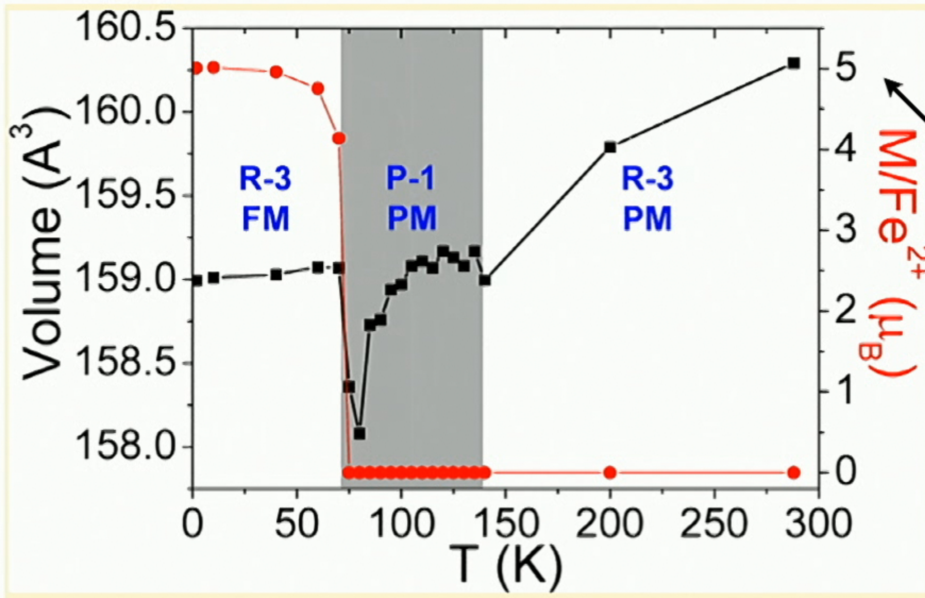
First oxide 2D Ising Ferromagnet

Angew. Chem. **2012**, *124*, 11915–11919

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
Article
pubs.acs.org/JACS

Across the Structural Re-Entrant Transition in $BaFe_2(PO_4)_2$: Influence of the Two-Dimensional Ferromagnetism

Rénald David,† Alain Pautrat,‡ Dmitry Filimonov,§ Houria Kabbour,† Hervé Vezin,∥ Myung-Hwan Whangbo,⊥ and Olivier Mentré*,†

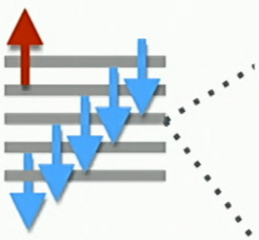


large moment

dx.doi.org/10.1021/ja404697b | J. Am. Chem. Soc. 2013, 135, 13023−13029

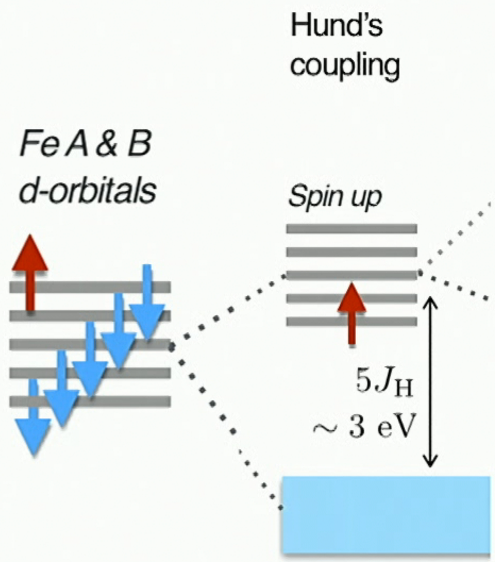
energy scale: U > Hund > Crystal filed > SOC

Atomic &



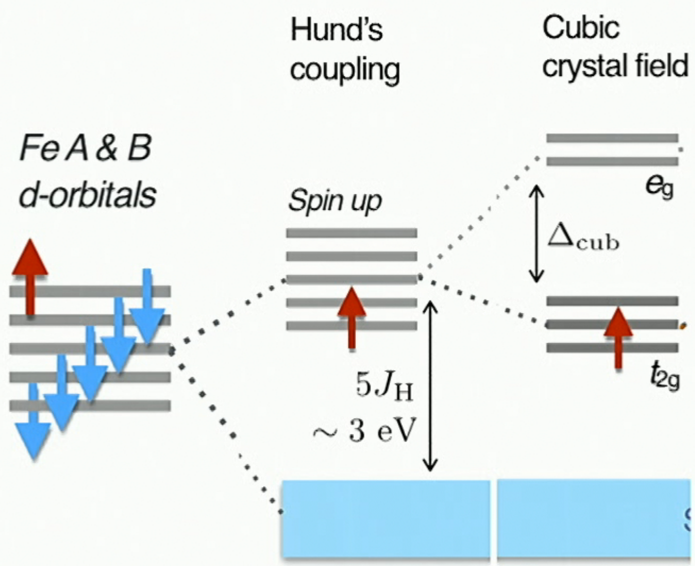
energy scale: U > Hund > Crystal filed > SOC

Atomic &



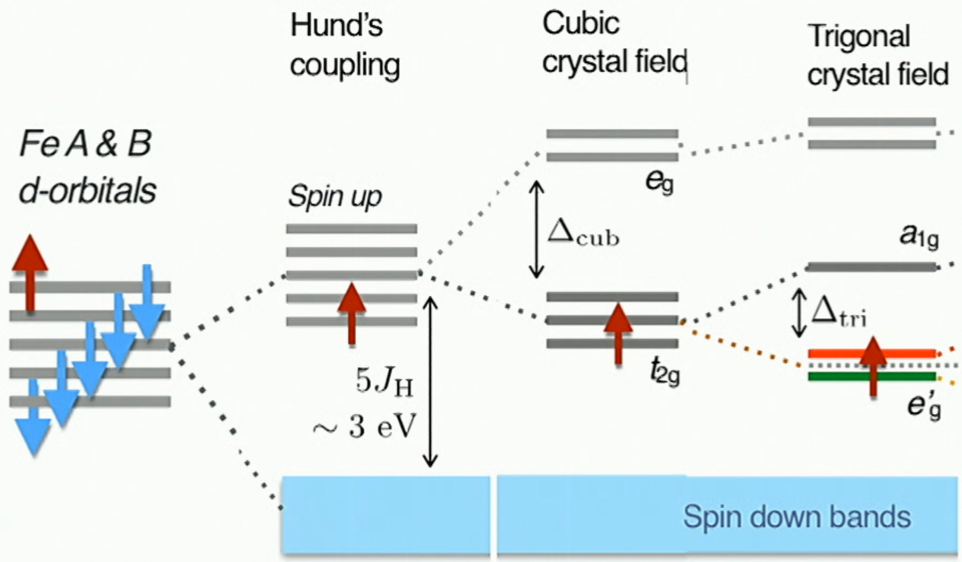
energy scale: U > Hund > Crystal filed > SOC

Atomic &



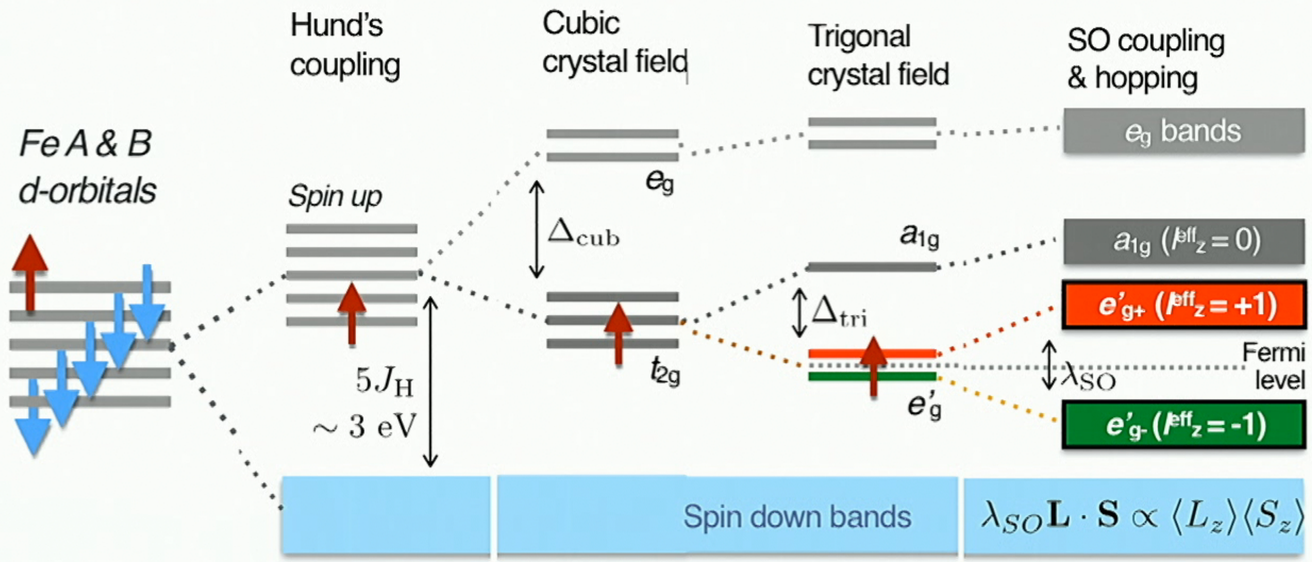
energy scale: U > Hund > Crystal filed > SOC

Atomic &



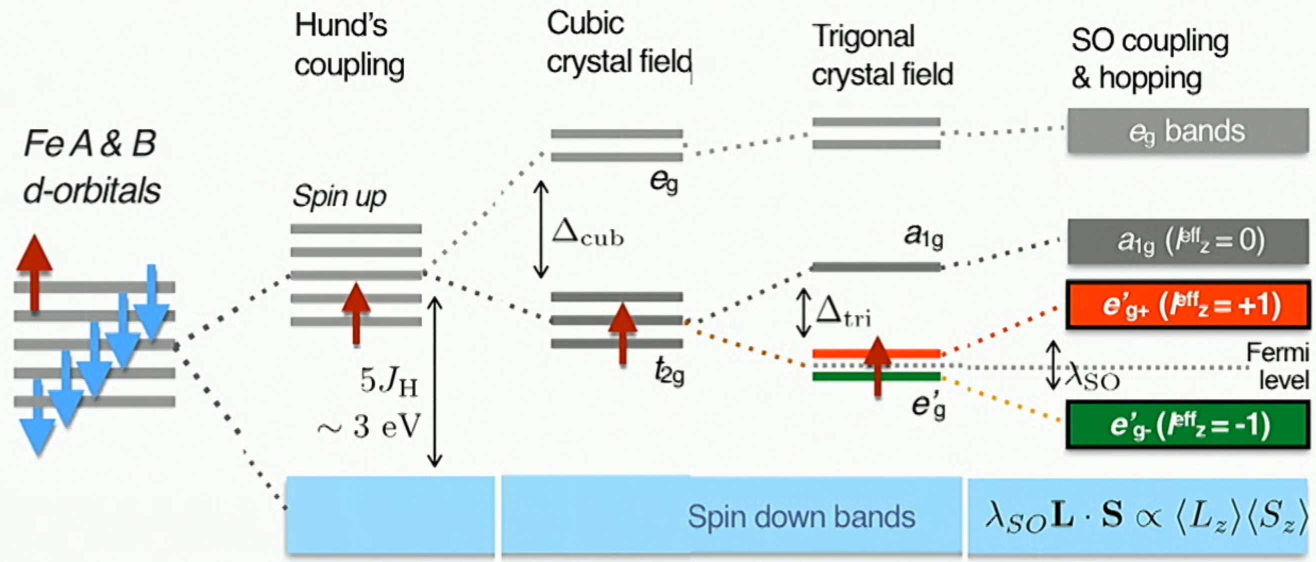
energy scale: U > Hund > Crystal filed > SOC

Atomic &



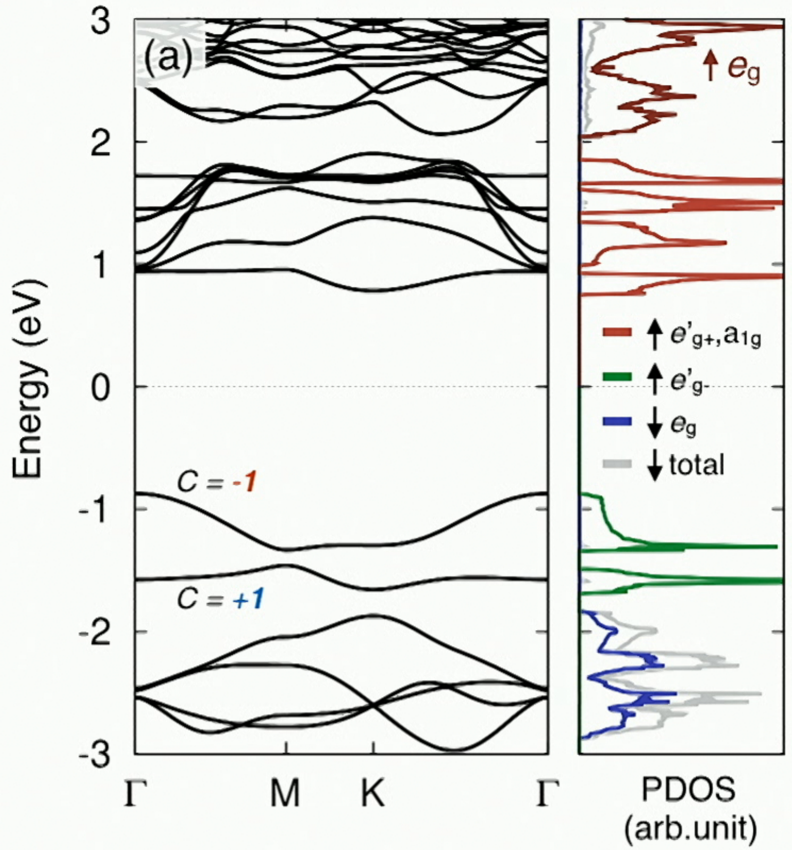
energy scale: U > Hund > Crystal filed > SOC

Atomic &



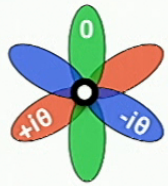
If hopping integral is small, atomic (eg) basis
is a good starting point:
Let's check

large U:

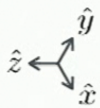


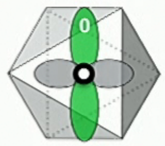
(a)
3
2
1
0
-1
-2
-3
Energy (eV)
C = -1
C = +1
Γ
M
K
Γ
↑ e_g
↑ e'_{g+},a_{1g}
↑ e'_{g-}
↓ e_g
↓ total
PDOS
(arb.unit)

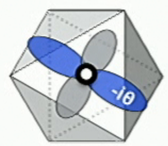
Tight binding model for atomic orbital e'_{g-}



$$\propto |d_{xy}\rangle + e^{2\pi i/3}|d_{xz}\rangle + e^{-2\pi i/3}|d_{yz}\rangle \equiv |l^z_{\rm eff} = -1\rangle$$







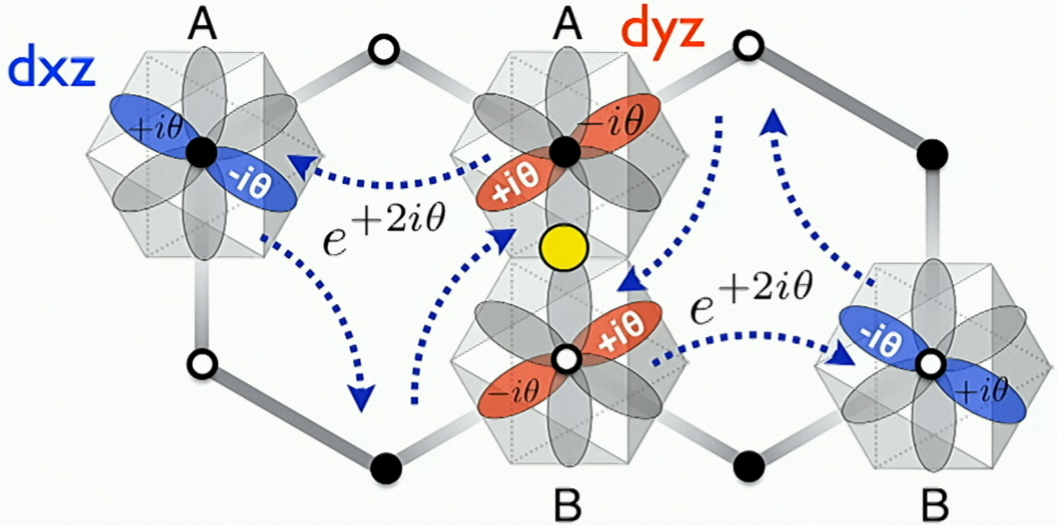
$$H = t_1 \sum_{\langle ij \rangle} c_i^\dagger c_j + t_2 \sum_{\langle\langle ij \rangle\rangle} e^{i\Phi_{ij}} c_i^\dagger c_j + h.c.,$$

	t_1	t_2	t'_2	t_3	$t_{\rm inter}$
BFPO ($e'_{\rm g-}$)	-116.7	+24.0	+39.1	-7.7	

2nd n.n hopping: complex

2nd n.n. hopping: complex hopping integrals

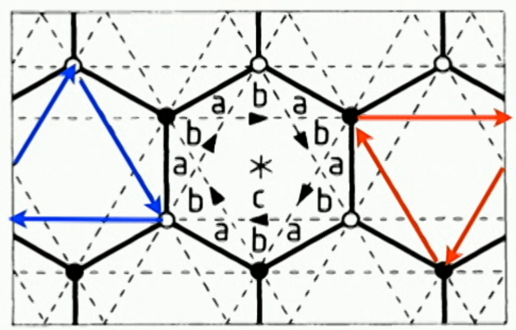
$$e'_{g-} \propto d_{xy} + e^{i\theta} d_{xz} + e^{-i\theta} d_{yz}$$



$$e^{2i\theta} c^{\dagger}_{iA} c_{jA} + e^{-2i\theta} c^{\dagger}_{iB} c_{jB} + h.c$$

Thus $\Phi_{ij} = 2\theta$ for A

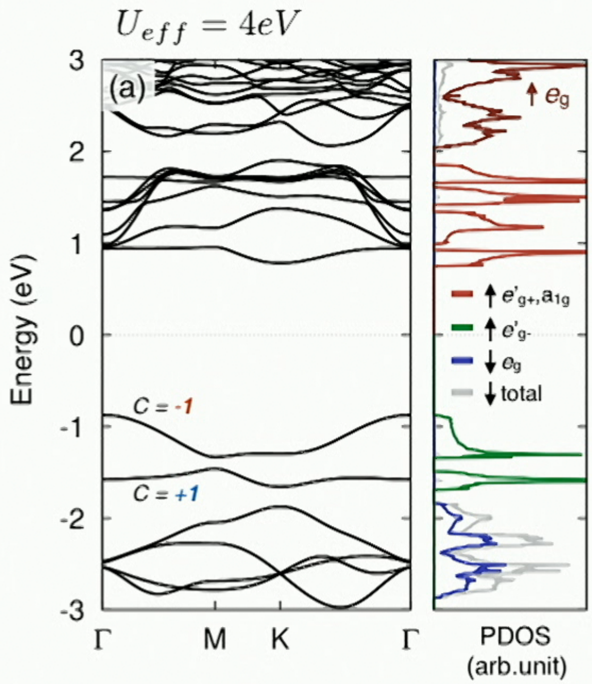
$\Phi_{ij} = -2\theta$ for B



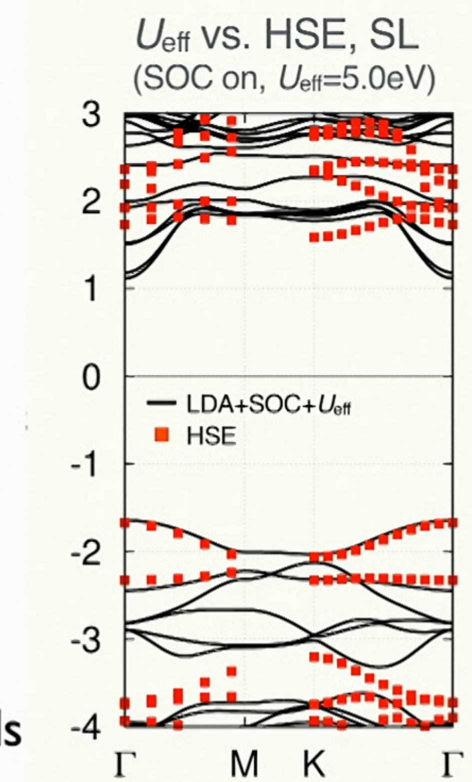
c+/c: electron with eg- orbital

e'_{g-} band maps to Haldane model

	t_1	t_2	t'_2	t_3	t_{inter}
BFPO (e'_{g-})	-116.7	+24.0	+39.1	-7.7	

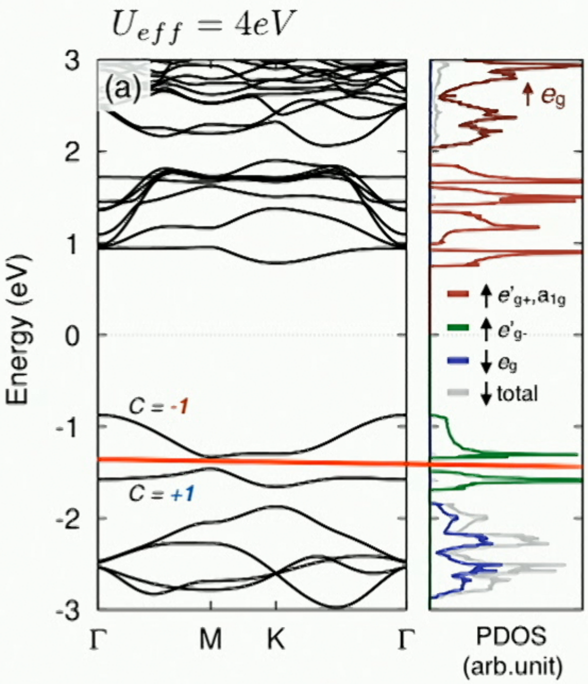


Two copies of Haldane Chern bands

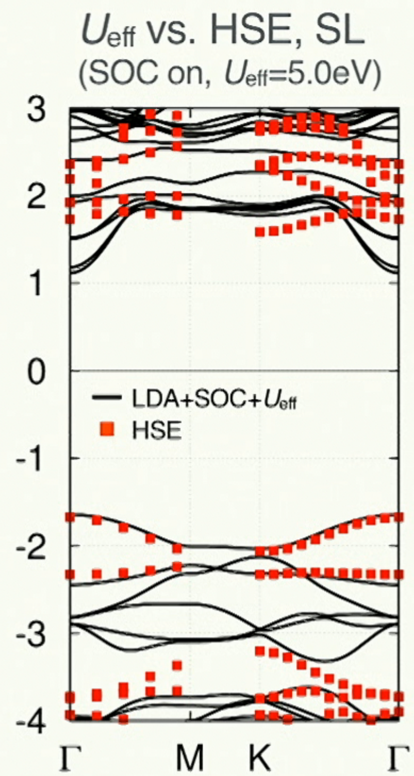


e'_{g-} band maps to Haldane model

	t_1	t_2	t'_2	t_3	$t_{\rm inter}$
BFPO (e'_{g-})	-116.7	+24.0	+39.1	-7.7	

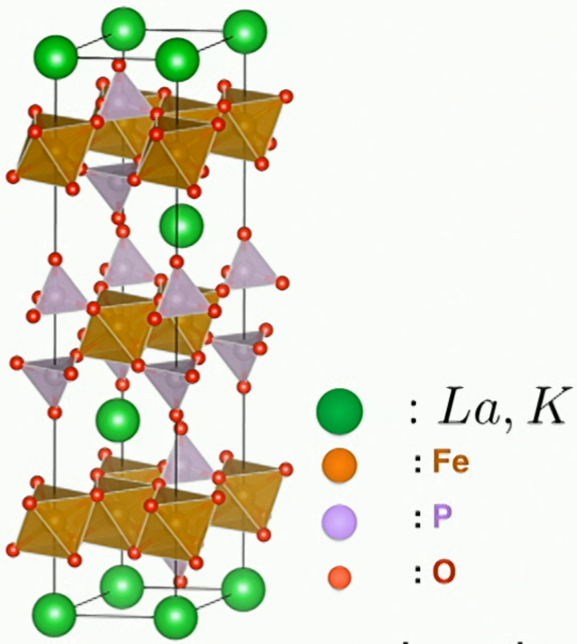


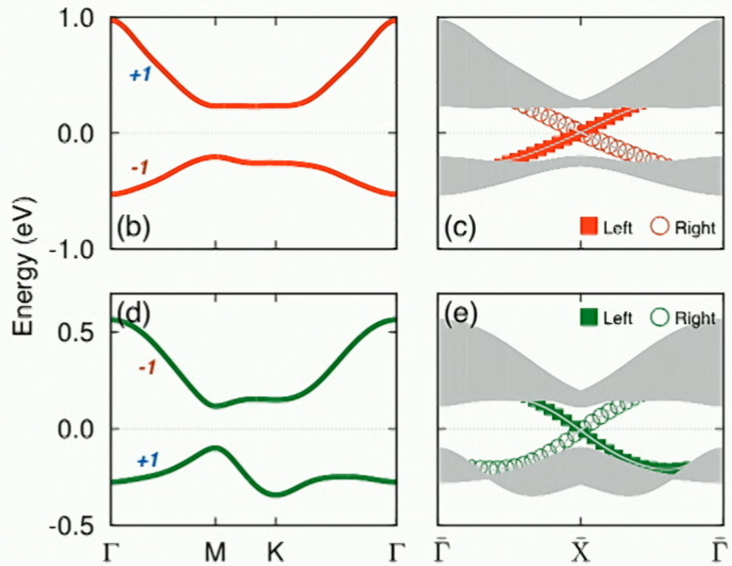
Gate doping



Two copies of Haldane Chern bands

New material proposal: $Ba^{2+} \rightarrow K^{+},\ La^{3+}$ Chemical doping





described by Haldane model

	t_1	t_2	t_2'	t_3	t_{inter}
LFPO (e'_{g+})	-210.4	-50.3	+22.0	-15.7	-5.2
KFPO (e'_{g-})	-137.6	+46.3	+24.0	+3.8	+1.2

H.-S. Kim & HYK, npj Quantum Materials (2017)2:20

Conclusion:

BaFe2(PO4)2: Topological Phase Transition :
Kagome Chern Insulator to Mott Insulator with two copies of Chern bands, as U increases

First realization of Haldane Chern Insulators in Stoichiometry Materials (KFPO, LFPO) with large moment and high Tc