Spin-orbit driven emergent phases in quantum materials

Indra Dasgupta

School of Physical Sciences
Indian Association for the Cultivation of Science
Kolkata, India
E-mail: sspid@iacs.res.in

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Workshop and International Conference on Electronic structure theory of emergent spin orbit driven phenomenon (Nov 11-15, 2024 , IIT Bombay)

Spin-Orbit Coupling & IIT Bombay

Sayantika Bhowal
Graduate Student (IACS)
Assistant Prof. IIT Bombay

Swarup Kr. Panda
Graduate Student (IACS)
MSc IIT Bombay
Associate Prof. Benett Univ

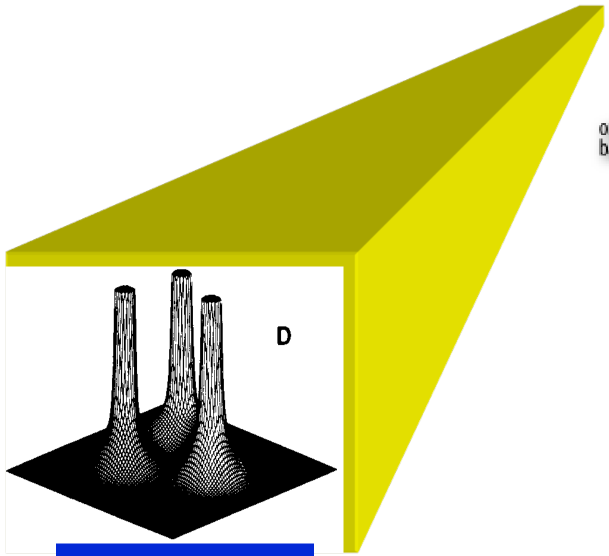
Ranjit Kr. Nanda
Graduate Student
PhD IIT Bombay
Prof. IIT Madras

(Half Heuslers)

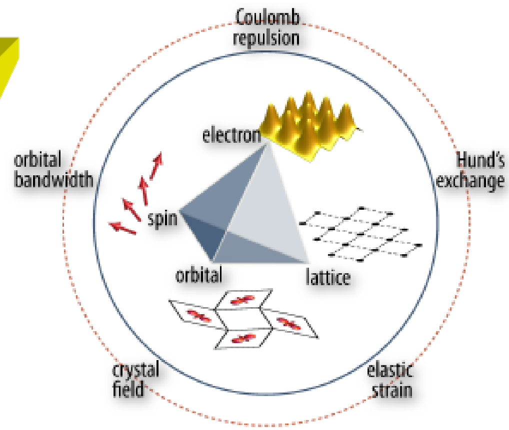
Electronic Structure of Quantum Materials

Strong interplay of the spin, charge, orbital and lattice degrees freedom + Topology → Emergent Phases and functions

Quantum Description



Microscopic
Electronic



Rondinelli and Spaldin (2011)

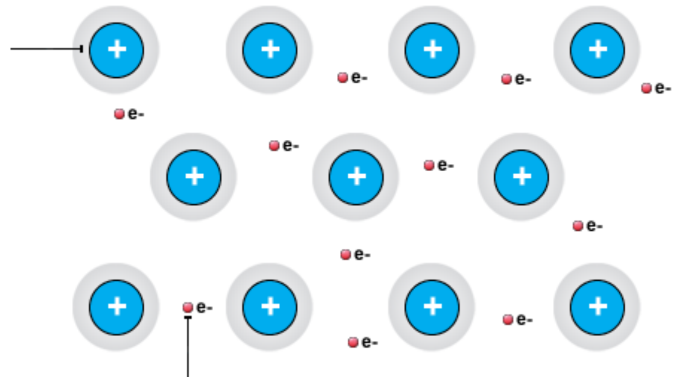
Starting Point: Independent Particle Approximation

Quantum Mechanics in Understanding Properties of Materials

$$H\Psi = \mathrm{E}\Psi$$

$$H = \sum_i [-\frac{1}{2}\Delta_i^2 + V(r_i)] + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

Non-interacting part **Interacting part**

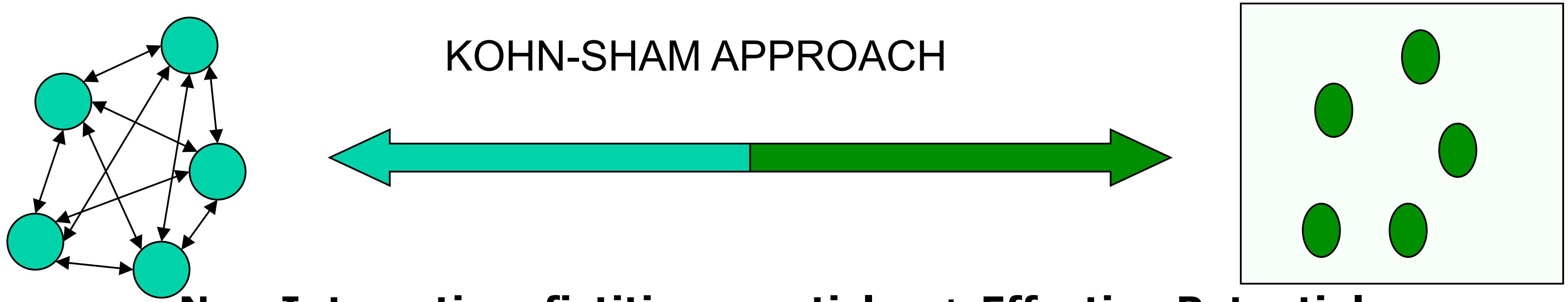


- **Density functional theory**

→ **Reduction to an effective non-interacting system.**

- **Self-consistent solution to an one electron Schrödinger equation with a periodic potential.**

Nobel Prize 1998

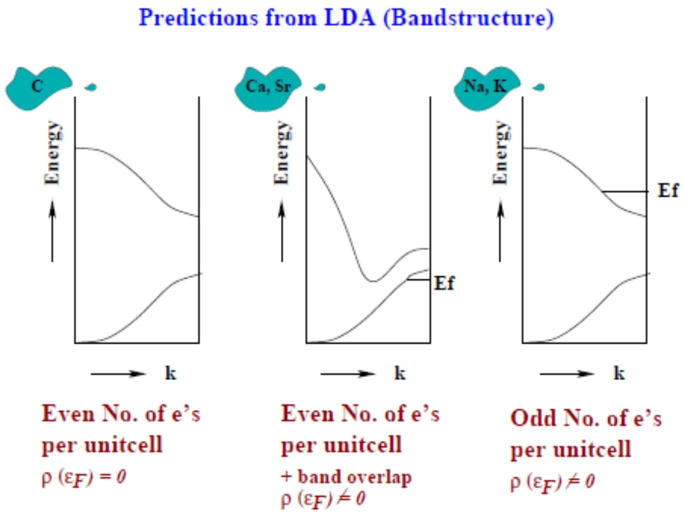


Non-Interacting, fictitious particles + Effective Potentials

KS-equation→ $$\left[-\frac{1}{2}\nabla^2 + V_H(n_{GS};\vec{r}) + V_{ext}(n_{GS};\vec{r}) + V_{xc}(n_{GS};\vec{r})\right]\Phi_i(\vec{r}) = \varepsilon_i \Phi_i(\vec{r})$$

Talk by Prof. Biplab Sanyal

Success & Failure of DFT



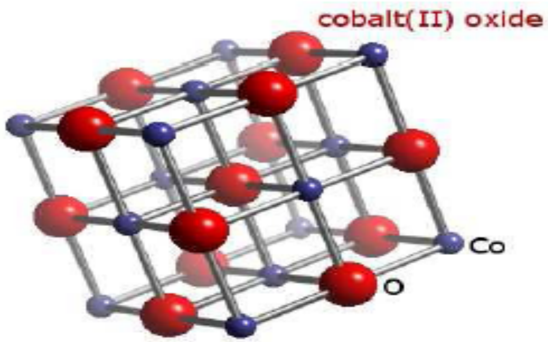
Accordingly to LDA, odd no. of e's per unit cell always give rise to Metal !

Pauli Exclusion Principle

Success:

Electronic Structure of Graphene/Dirac Materials, Topological Insulators
Identify Topological phases of Quantum Matter (Berry Phase):
Spin-orbit coupling is Important

Failure of Band Theory



Total No. of electrons = 9 +6 = 15

Band theory predicts CoO to be metal, while it is the toughest insulator known

Failure of LDA –) Failure of single particle picture
––) Importance of e–e interaction effects (Correlation)

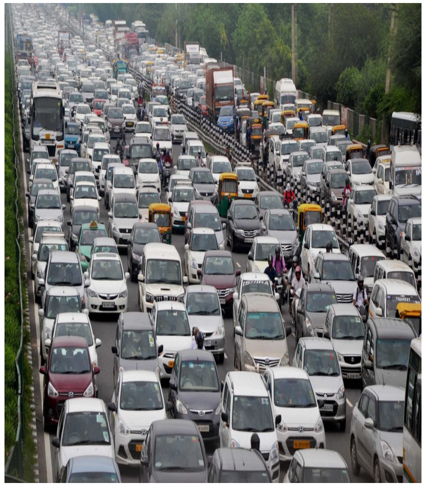
Other Example

High Tc Cuprates
La_2CuO_4 ➔
Insulator predicted to be a metal

STRONG CORRELATION

Strongly Correlated Systems & Model Hamiltonian Approach

$$H = \sum_i [-\frac{1}{2}\Delta_i^2 + V(r_i)] + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$



Find some complete one-particle basis:

$$H = \sum_i \varepsilon_i n_i + \sum_{i \neq j} t_{ij} c_i^+ c_j + \frac{1}{2} \sum_{ijkl} v_{ijkl} c_i^+ c_j^+ c_l c_k$$

Non-interacting part (DFT)

Interacting Part (only partially takes into account Correlation)

This model can be solved for small atoms and molecules, using, *e.g.* quantum chemical methods. But too complicated for systems we shall consider here:

Need to remove

→Degrees of freedom (Retain only active orbitals)

→Interaction terms

→Model Hamiltonian with chemical realism

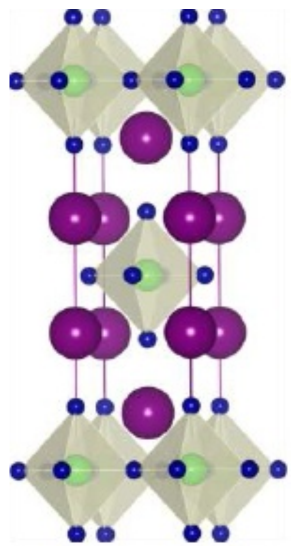
Key Ingredients of Quantum Matter Leading to Emergent Phases

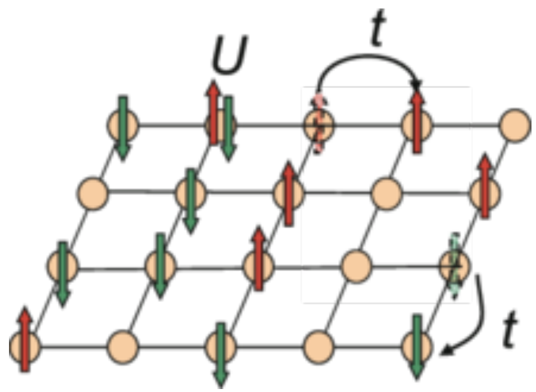
- **Crystal Field Spliting**
- **Kinetic Hopping (t)**
- **Onsite Coulomb Int. (U) & Hunds Exchange J_H**
- **Spin Orbit Interaction (λ)**

+

- **Topology (Frustrated Lattice ➔ Triangular, Kagome or Honeycomb)**

SrVO3



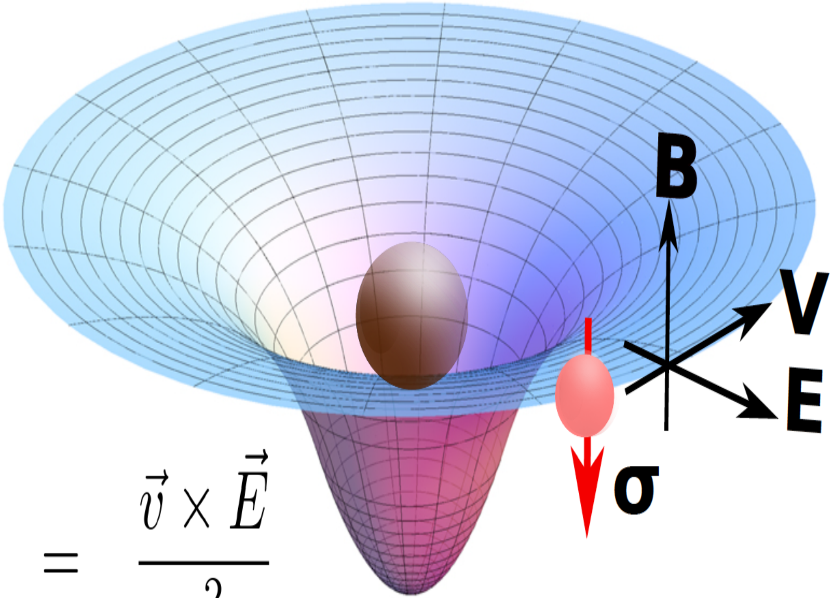


Wikipedia

Generic model Hamiltonian to start with.....

$$H=\sum t_{ij,\alpha\beta} C^{\dagger}_{i\alpha} C_{j\beta} + h.c + U \sum n_{i\alpha}(n_{i\alpha}-1) + \lambda \sum L_i . S_i$$

Spin-Orbit Coupling



$$\vec{B} = \frac{\vec{v} \times \vec{E}}{c^2}$$

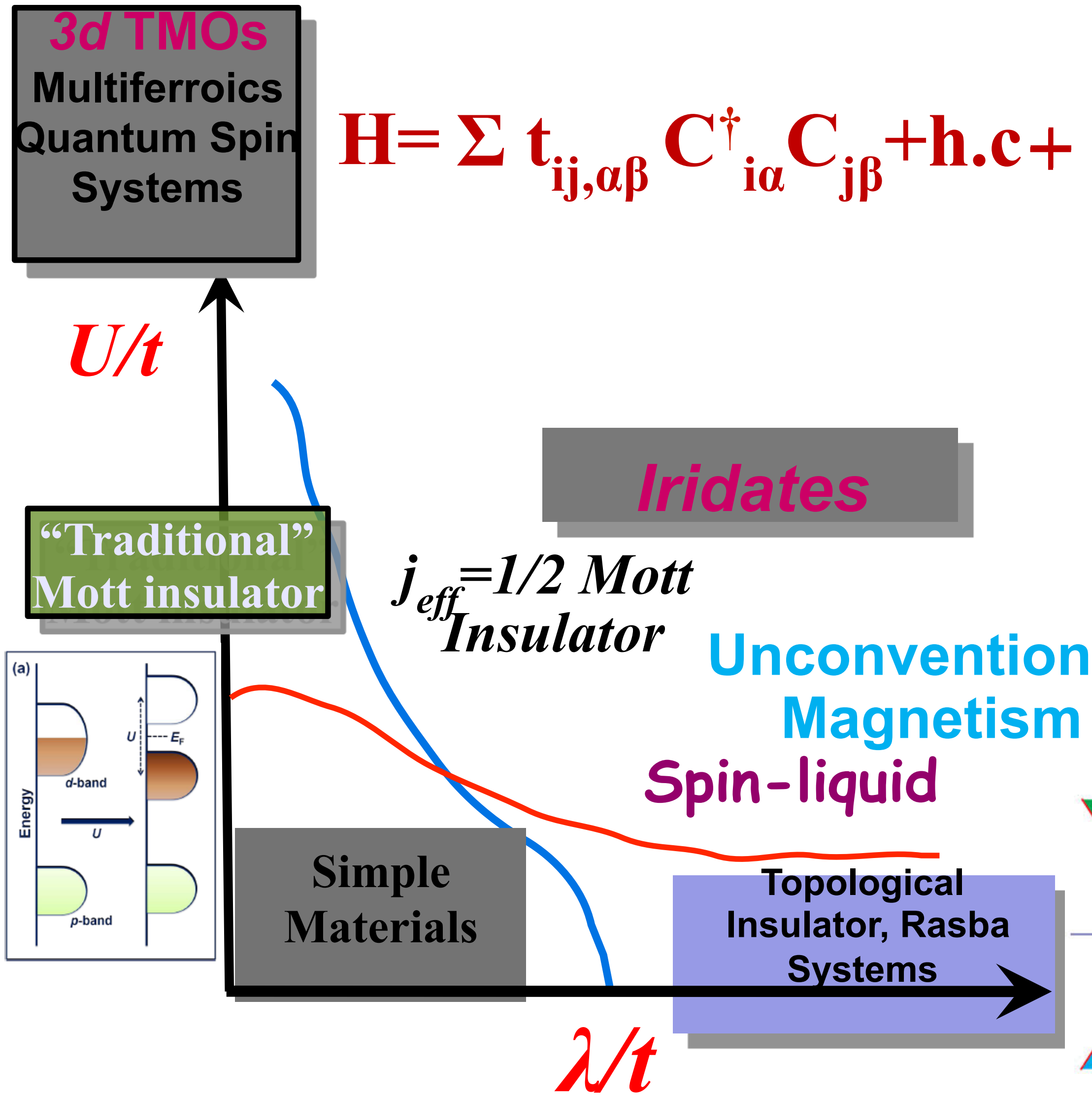
The radial electric field produced by the nucleus appears as a magnetic field in the rest frame of the electron. This magnetic field interacts with the spin of the electron resulting in SOC

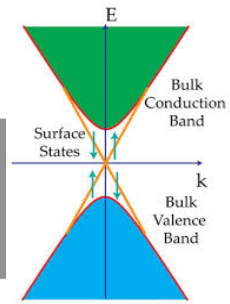
There can be other sources of electric field particularly in Non-centrosymmetric solids leading to Rashba-Dresselhaus effect

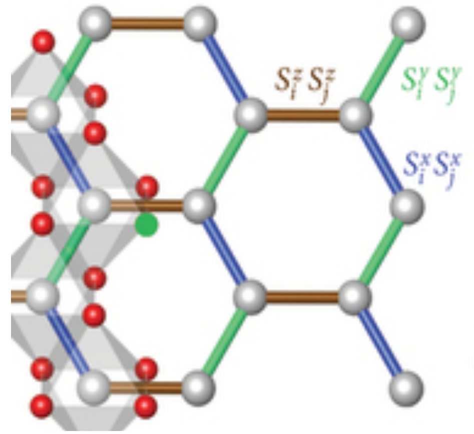
Emergent Phases:

$$H= \Sigma\, t_{ij,\alpha\beta}\, C^{\dagger}_{i\alpha} C_{j\beta} + h.c + U\, \Sigma\, n_{i\alpha}(n_{i\alpha}-1) + \lambda\, \Sigma\, L_i . S_i$$

$$H_{spin} = \Sigma\, J_{ij} S_i . S_j + K\, S_i^{\gamma} S_j^{\gamma}$$







QSL state with gapped/ gapless excitation

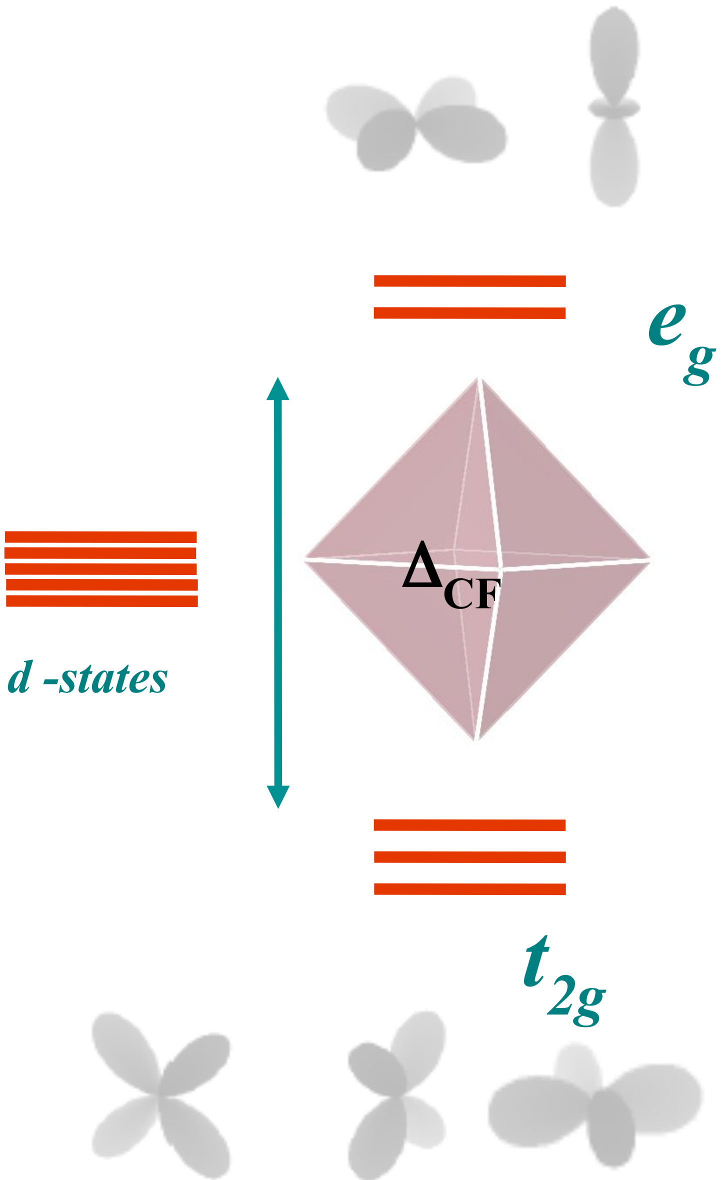
Third Axis : Disorder

Ann. Rev. Cond. Mat. Physics, Vol. 5: 57-82 (2014)

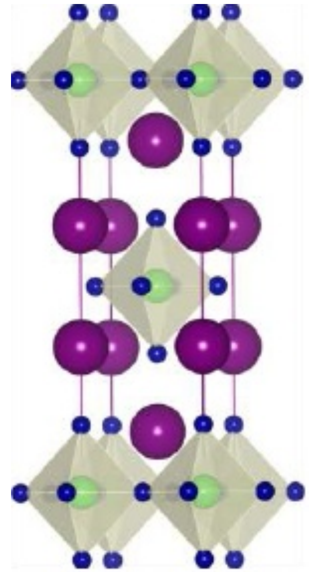
Nat. Phys. 11, 444–445 (2015)

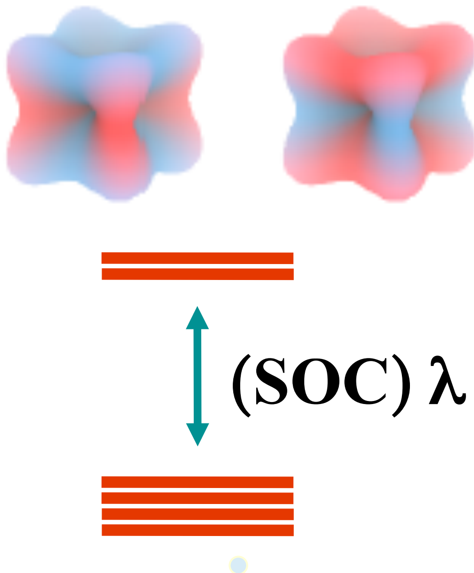
PRL 102, 017205 (2009)

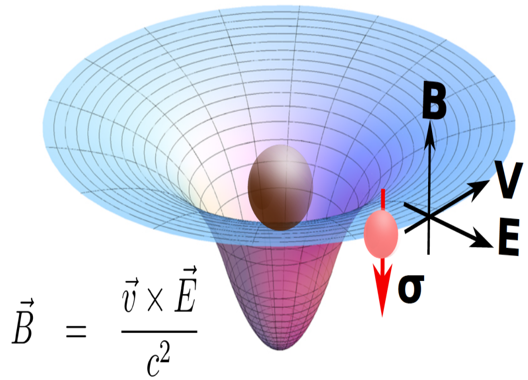
Crystal Field and Spin-Orbit Coupling (Onsite Terms)



These parameters
can be estimated
from DFT calc.

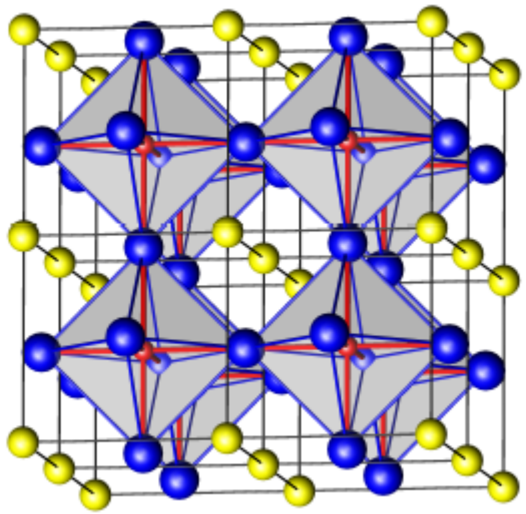


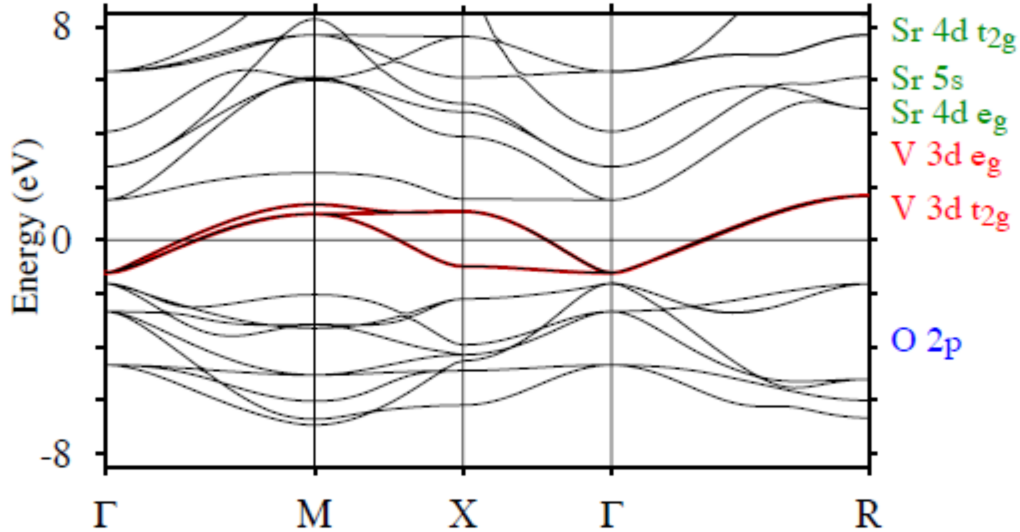


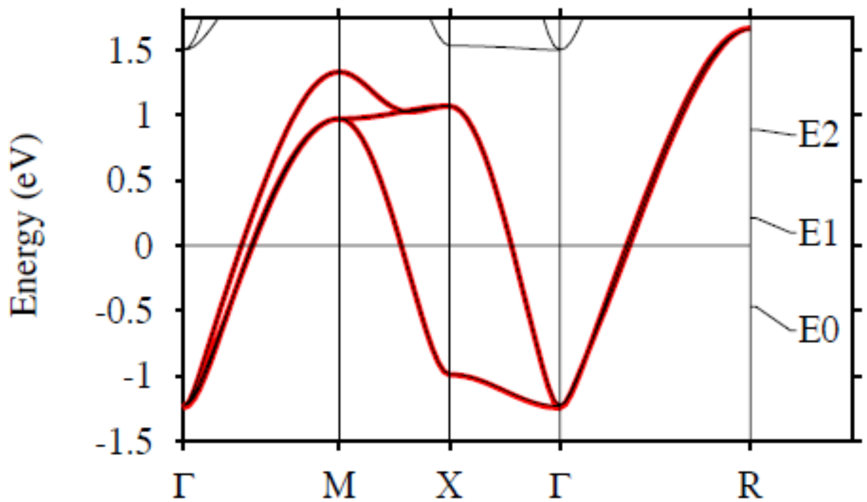


Few Band Tight-Binding Hamiltonian → Integrating out orbital *dof*

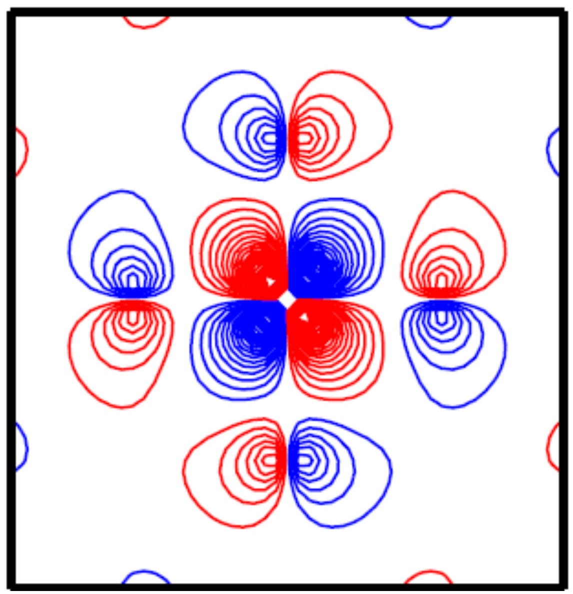
SrVO3







t2g Wannier Function



Pavarini *et. al.* *(2005)*

From LDA to minimal models

Löwdin downfolding: active (d) and passive (s, p).

$$H = \begin{pmatrix} H_{AA} & H_{AP} \\ H_{PA} & H_{PP} \end{pmatrix}$$

Integrate out weakly correlated/high energy states

$$H = H_{AA} + H_{AP}(\epsilon - H_{PP})^{-1} H_{AP}$$

Get rid of energy dependence.

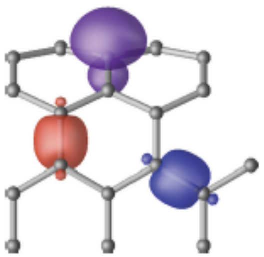
$$\tilde{H} = H_{AA} + H_{AP}(\epsilon_0 - H_{PP})^{-1} H_{PA}$$

Max-loc WFs ↔ "Exact" Tight-Binding

Compact mapping of Bloch states into local orbitals

$$\omega_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})d\mathbf{k}$$

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N_R}}\sum_R e^{i\mathbf{k}\cdot\mathbf{R}}\,\omega_n(\mathbf{r}-\mathbf{R})$$



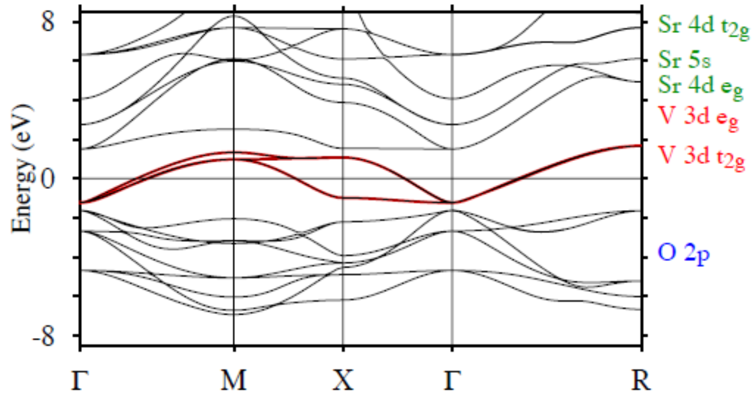
Multiband case:

$$w_n(\mathbf{r}-\mathbf{R}) = \frac{V}{8\pi^3}\int_{BZ} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_m U_{mn}^{(\mathbf{k})}\psi_{m\mathbf{k}}(\mathbf{r})\, d\mathbf{k}$$

SrVO3 → Active Orbitals t_{2g} , Passive → Rest

NMTO Downfolding Method

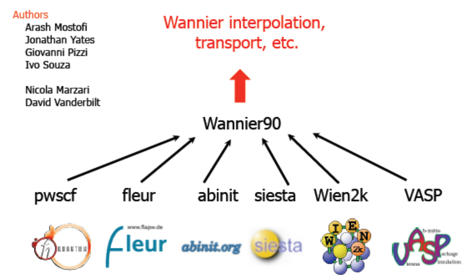
O.K Andersen & T. Saha-Dasgupta



Max. Localized WF
D. Vanderbilt

PRB 56, 12847 (1997)
Rev. Mod. Phys 84, 1419 (2012)

Wannier90 code



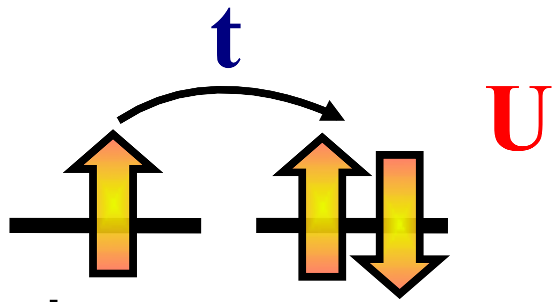
Strong Correlation..

Unpaired electron →metallic character

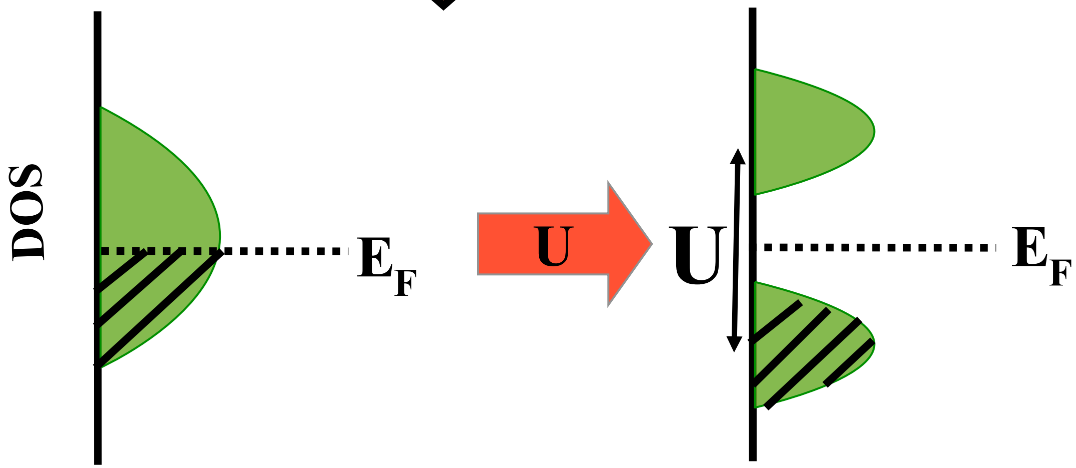
$$H=\Sigma\, t_{ij,\alpha\beta}\, C^{\dagger}_{i\alpha} C_{j\beta} + h.c + U\, \Sigma\, n_{i\alpha}(n_{i\alpha}-1)$$

Hubbard Model

Correlated System



Mott Insulator



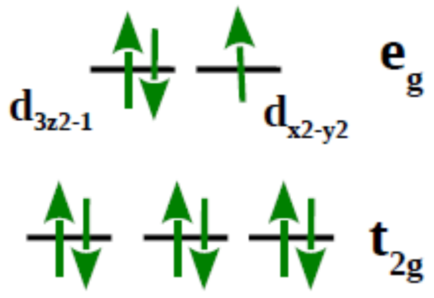
3*d* TMO-High T_c Cuprates:

- Half filled systems, Cu: d^9
- Insulator!

Hubbard Model

$$H = \sum t_{ij}[c_{i\sigma}^{+}c_{j\sigma} + c_{j\sigma}^{+}c_{i\sigma}] + U\sum n_{i\uparrow}n_{i\downarrow}$$

Mottronics



Hubbard Model to Heisenberg Model

1 Orbital and 1 electron / site ➔High Tc Cuprates (d^9)

U >> t, Consider t as a perturbation (Strong Coupling Expansion)

$$H_{Heis} = \sum J_{ij} S_i S_j$$

$J=4t^2/U$

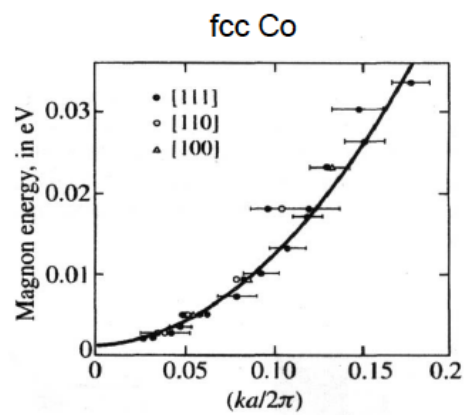
$$\hat{\mathcal{H}} \sim J \sum_{\langle i,j \rangle} a_i^{\dagger} a_j + h.c.$$

Spin Wave Analysis (Magnons)

$$S^z = S - a^{\dagger}a$$

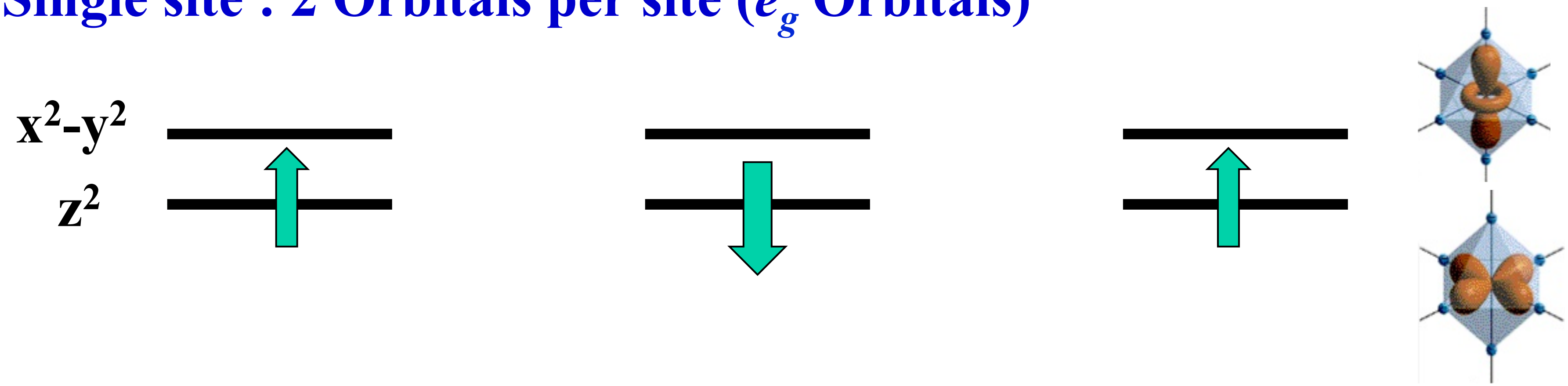
$$S^{+} = \sqrt{2S}\sqrt{1 - \frac{a^{\dagger}a}{2S}}\,a = \sqrt{2S}\left(1 - \frac{a^{\dagger}a}{4S}\right)a + \dots$$

$$S^{-} = \sqrt{2S}a^{\dagger}\sqrt{1 - \frac{a^{\dagger}a}{2S}} = \sqrt{2S}a^{\dagger}\left(1 - \frac{a^{\dagger}a}{4S}\right) + \dots$$



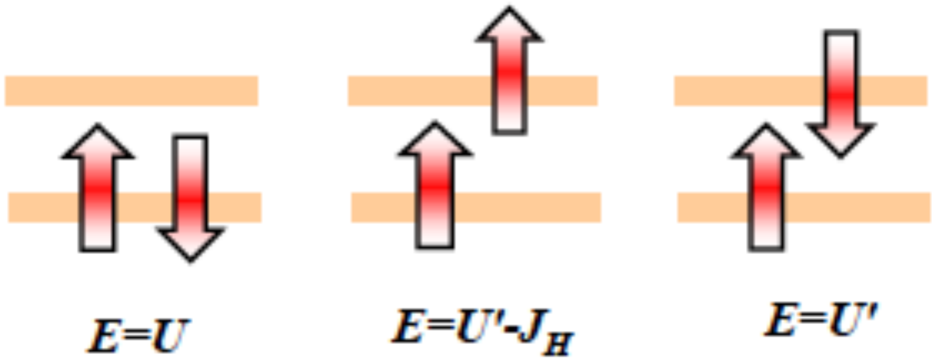
Interactions in a Multiband Hubbard Model

Single site : 2 Orbitals per site (e_g Orbitals)



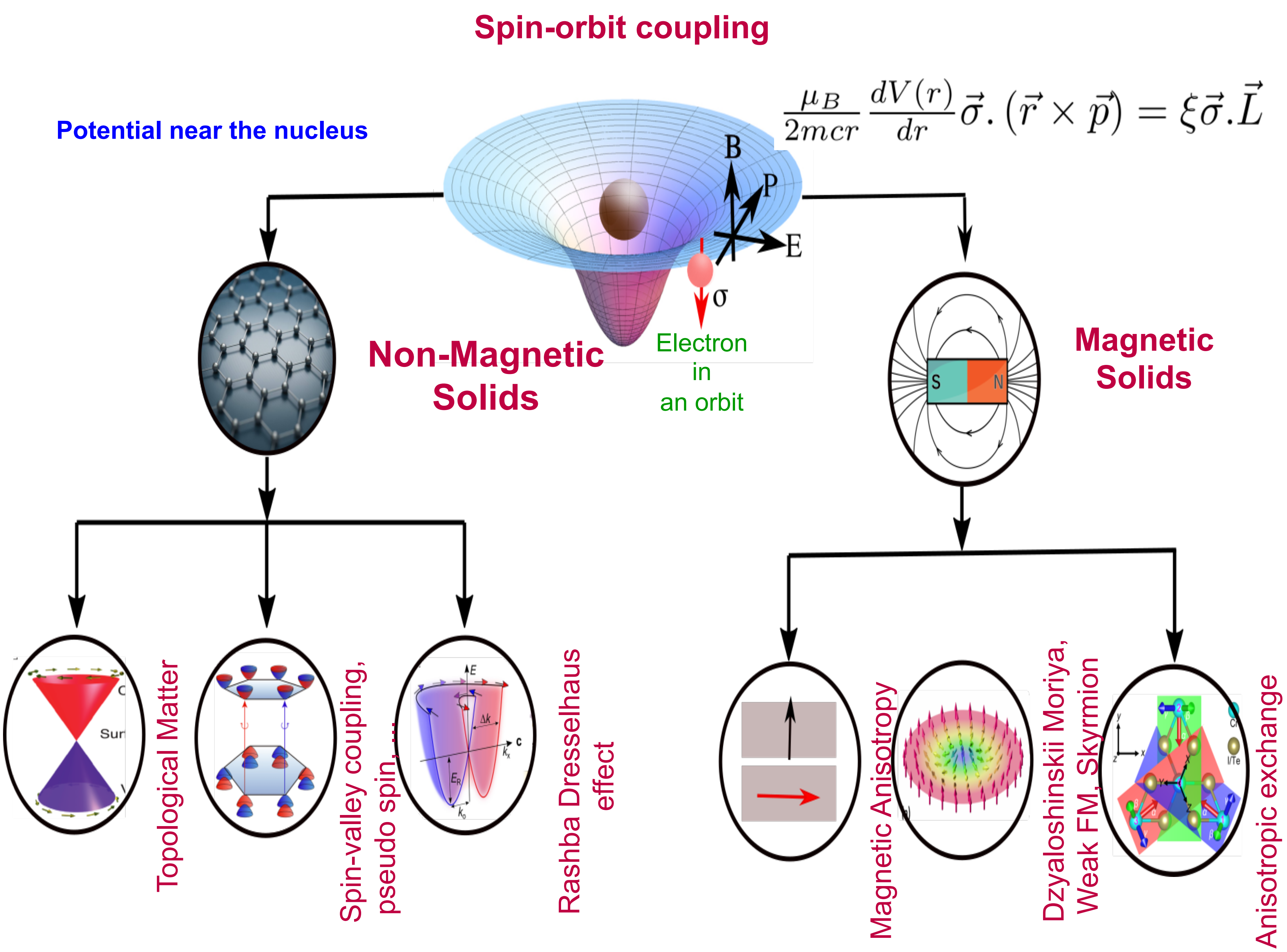
Cooperative JT Interaction / Orbital Ordering

After hopping three possible configurations



U' = Inter-orbital Coulomb Interaction

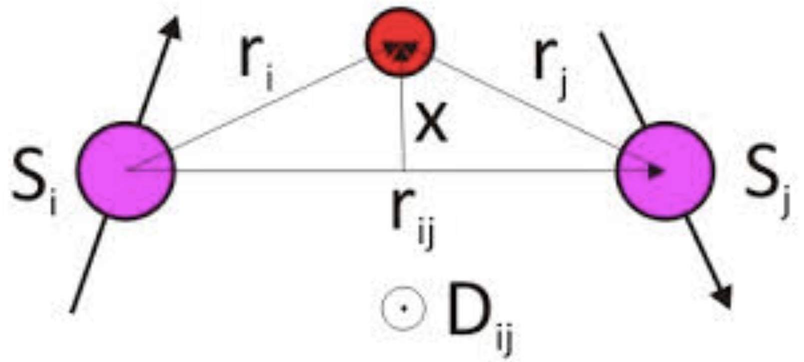
J_H = Hund's Exchange



Spin-orbit coupling
$$\frac{\mu_B}{2mcr}\frac{dV(r)}{dr}\vec{\sigma}.(\vec{r}\times\vec{p}) = \xi\vec{\sigma}.\vec{L}$$
Potential near the nucleus
B
P
E
σ
Electron in an orbit
Non-Magnetic Solids
Magnetic Solids
S
N
Topological Matter
Spin-valley coupling, pseudo spin, ...
Rashba Dresselhaus effect
Magnetic Anisotropy
Dzyaloshinskii Moriya, Weak FM, Skyrmion
Anisotropic exchange

Exchange Interaction and Spin-Orbit Coupling

Dzyaloshinskii–Moriya interaction



Anti-symmetric exchange interaction ➔ Canting of Spins

$$\mathbf{H_{DM} = \Sigma}\ \boldsymbol{D_{ij} \cdot S_i}\ \mathbf{X}\ \boldsymbol{S_j}$$

Requirements:

(a) Spin Orbit Coupling

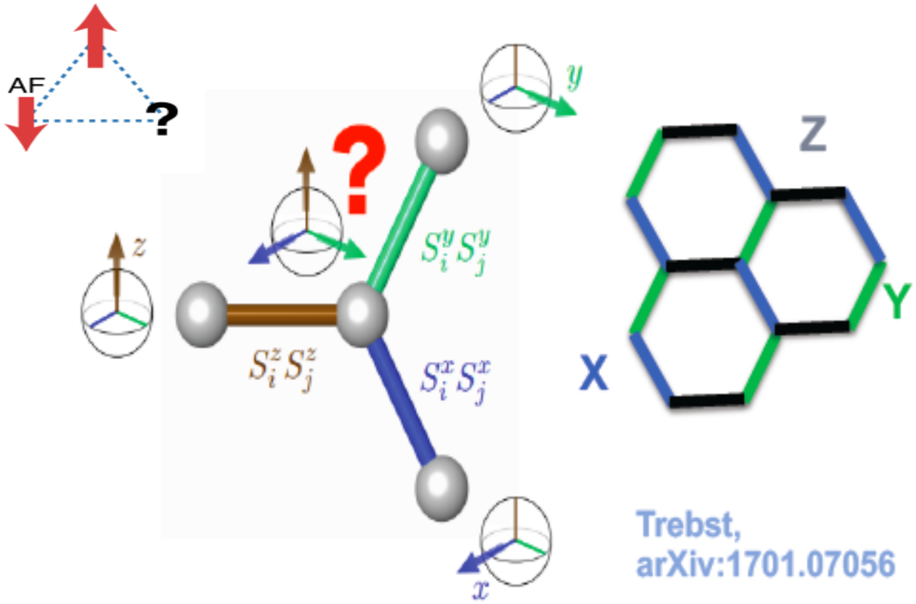
(b) Lack of Inversion Symmetry

SOC can lead to single ion anisotropy (easy axis)

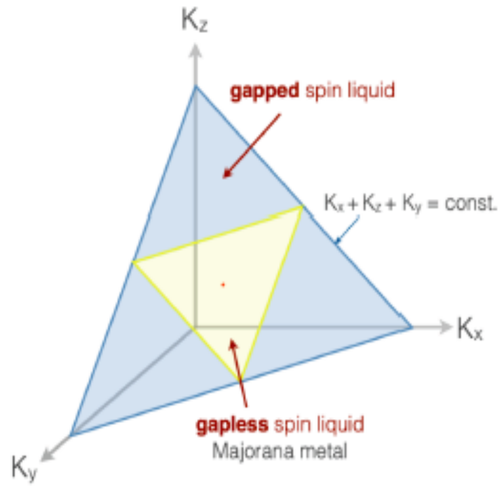
Heisenberg Model ➔ Ising Model

Kitaev model

- Bond-directional dependent Ising coupling → exchange frustration
- Ground state for S=1/2 moments on a 2D honeycomb lattice is an exactly solvable quantum spin liquid (QSL)
- Fractionalized spin excitations in the QSL are topologically protected gauge flux and Majorana fermion pairs



Trebst, arXiv:1701.07056



Alexei Kitaev

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Annals of Physics 321 (2006) 2–111
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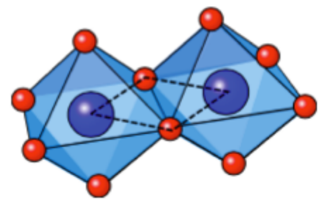
Anyons in an exactly solved model and beyond

Alexei Kitaev *
California Institute of Technology, Pasadena, CA 91125, USA

Received 21 October 2005; accepted 25 October 2005

Material Realization of Kitaev Spin Liquid

Proposed physical realization: Edge-sharing octahedra in honeycomb $J_{eff} = ½$ Mott insulators leads to bond directional, Kitaev-like exchange



Honeycomb systems with edge sharing octahedra

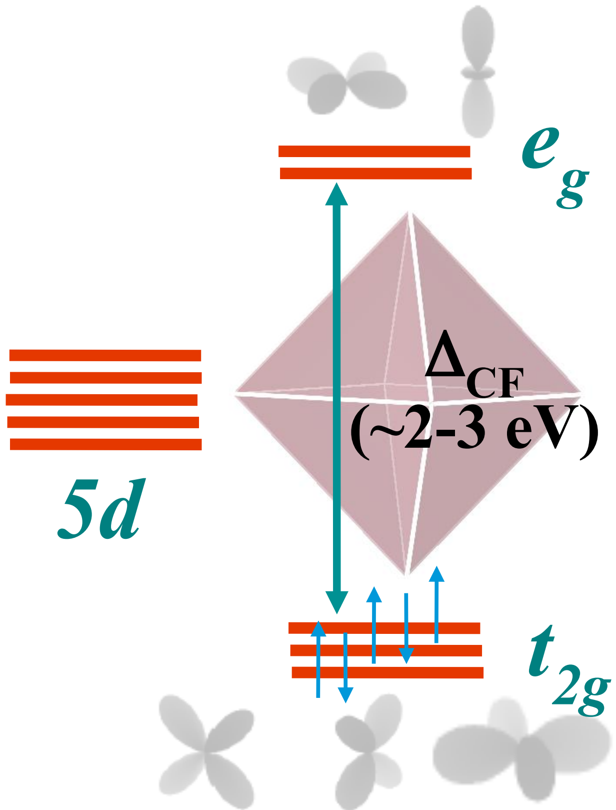
Multiband Hubbard Model + SOC

Search for Novel Quantum Materials

SOC Induced Novel Insulating State in *5d* transition metal Oxides:

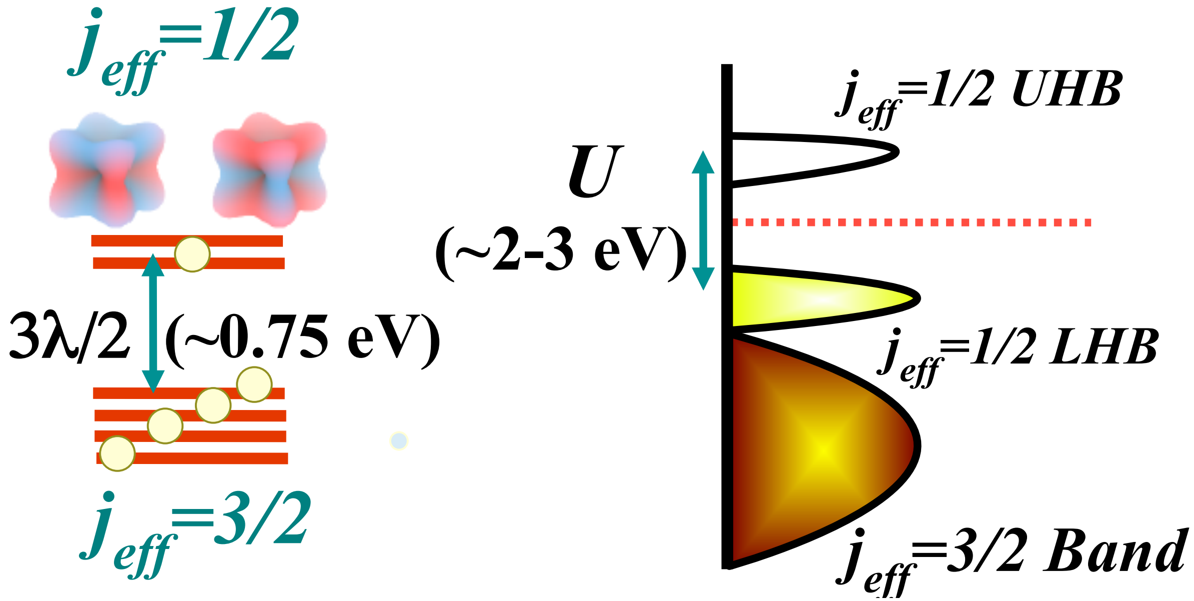
Traditional Belief:
5d **systems have large bandwidth**
→ U/t small
→uncorrelated metal (Boring!!!)

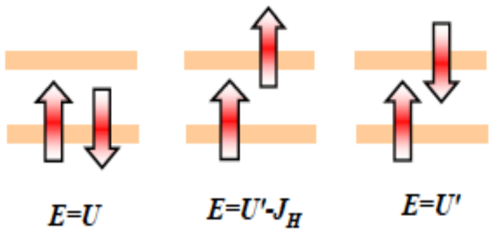
$CaIrO_3$, Sr_2IrO_4, Na_2IrO_3 having d^5 configuration are insulator!



j_{eff}=1/2 Mott insulator

Phys. Rev. Lett 101, 076402 (2008)





A Multiband Hubbard Hamiltonian:

$$H = H_{\Delta} + H_{int} + H_{SOC} + H_{t}$$

Crystal field

$$H_{\Delta} = \sum_{i}\sum_{l,m} e_{l,m} d^{\dagger}_{i,l\sigma} d_{i,m\sigma}$$

Interaction term

Spin-orbit coupling

$$H_{SOC} = \frac{i\lambda}{2}\sum_{i}\sum_{lmn} \epsilon_{lmn} \sum_{\sigma\sigma'} \sigma^{n}_{\sigma\sigma'} d^{\dagger}_{i,l\sigma} d_{i,m\sigma'}$$

Hopping

$$H_{t} = \sum_{\substack{l,m,\sigma \\ i\neq j}} t^{ij}_{l,m} d^{\dagger}_{i,l\sigma} d_{j,m\sigma}$$

$$H_{int} = U_d \sum_{i}\sum_{l} n_{i,l\uparrow} n_{i,l\downarrow} + \frac{(U'_d - J_H)}{2}\sum_{i}\sum_{\substack{l,m \\ l\neq m}} n_{i,l\sigma} n_{i,m\sigma} + \frac{U'_d}{2}\sum_{i}\sum_{\substack{l,m \\ l\neq m \\ \sigma\neq\sigma'}} n_{i,l\sigma} n_{i,m\sigma'}$$
$$- \frac{J_H}{2}\sum_{i}\sum_{\substack{l,m \\ l\neq m}} (d^{\dagger}_{i,m\uparrow} d_{i,m\downarrow} d^{\dagger}_{i,l\downarrow} d_{i,l\uparrow} - d^{\dagger}_{i,m\downarrow} d^{\dagger}_{i,m\uparrow} d_{i,l\uparrow} d_{i,l\downarrow} + h.c.)$$

Kanamori Hamiltonian

PRL 102, 017205 (2009) PHYSICAL REVIEW LETTERS week ending 9 JANUARY 2009

Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

G. Jackeli[1,*] and G. Khaliullin[1]
[1]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
(Received 21 August 2008; published 6 January 2009)

Spin –Orbital Entangled $J_{eff} = ½$ States

$$|\uparrow\rangle = \quad \phi_{3\alpha} = \frac{1}{\sqrt{3}}(d_{xy\uparrow} + d_{yz\downarrow} + i d_{zx\downarrow}),$$

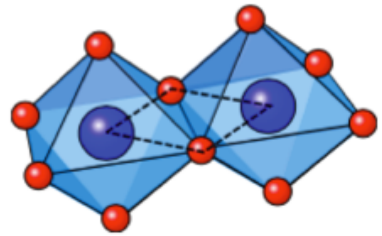
$$|\downarrow\rangle = \quad \phi_{3\beta} = \frac{1}{\sqrt{3}}(d_{xy\downarrow} - d_{yz\uparrow} + i d_{zx\uparrow}).$$

Isospin up state

Strong Coupling expansion in the $J_{eff} = ½$ manifold U, λ >> t

Spin model: Kitaev Interaction

$$H = \Sigma_{\alpha\beta(\gamma)\in<ij>}$$
$$K\, S_i^{\gamma} S_j^{\gamma} + \Gamma(S_i^{\alpha} S_j^{\beta} + S_i^{\beta} S_j^{\alpha})]$$



Edge sharing octahedra in a Honeycomb lattice

Realization of novel Magnetic States → Spin Liquids

PHYSICAL REVIEW B **104**, 115106 (2021)

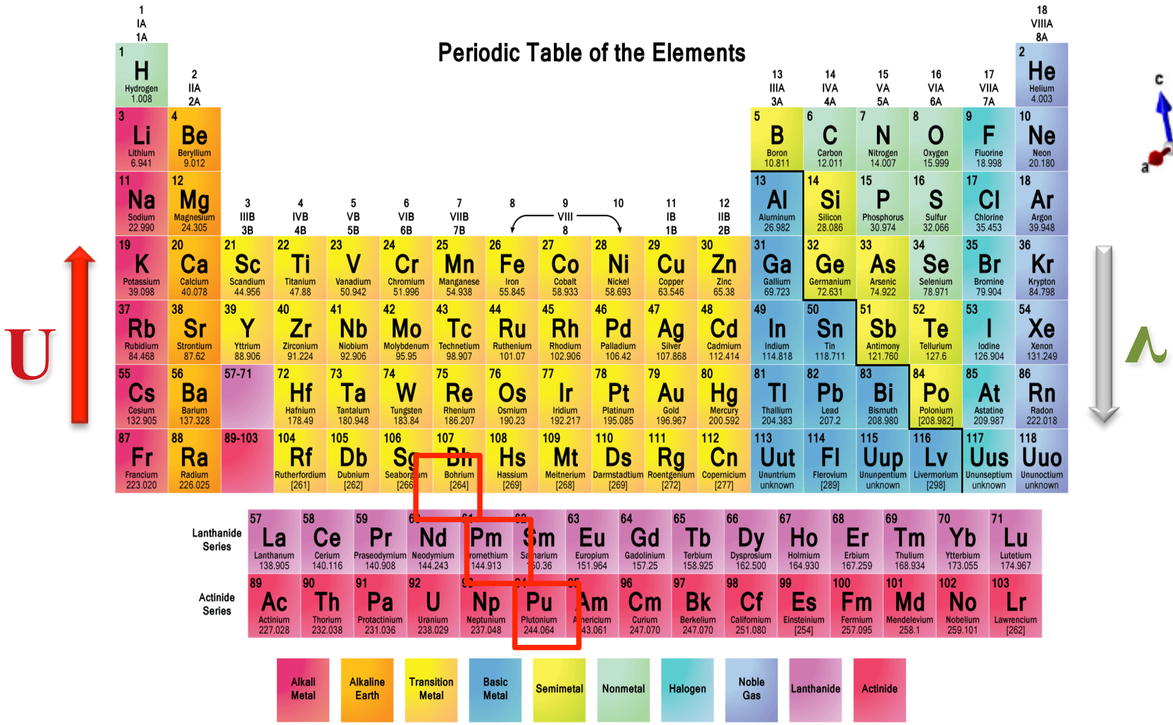
Unusual spin dynamics in the low-temperature magnetically ordered state of $Ag_3LiIr_2O_6$

Atasi Chakraborty,[1,*] Vinod Kumar,[2,*] Sanjay Bachhar,[2] N. Büttgen,[3] K. Yokoyama,[4] P. K. Biswas,[4] V. Siruguri,[5] Sumiran Pujari,[2] I. Dasgupta,[1] and A. V. Mahajan[2,†]

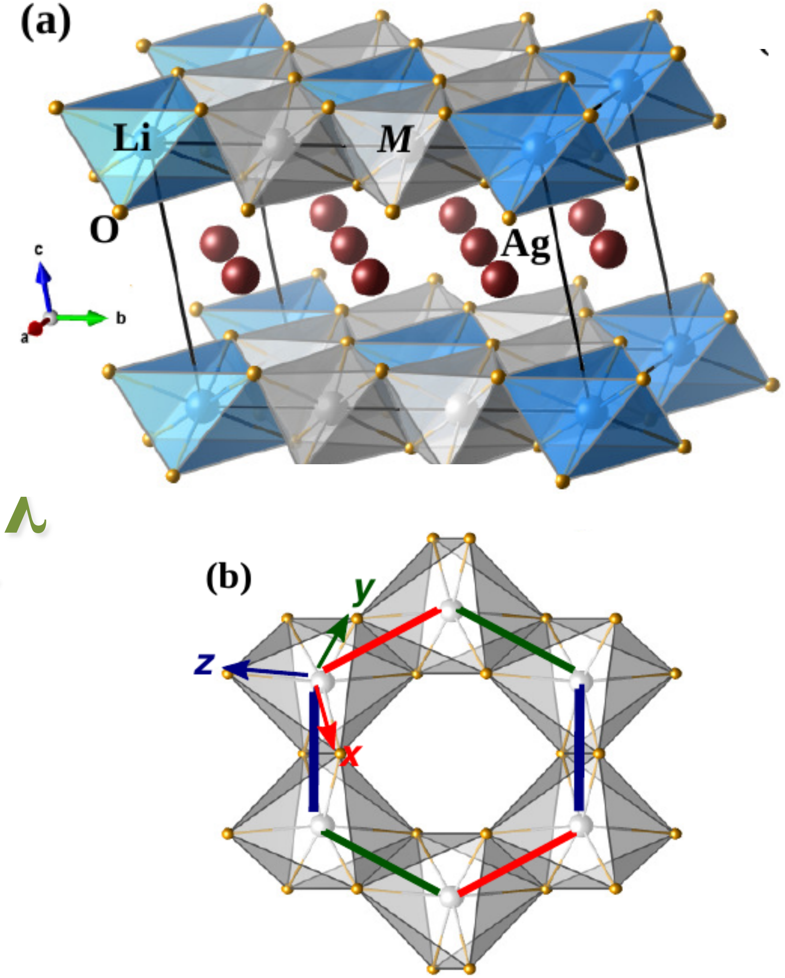
Theory (DFT) : Atasi Chakraborty , Mainz (Germany)

Expt : (NMR, muSR)Vinod Kumar, Sanjay Bachhar & A.V. Mahajan (IIT-B)

$Ag_3LiIr_2O_6$



$Ag_3^{1+}Li^{1+}Ir_2^{4+}O_6^{2-}$

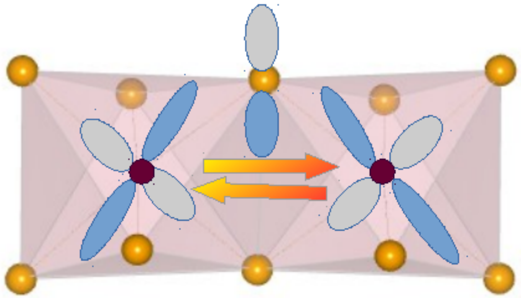


Monoclinic [space group C2/m]

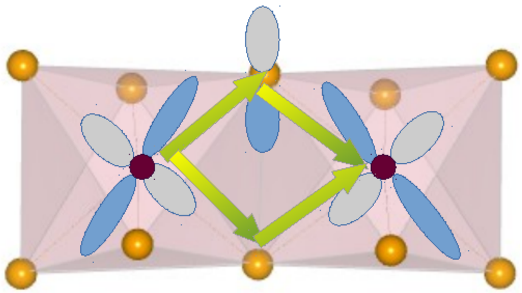
$Ag_3LiIr_2O_6$

Honeycomb network: dominant SOC ($5d^5$)+ Spin 1/2 $\Rightarrow$ Kitaev exchange

$$H = \sum_{\langle i,j\rangle \in \gamma} (J\, S_i . S_j + K\, S_i^{\gamma} S_j^{\gamma})$$



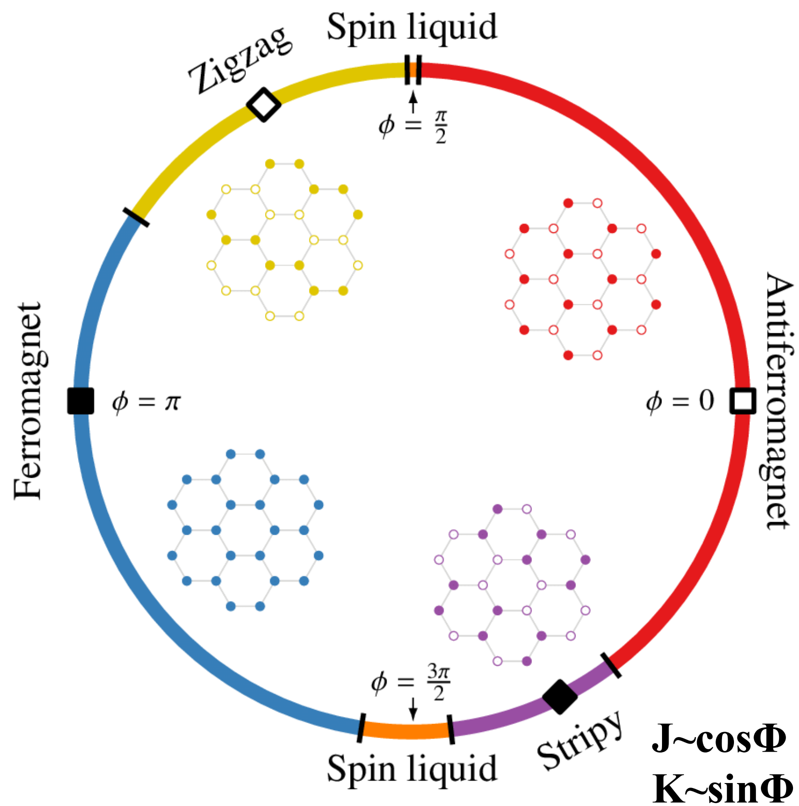
J from
direct d-d hopping



K from
super exchange via oxygen

Competing energy scale

Long range ordering **QSL**



J~cosΦ
K~sinΦ

LETTER

[$H_3LiIr_2O_6$]

doi:10.1038/nature25482

A spin–orbital-entangled quantum liquid on a honeycomb lattice

K. Kitagawa[1]*, T. Takayama[2]*, Y. Matsumoto[2], A. Kato[1], R. Takano[1], Y. Kishimoto[3], S. Bette[2], R. Dinnebier[2], G. Jackeli[2,4] & H. Takagi[1,2,4]

PHYSICAL REVIEW LETTERS **123**, 237203 (2019)

Thermodynamic Evidence of Proximity to a Kitaev Spin Liquid in $Ag_3LiIr_2O_6$

Faranak Bahrami,[1] William Lafargue-Dit-Hauret,[2,3] Oleg I. Lebedev,[4] Roman Movshovich,[5] Hung-Yu Yang,[1] David Broido,[1] Xavier Rocquefelte,[2] and Fazel Tafti[1,*]

[1]*Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA*
[2]*Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226, F-35000 Rennes, France*
[3]*Physique Théorique des Matériaux, CESAM, Université de Liège, B-4000 Sart Tilman, Belgium*
[4]*Laboratoire CRISMAT, ENSICAEN-CNRS UMR6508, 14050 Caen, France*
[5]*MPA-CMMS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

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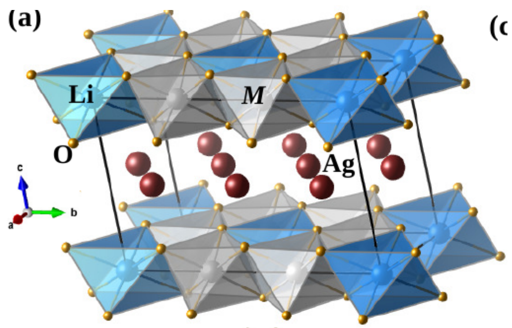
Is $Ag_3LiIr_2O_6$ a Kitaev Spin Liquid ?

(a)

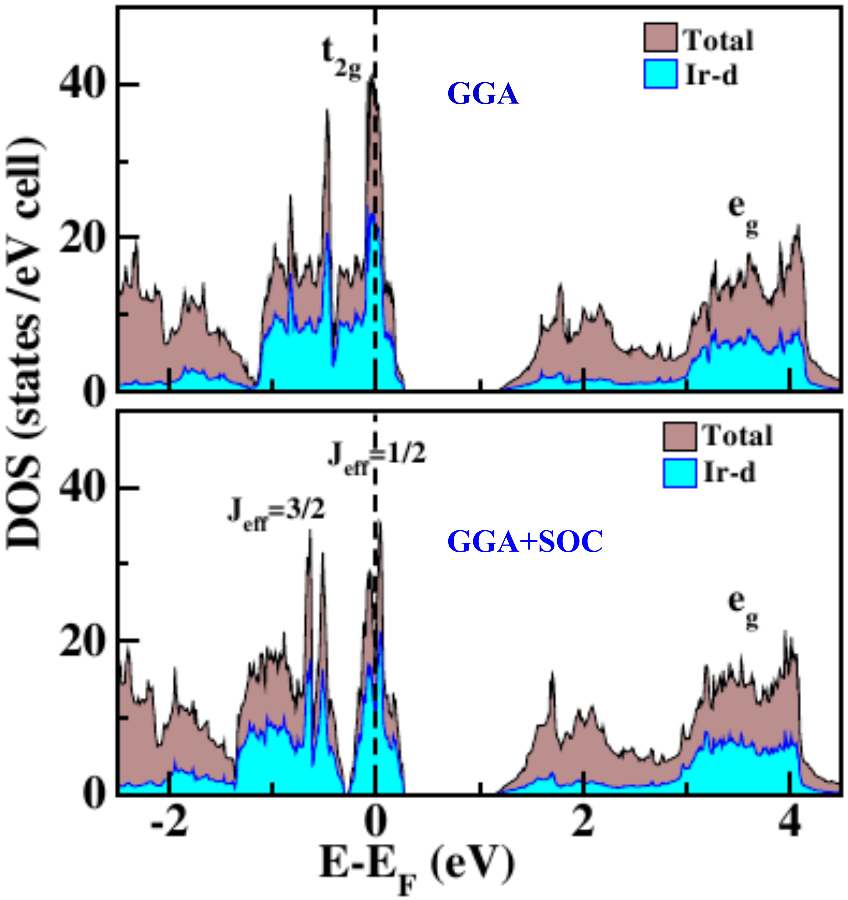


Hamiltonian within bond basis

$$S_i = \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix} \qquad \hat{H} = \mathbf{S}_i \cdot \tilde{J}_{ij} \cdot \mathbf{S}_j$$

$$H = \sum_{\langle ij \rangle \in \alpha\beta(\gamma)} [J^\alpha S_i^\alpha S_j^\alpha + J^\beta S_i^\beta S_j^\beta + J^\gamma S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) + D(S_i^\alpha S_j^\beta - S_i^\beta S_j^\alpha)] \quad (2)$$

$$\tilde{J} = \begin{pmatrix} J_{xx} & J_{xy} & J_{xz} \\ J_{yx} & J_{yy} & J_{yz} \\ J_{zx} & J_{zy} & J_{zz} \end{pmatrix}$$



For the Z bond

$J_z = 5.5$ meV (AFM)

$K_z = -5.1$ meV (FM),

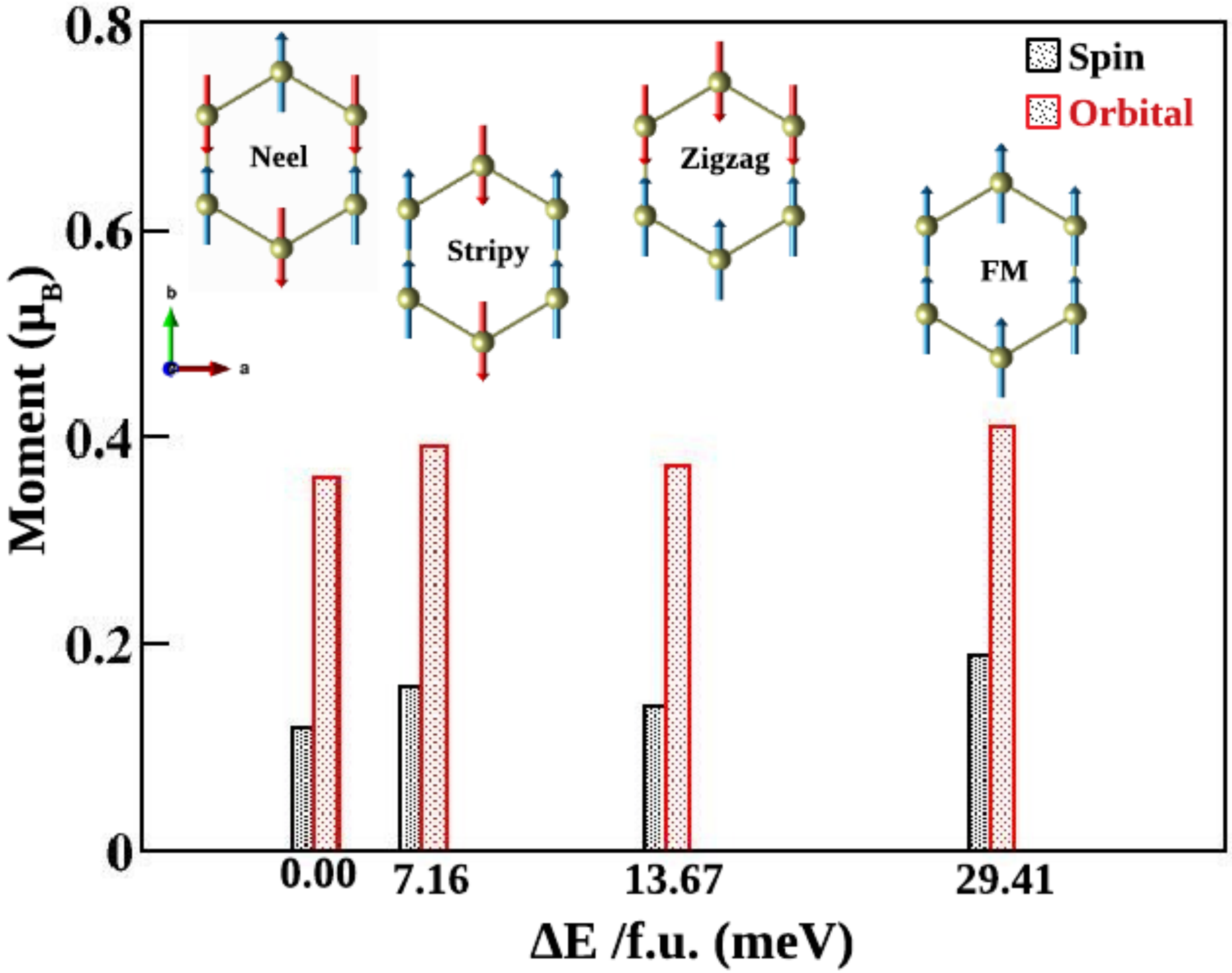
$\Gamma z = -1.3$ meV (FM),

$\Gamma_z' = -3.0$ meV (FM)

J is comparable to K

-> Ordering

Ground state magnetism

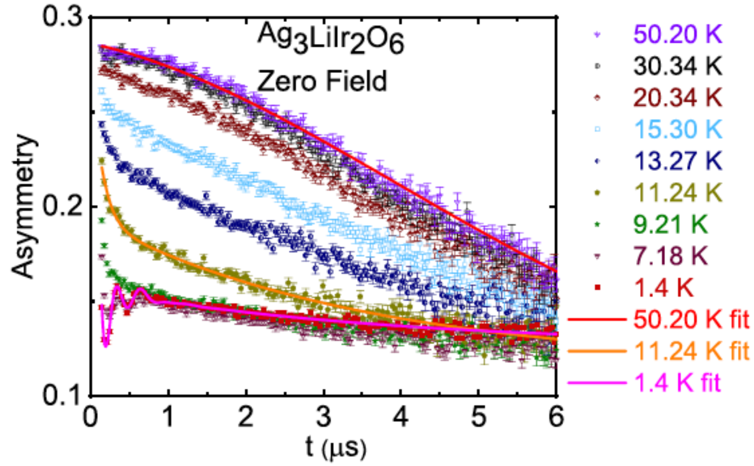


Stable AFM long range ordered ground state

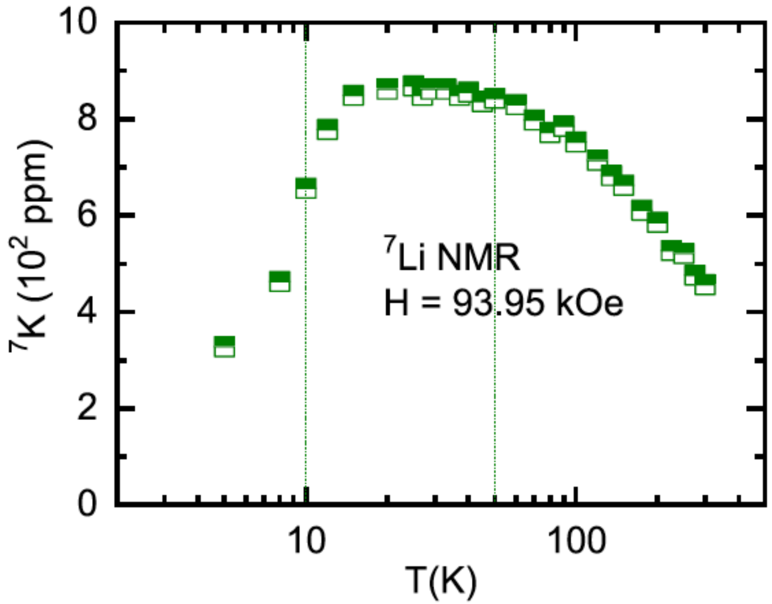
A. V. Mahajan (IIT Bombay) Ordering confirmed by muSR measurements

Experimental Scenario

Oscillations in μSR relaxation data below ~9K ➔Magnetic Ordering. Analysis of muon data in the orderd state complemented with DFT of Muon stopping sites points toward incommensurate Neel and stripe ordered magnetic domains



^{7}Li NMR shift shows 2 anomalies 10K ~ onset of long range ordering.
Broad maximum at 50K ~ onset of SRO



PRB 104, 115106 (2021)

Spin Liquids

PRL **116,** 097205 (2016) PHYSICAL REVIEW LETTERS week ending 4 MARCH 2016

Origin of the Spin-Orbital Liquid State in a Nearly $J = 0$ Iridate $Ba_3ZnIr_2O_9$

Abhishek Nag,[1] S. Middey,[2‡] Sayantika Bhowal,[3] S. K. Panda,[2§] Roland Mathieu,[4] J. C. Orain,[5] F. Bert,[5] P. Mendels,[5] P. G. Freeman,[6,7] M. Mansson,[6,8] H. M. Ronnow,[6] M. Telling,[9] P. K. Biswas,[10] D. Sheptyakov,[11] S. D. Kaushik,[12] Vasudeva Siruguri,[12] Carlo Meneghini,[13] D. D. Sarma,[14] Indra Dasgupta,[2,3,*] and Sugata Ray[1,2,†]

PHYSICAL REVIEW LETTERS **125,** 267202 (2020)

Geometric Frustration

Gapless Quantum Spin Liquid in the Triangular System $Sr_3CuSb_2O_9$

S. Kundu,[1,*] Aga Shahee,[1] Atasi Chakraborty,[2] K. M. Ranjith,[3] B. Koo,[3] Jörg Sichelschmidt,[3] Mark T. F. Telling,[4] P. K. Biswas,[4] M. Baenitz,[3] I. Dasgupta,[2] Sumiran Pujari,[1] and A. V. Mahajan[1,†]

PHYSICAL REVIEW B **104**, 115106 (2021)

Exchange Frustration (Kitaev)

Unusual spin dynamics in the low-temperature magnetically ordered state of $Ag_3LiIr_2O_6$

Atasi Chakraborty,[1,*] Vinod Kumar,[2,*] Sanjay Bachhar,[2] N. Büttgen,[3] K. Yokoyama,[4] P. K. Biswas,[4] V. Siruguri,[5] Sumiran Pujari,[2] I. Dasgupta,[1] and A. V. Mahajan[2,†]

Is there any other source of Spin-Orbit Coupling ?

Collaboration

Kunal Dutta (IACS)

Subhadeep Bandyopadhyay (IACS)
➔Univ of Leige', Belgium

Atanu Paul (IACS)
→ Bar –Ilan University, Israel

Phys. Rev. B 101, 014109 (2020)
Phys Rev B 103, 014105 (2021)

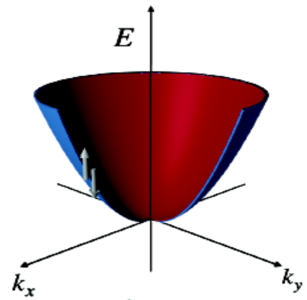
Phys Rev B 108, 245146 (2023)

Symmetry and Band Splitting

$$\text{Crystal inversion symmetry}: \varepsilon(\vec{k}\uparrow) = \varepsilon(-\vec{k}\uparrow)$$

$$\text{Time reversal symmetry}: \varepsilon(\vec{k}\uparrow) = \varepsilon(-\vec{k}\downarrow)$$

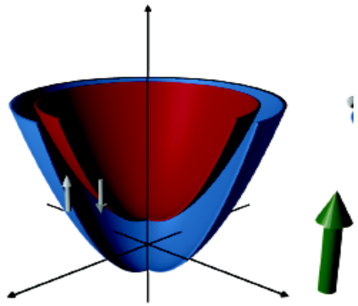
$$\text{Kramer's degenarcy}: \varepsilon(\vec{k}\uparrow) = \varepsilon(\vec{k}\downarrow)$$



Spin degenerate
$E_{\uparrow\downarrow} = ak^2$

Breaking Time rerversal symmetry applying external magnetic field

$$\boxed{\varepsilon(\vec{k}\uparrow) \neq \varepsilon(-\vec{k}\downarrow)}$$

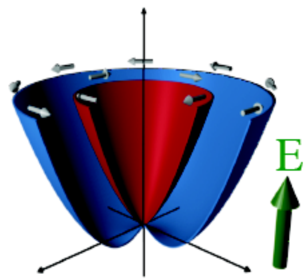


Zeeman splitting B
$E_{\uparrow\downarrow} = ak^2 \pm \alpha_z$

Breaking inversion symmetry

(Can be broken by applying external Electric field)

$$\boxed{\varepsilon(\vec{k}\uparrow) \neq \varepsilon(-\vec{k}\uparrow)}$$



Emmanuel I. Rashba (1927-)

Momentum-dependent splitting of the spin bands in non-centrosymmetric systems.

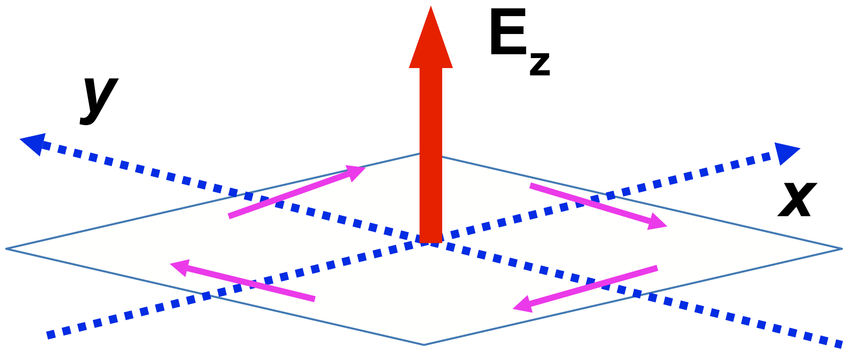
Rashba splitting
$E_{\uparrow\downarrow} = ak^2 \pm \alpha_R |k|$

Ref: Rashba, Sov. Phys. Solid State (1960)

The Rashba-Dresselhaus Effect

Rashba-Dresselhaus Spin-Orbit Coupling

No Inversion Symmetry ➔ Potential gradient from positively charged nucleus generates an electric field E = E z



Electron sees a magnetic field in rest frame :
$B = (v \times E)/c^2$

B field couples to electron's spin moment (M_s)

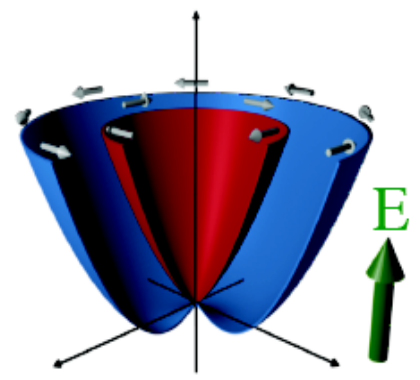
$$H = M_S . B = (g\mu_B \sigma/2).(v \times E/c^2)$$
$$= \alpha\sigma . (k \times z) = B(k). \sigma$$

σ : Pauli spin matrices

➔B(k): Momentum dependent magnetic field
***k* dependence of B is determined by symmetry**

$$H_R = \alpha_R \vec{\sigma}.(\vec{k} \times \hat{z}) = \alpha_R(\sigma_x k_y - \sigma_y k_x)$$

$$B(k) = (k_y, -k_x)$$



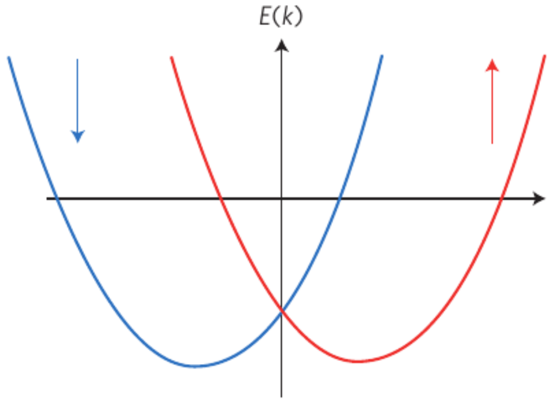
$$E_{\uparrow\downarrow} = ak^2 \pm \alpha_R |k|$$

Momentum dependent splitting of bands: Rashba Splitting

Provides an electric field control over the spin degrees of freedom *(Spintronics)*

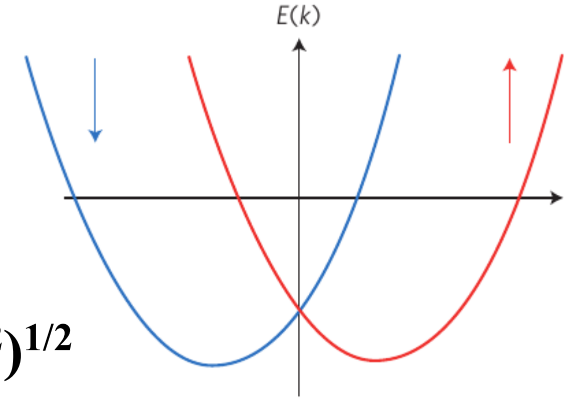
Rashba effect

Hamiltonian: $H_R = \alpha_R (\sigma_x k_y - \sigma_y k_x)$



Dresselhaus effect

Hamiltonian: $H_D = \alpha_D (\sigma_x k_y + \sigma_y k_x)$

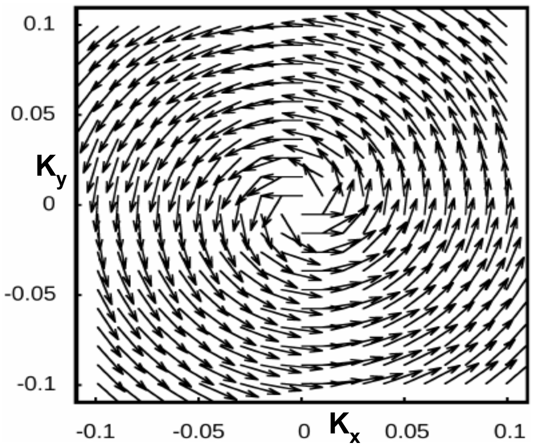


Eigen values

$$E = E_o + \hbar^2/2m.\ \alpha(k_x^2 + k_y^2)^{1/2}$$

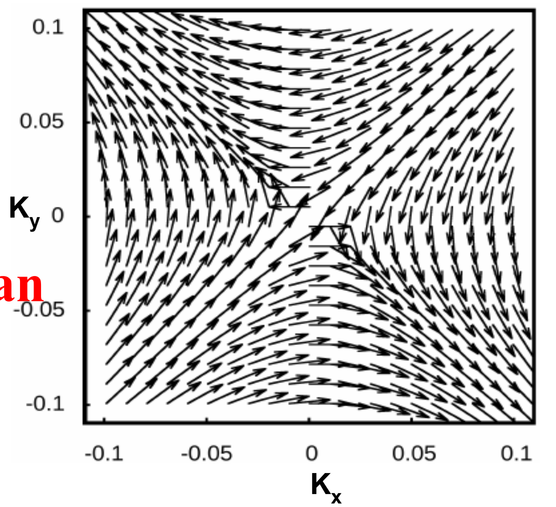
Spin-texture: Orientation of the expectation value of the spin components on the momentum plane

$$< \sigma_i > = < \Psi|\sigma_i\ |\Psi >$$



Rashba Spintexture

Ψ is the eigen function of Rashba/Dresselhaus Hamiltonian
σ's are the Pauli spin matrices.



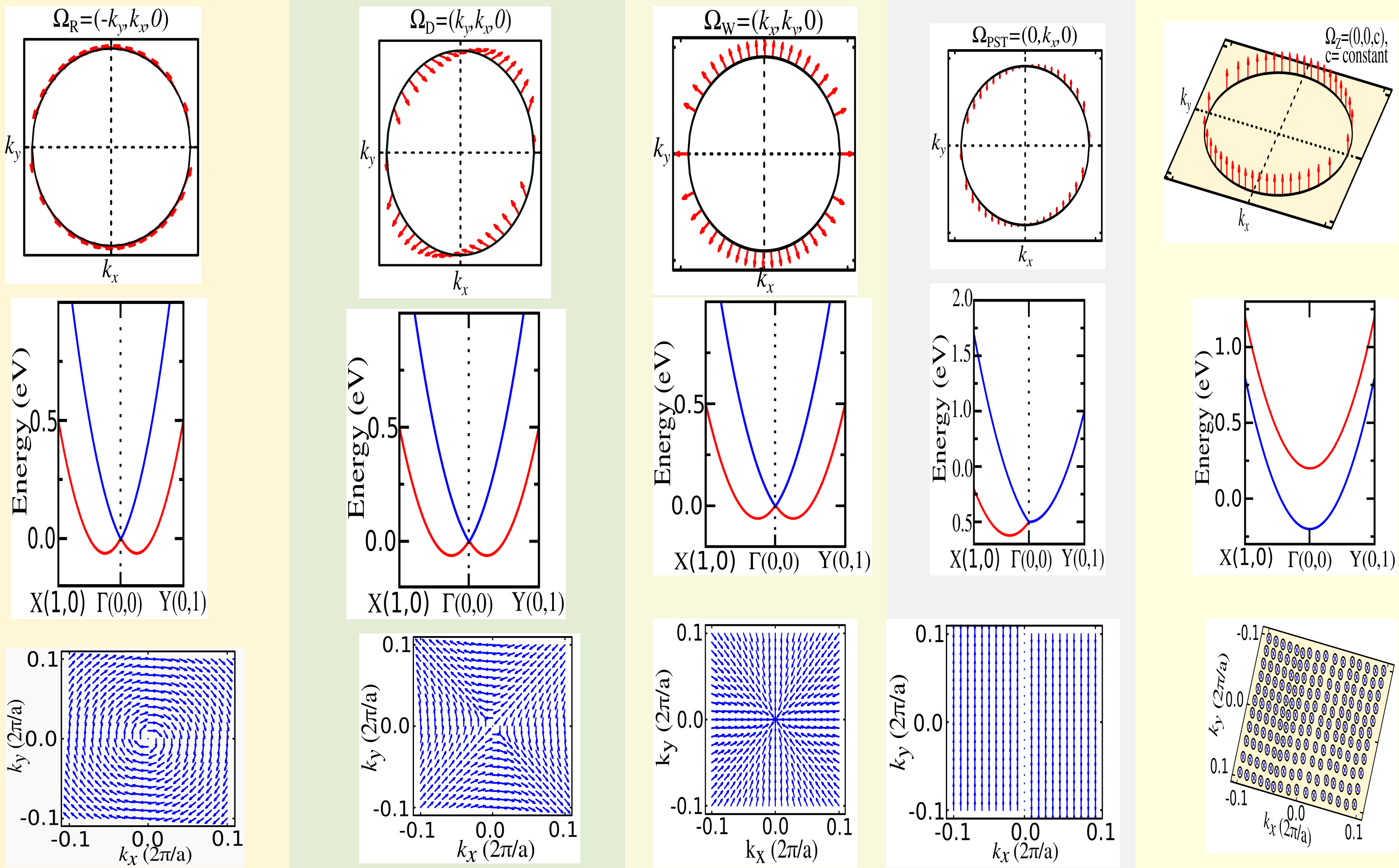
Dresselhaus Spintexture

Rashba effect | **Dresselhaus effect** | **Weyl effect** | **Persistent** | **Zeeman effect**

Field[B(k)]

Band Dispersion

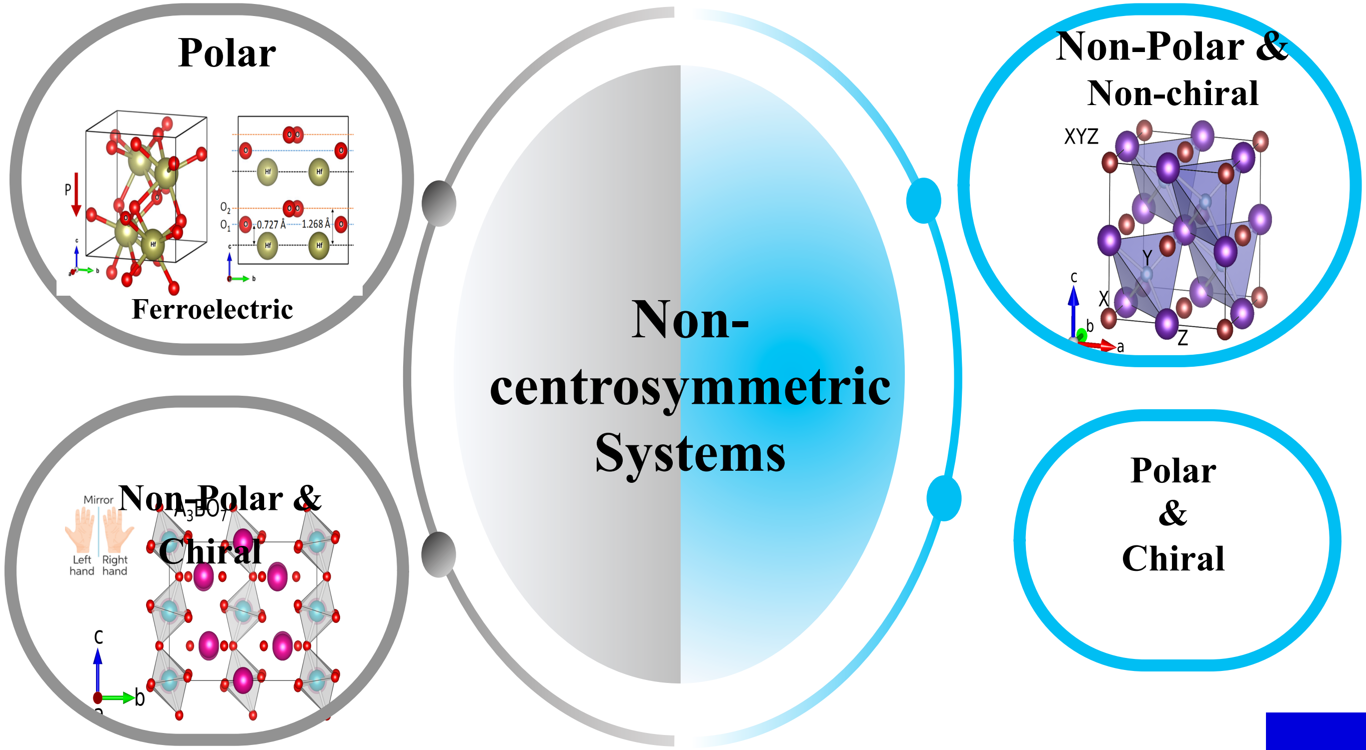
Spin Texture



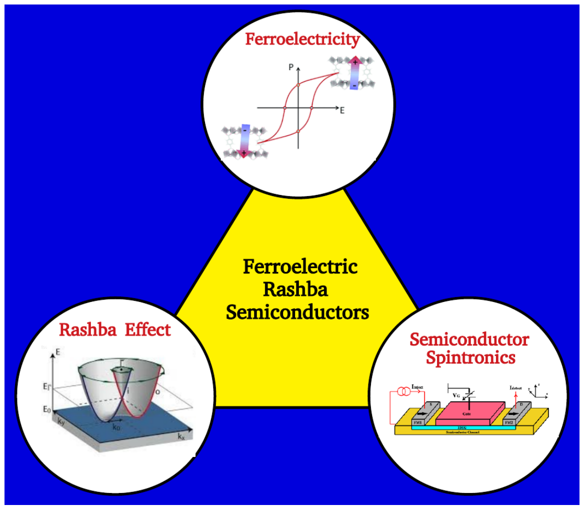
- ◆ Field (B) and ST are determined by the local symmetry of the BZ (little group)
- ◆ PSH robust against spin dependent disorder leads to infinite spin lifetime

How to design PSH ? Try $\alpha_R = \alpha_D$ RMP (2017) Strained LaAlO3/SrTiO3 (001)
Exploit non-symmorphic Symmetry in some bulk systems ? Nat. Comm (2018)
Zeeman like splitting of bands induced by electric field ?

Search for Rashba Systems

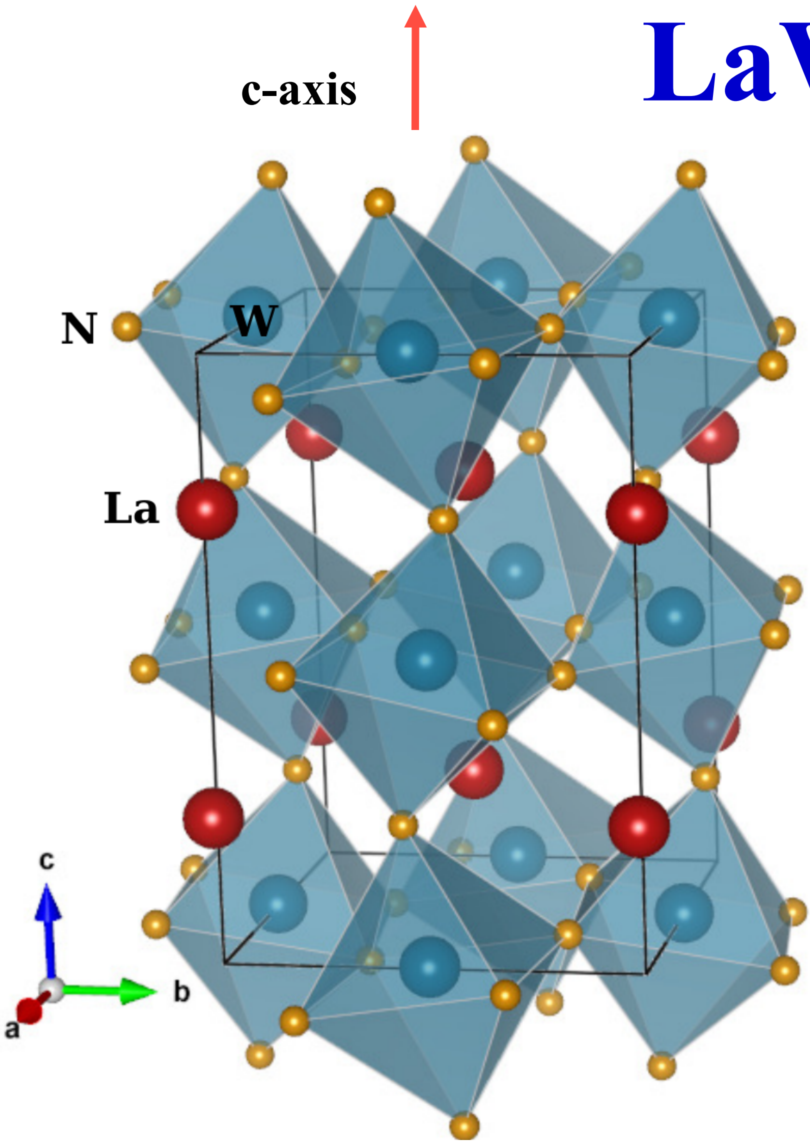


Ferroelectric Materials:
Reversal of Spin Texture
upon application of electric field



$LaWN_3$

$Pna2_1$ phase



Primitive orthorhombic unit cell with a = 5.5703 A^0 , c = 5.5992 A^0

Space Group = $Pna2_1$, No:- 33 (nonsymmorphic)

Unit cell contains 4 f.u. W and N forms octahedral network.

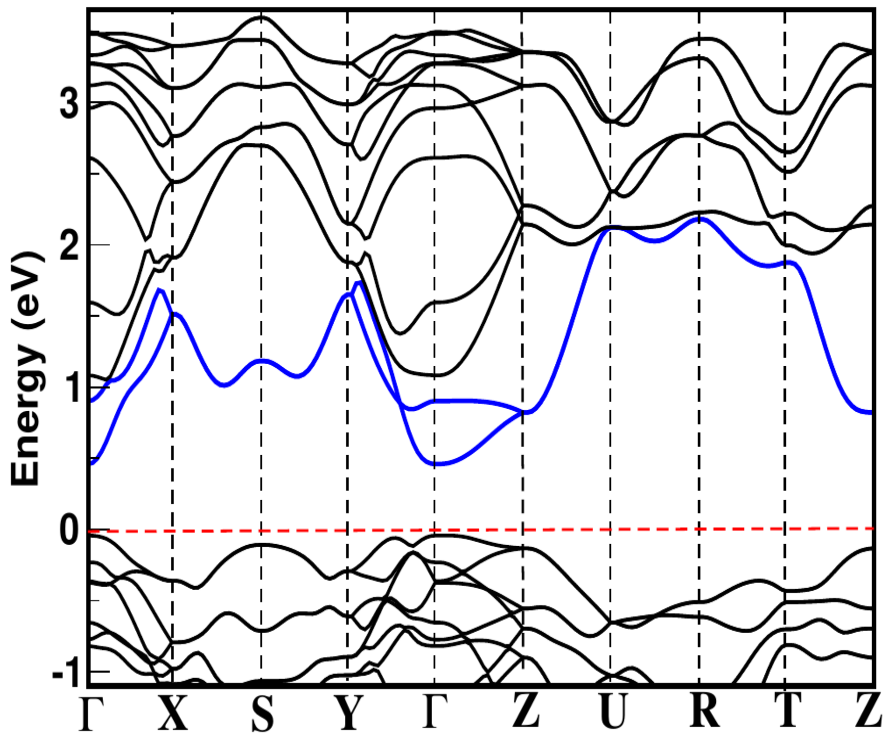
This phase is non-centrosymmetric with C_{2v} Point group symmetry.

System has ferroelectric polarisation of around 20 μC/cm ^{2} along (001) direction.

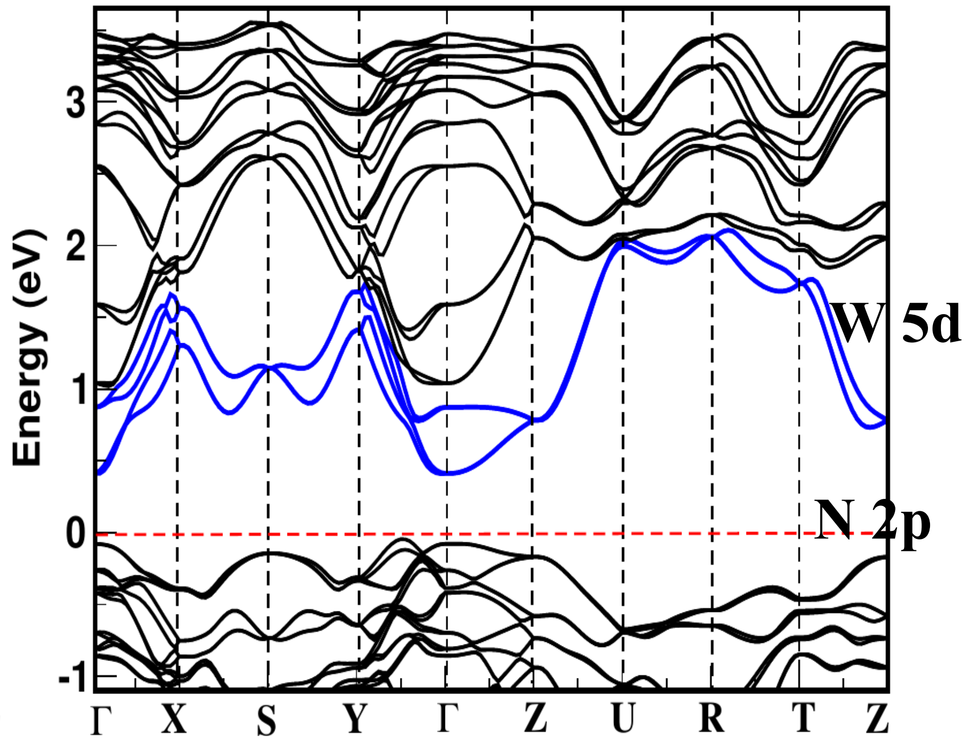
Ref: PRB 95,014111(2017)

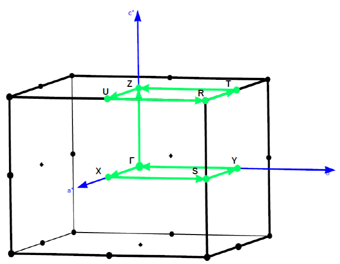
Effect of Spin orbit coupling

Non-spin polarised



Non-spin polarised +SOC





No splitting along Γ-Z direction of SOC included bands (parallel to polarisation axis)
Splitting along Γ-X direction
(perp. to polarisation axis)

This is consistent with Rashba-Dresselhaus effect

Role of Symmetry

Point group Symmetry (C_{2v}) operations of the system are :

Operation	(k_x, k_y, k_z)	$(\sigma_x, \sigma_y, \sigma_z)$
E	(k_x, k_y, k_z)	$(\sigma_x, \sigma_y, \sigma_z)$
C2	$(-k_x, -k_y, k_z)$	$(-\sigma_x, -\sigma_y, \sigma_z)$
$i\Sigma_x$	$(-k_x, k_y, k_z)$	$(\sigma_x, -\sigma_y, -\sigma_z)$
$i\Sigma_y$	$(k_x, -k_y, k_z)$	$(-\sigma_x, \sigma_y, -\sigma_z)$

Rashba term, $\alpha_R(\sigma_y k_x - \sigma_x k_y)$

Dresselhaus term, $\alpha_D(\sigma_y k_x + \sigma_x k_y)$

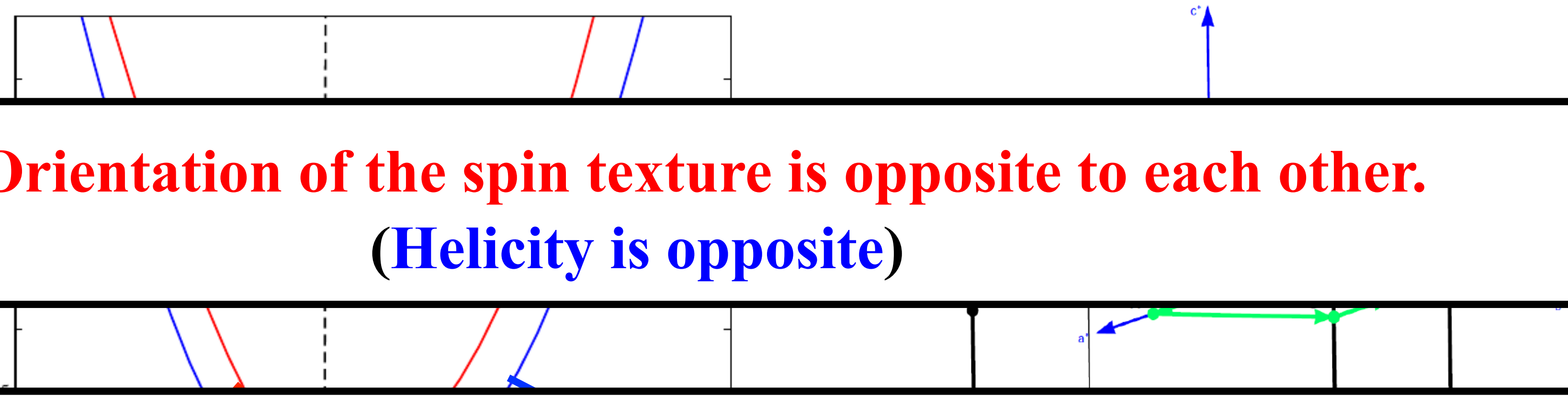
Invariant under all symmetry operations

We can expect both Rashba and Dresselhaus coupling in the system

No term containing out of plane spin component is invariant under all symmetry operations

Ref: PRB 93, 245159 (2016)

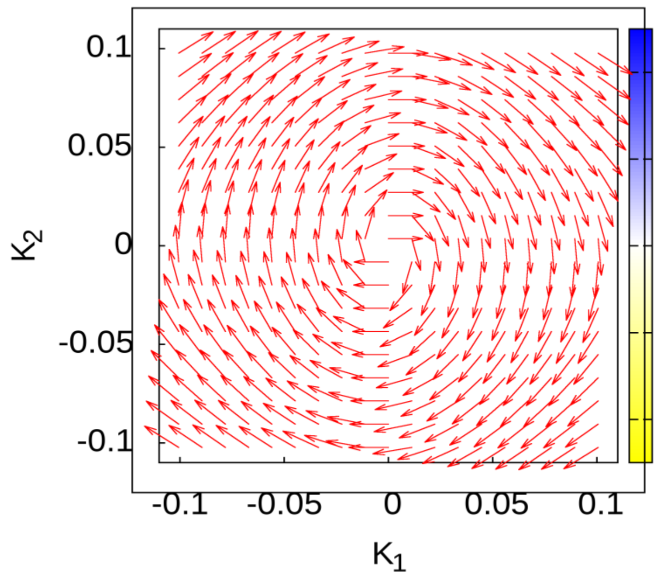
Rashba or Dresselhaus?



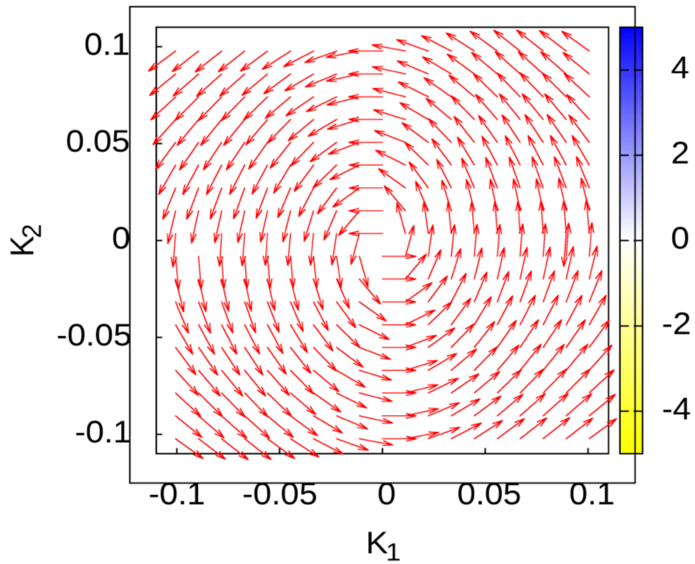
Orientation of the spin texture is opposite to each other.
(Helicity is opposite)

No out of plane component of spin, and spin is always ⊥ to momentum suggests it is Rashba effect

Inner Branch



Outer Branch



Model Hamiltonian

$$\mathrm{H}_\Gamma(k) = E_0(k) + \alpha k_x \sigma_y + \beta k_y \sigma_x$$

Eigenvalue equation of the Hamiltonian,

$$E_\Gamma(k) = E_0(k) \pm \sqrt{\alpha^2 k_x^2 + \beta^2 k_y^2}$$

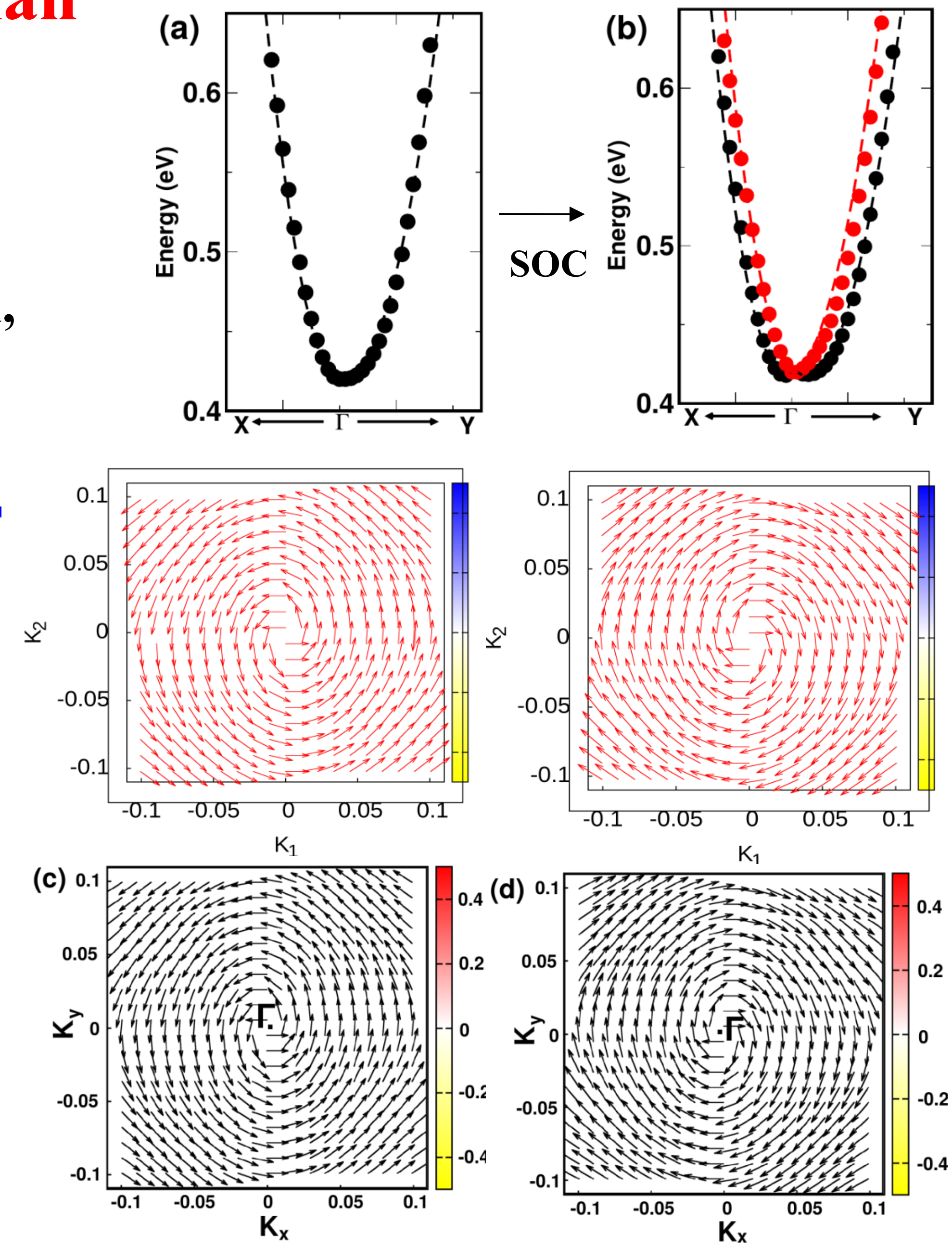
Where Rahba parameter (α_R) and Dresselhaus parameter s(α_D) fiting DFT bands are:

DFT

k.p model

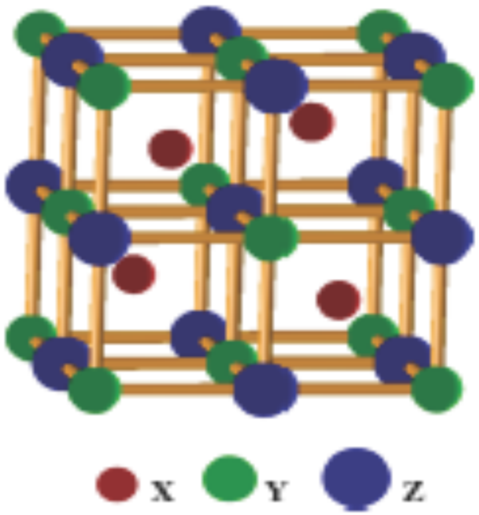
$$\alpha_R = 0.32 \text{ eV.A}^0, \quad \alpha_D = 0.014 \text{ eV.A}^0$$

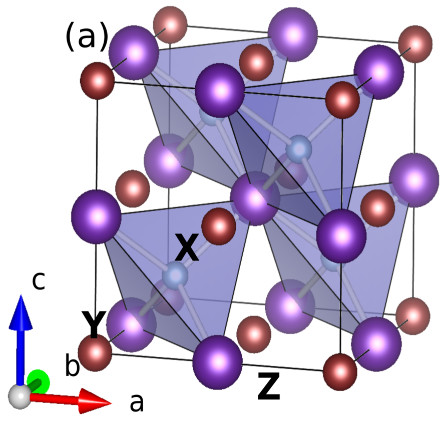
Clearly Rashba effect dominates over Dresselhaus effect



Non CentroSymmetric Half-Heusler Compounds XYZ (CoZrBi)

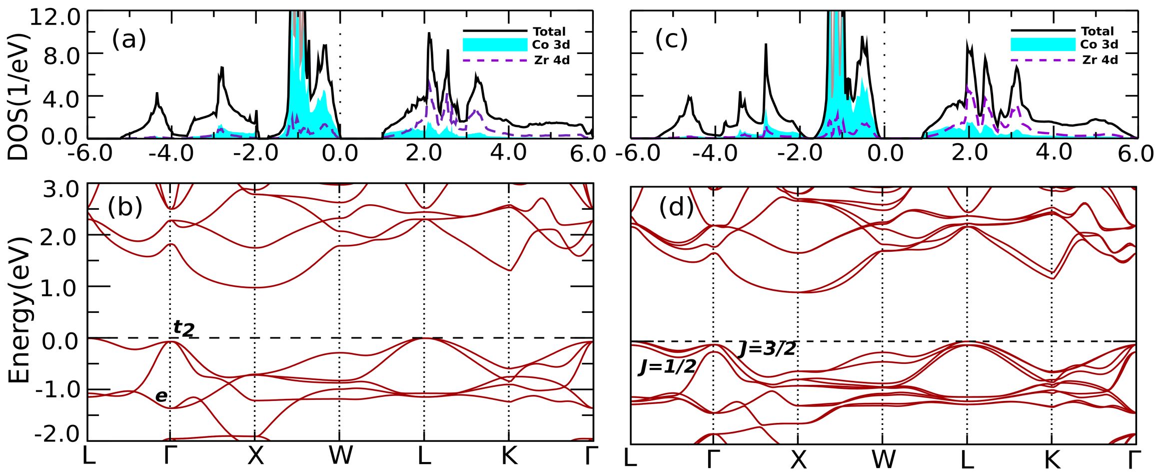
The unit cell is fcc lattice with three atom as basis.

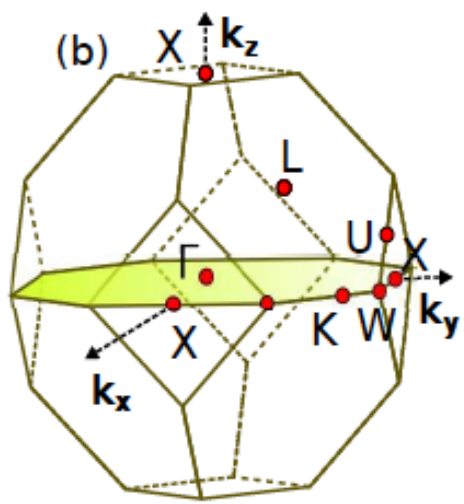




18-electron half-Heusler CoZrBi
Co electron configuration [Ar]$3d^7\ 4s^2$
Zr electron configuration [Kr]$4d^2\ 5s^2$
Bi electron configuration [Xe]$4f^{14}\ 5d^{10}\ 6s^2\ 6p^3$

Total number of valence electron = 9+4+5 = 18

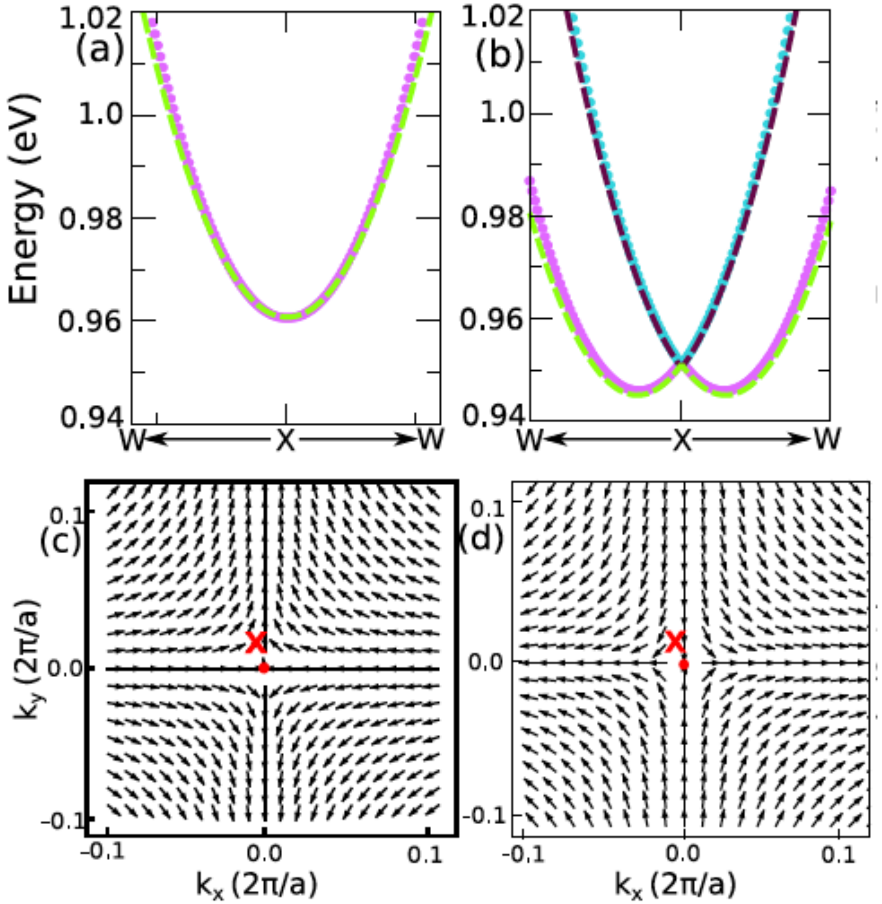




Local wavevector point group symmetry (little group) plays an important role

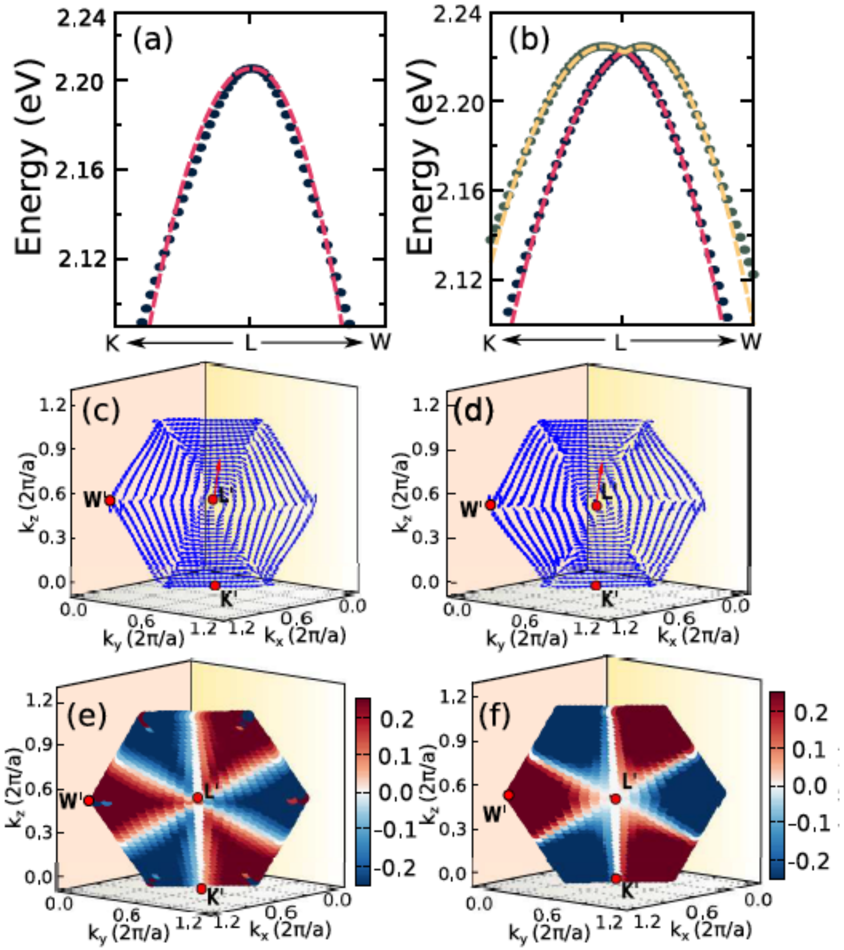
Dresselhaus and Rashba Efffect in non-polar non-centrosymmetric CoZrBi

Non polar X point



Dresselhaus Effect (CBM)

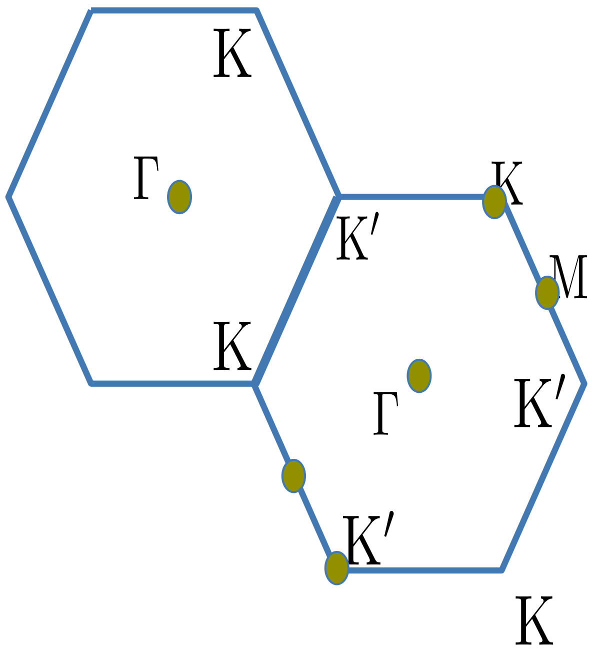
Polar L point

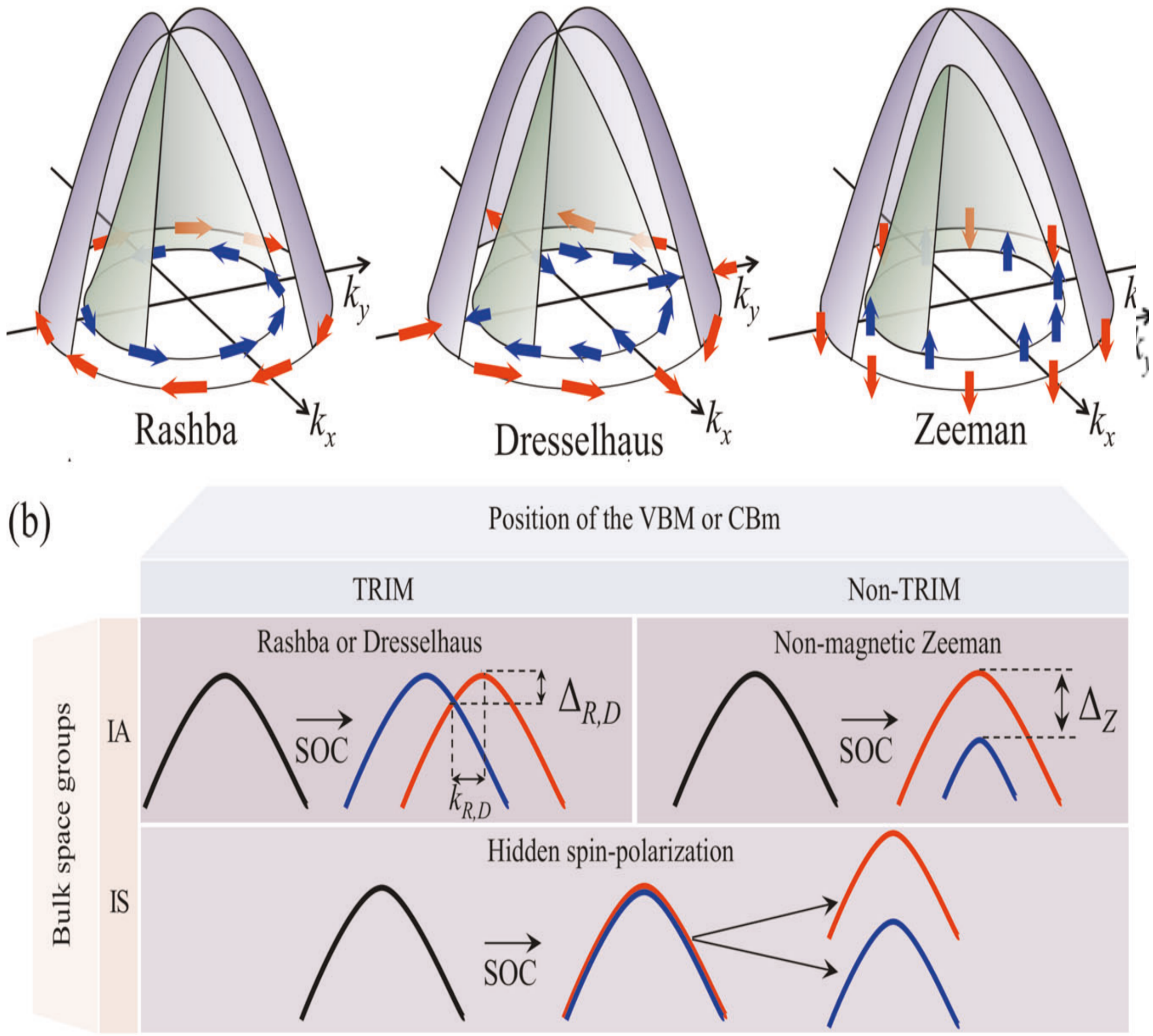


Rashba Effect (CB)

Crystallographic Space Group Symmetry vs Wave vector point group symmetry (Little Group)

Time Reversal Invariant Momenta(TRIM)



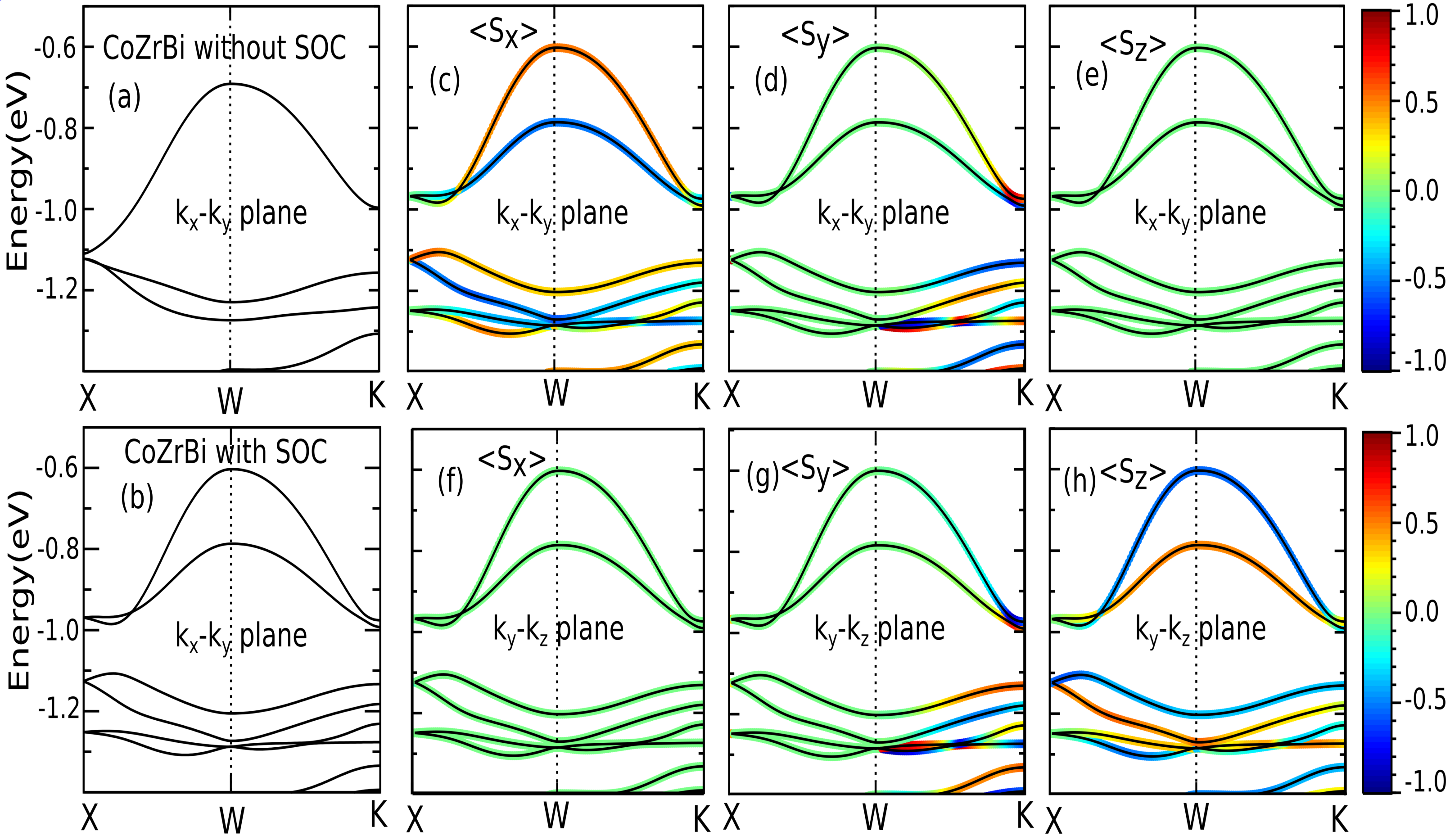


A time reversal Invariant k point satisfy –k + G = k

For HH W point is Non TR ➔ Zeeman Effect

Zeeman Effect

18electron : (ZrCoBi)



In the k_x-k_y plane along the X-W-K direction, the S_x component of the spin expectation value shows a prominent contribution.

In the k_x-k_y plane along the X-W-K direction, the S_z component of the spin expectation value shows a prominent contribution.

Model Hamiltonian for Zeeman Spin splitting

$$H = H_0 + \vec{\Omega}_D(\mathbf{k}).\vec{\sigma}$$

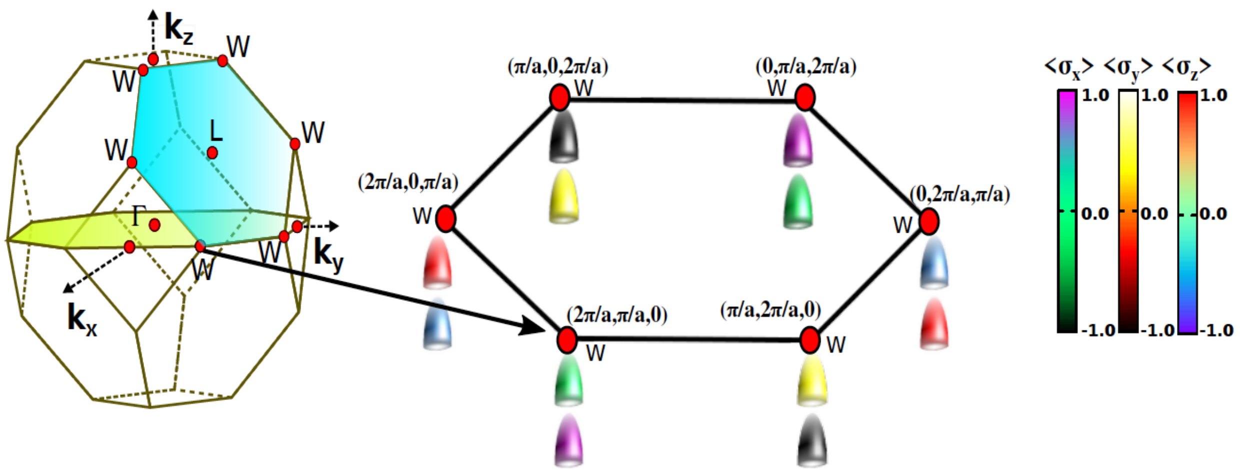
$$H_0 = \frac{\hbar^2\left(k_x^2+k_y^2\right)}{2m^*}1$$

$$\Omega_D\left(\mathbf{k}\right) = \lambda_D\left(k_x\left(k_y^2-k_z^2\right), k_y\left(k_z^2-k_x^2\right), k_z\left(k_x^2-k_y^2\right)\right)$$

In k_x- k_y plane k_z=0. Effective magnetic field along W-X direction is,

$$\Omega_D(\mathbf{k}) \approx \left(k_x k_y^2, 0, 0\right) \qquad \mathrm{k}_x << \left(k_y = \frac{2\pi}{a}\right)$$

S_x expectation value of spin survives along the path X-W-K in k_x-k_y plane



SOC ties spin splitting to the valley index.

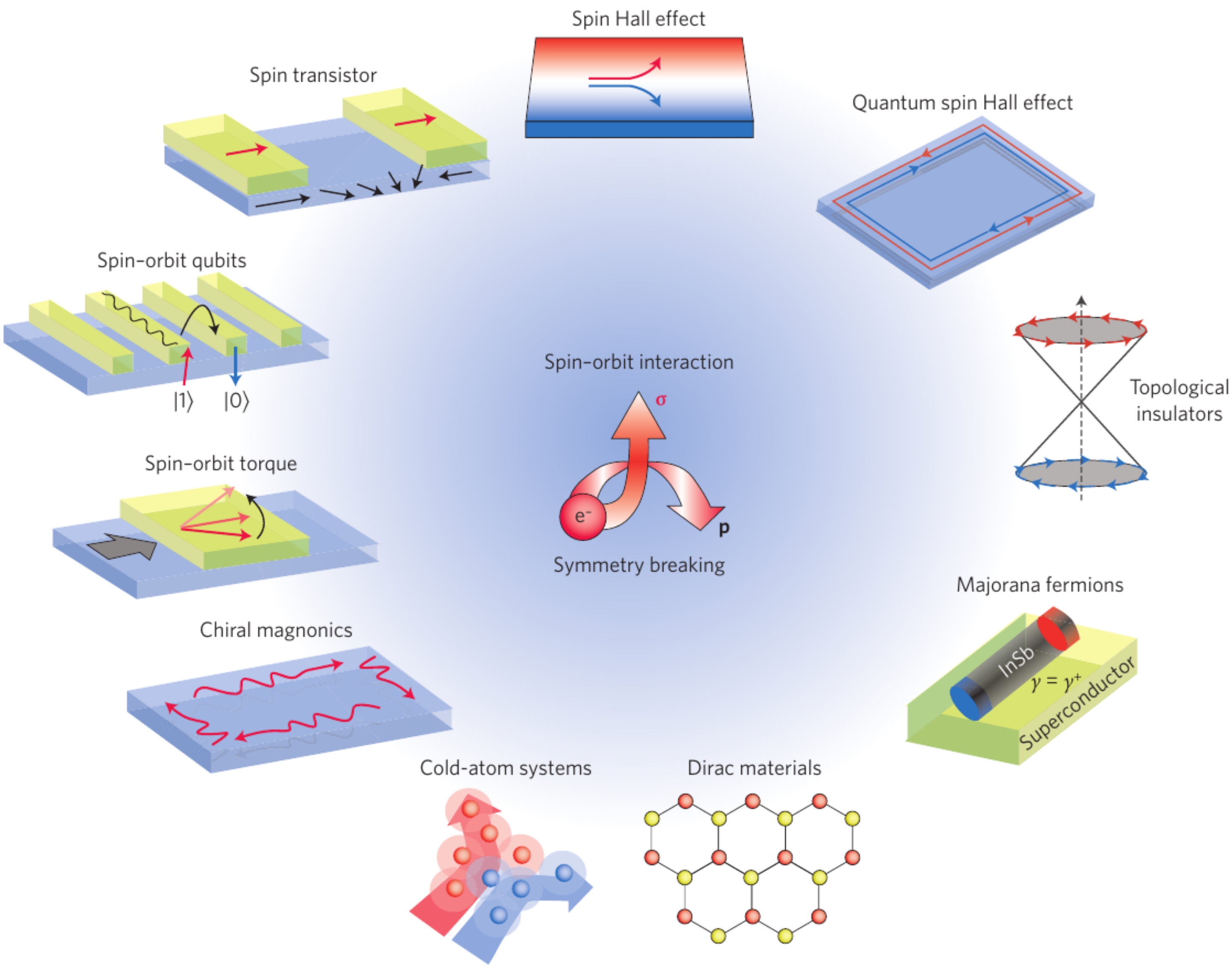
Charge carriers between valleys should have simultaneous spin flip and momentum transfer.

This favors long valley life-time for valleytronics application.

Spin splitting controlled by Electric field

Ideal for spin valleytronics

Emergent Phenomena in Spin Orbit Coupled Systems



Ref: A. Manchon et al Nat. Mat. 14, 871 (2015)

Thank You