Topological Weyl Semimetal and Unconventional Superconductivity in Doped Topological Insulators

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清华高研院

内 容

☐ **Weyl**半金属

☐ **BiS$_2$**超导体

☐ **掺杂拓扑绝缘体**

合作者

Sergej Savrasov, *UC Davis*

Ari Turner & Ashvin Vishvanath
UC Berkeley

段纯刚   华东师大

曹刚   肯塔基大学

Qiang Wang, Daniel S Dessau   科罗拉多大学/橡树岭

动机(5d元素)

PERIODIC TABLE OF THE ELEMENTS

内容

5d过渡金属氧化物

❑烧绿石结构铱化合物
    磁基态构型, **Weyl**半金属, **Fermi Arc**

❑设计**Axion**绝缘体

❑**Slater insulator**

❑**BiS₂**超导体

❑电声子耦合➔非常规超导体

❑总结

5d过渡元素氧化物的特点
自旋轨道耦合和电子关联

Phase-Sensitive Observation of a Spin-Orbital Mott State in Sr_2IrO_4

B. J. Kim,[1,2]* H. Ohsumi,[3] T. Komesu,[3] S. Sakai,[3,4] T. Morita,[3,5] H. Takagi,[1,2]* T. Arima[3,6]

Measurement of the quantum-mechanical phase in quantum matter provides the most direct manifestation of the underlying abstract physics. We used resonant x-ray scattering to probe the relative phases of constituent atomic orbitals in an electronic wave function, which uncovers the unconventional Mott insulating state induced by relativistic spin-orbit coupling in the layered 5d transition metal oxide Sr_2IrO_4. A selection rule based on intra-atomic interference effects establishes a complex spin-orbital state represented by an effective total angular momentum = 1/2 quantum number, the phase of which can lead to a quantum topological state of matter.

Novel $J_{eff} = 1/2$ Mott State Induced by Relativistic Spin-Orbit Coupling

- 尽管5d的实空间轨道半径很大，但是由于强的自旋轨道耦合，仍然有不可忽略的电子关联效应。

由于自旋轨道耦合和电子关联的联合效应导致了Sr_2IrO_4等$5d^5$电子体系是绝缘体

$5d^5$

强自旋轨道耦合下的**T$_{2g}$**轨道

强晶体场下的相对论**5d**电子

(a) wide t_{2g}-band Metal

(b) U UHB LHB $S = 1/2$ Mott ground state

(c) ζ_{so} $J_{eff} = 1/2$ band $J_{eff} = 3/2$ band J_{eff} band split due to SO

(d) A B U ζ_{so} $J_{eff} = 1/2$ UHB $J_{eff} = 1/2$ LHB $J_{eff} = 3/2$ band $J_{eff} = 1/2$ Mott ground state

(e) e_g $5d$ $10Dq$ $L_{eff} = 1$ t_{2g} $J_{eff} = 1/2$ ζ_{so} $J_{eff} = 3/2$ $J_{5/2}$ $J_{3/2}$ $5d$ Crystal Field SO coupling Crystal Field SO coupling

FIG. 1. Schematic energy diagrams for the $5d^5$ (t_{2g}^5) configuration (a) without SO and U, (b) with an unrealistically large U but no SO, (c) with SO but no U, and (d) with SO and U. Possible optical transitions A and B are indicated by arrows. (e) $5d$ level splittings by the crystal field and SO coupling.

(after Kim et.al, PRL 2009)
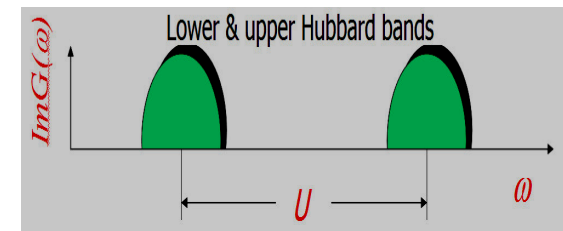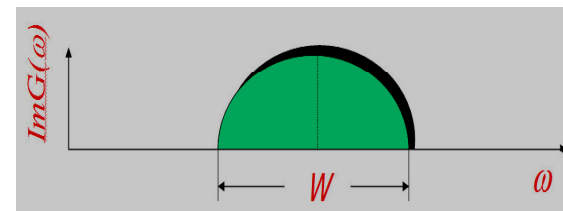
Ir $5d^5$ j=5/2 Γ_8 Γ_7 j=3/2

A small Hubbard U produces Mott insulating behavior for Γ_7 band at half filling

$ImG(\omega)$ W ω

$ImG(\omega)$ Lower & upper Hubbard bands   U ω

5d过渡元素氧化物的特点
强自旋轨道耦合

Orbital Magnetism and Spin-Orbit Effects in the Electronic Structure of BaIrO$_3$
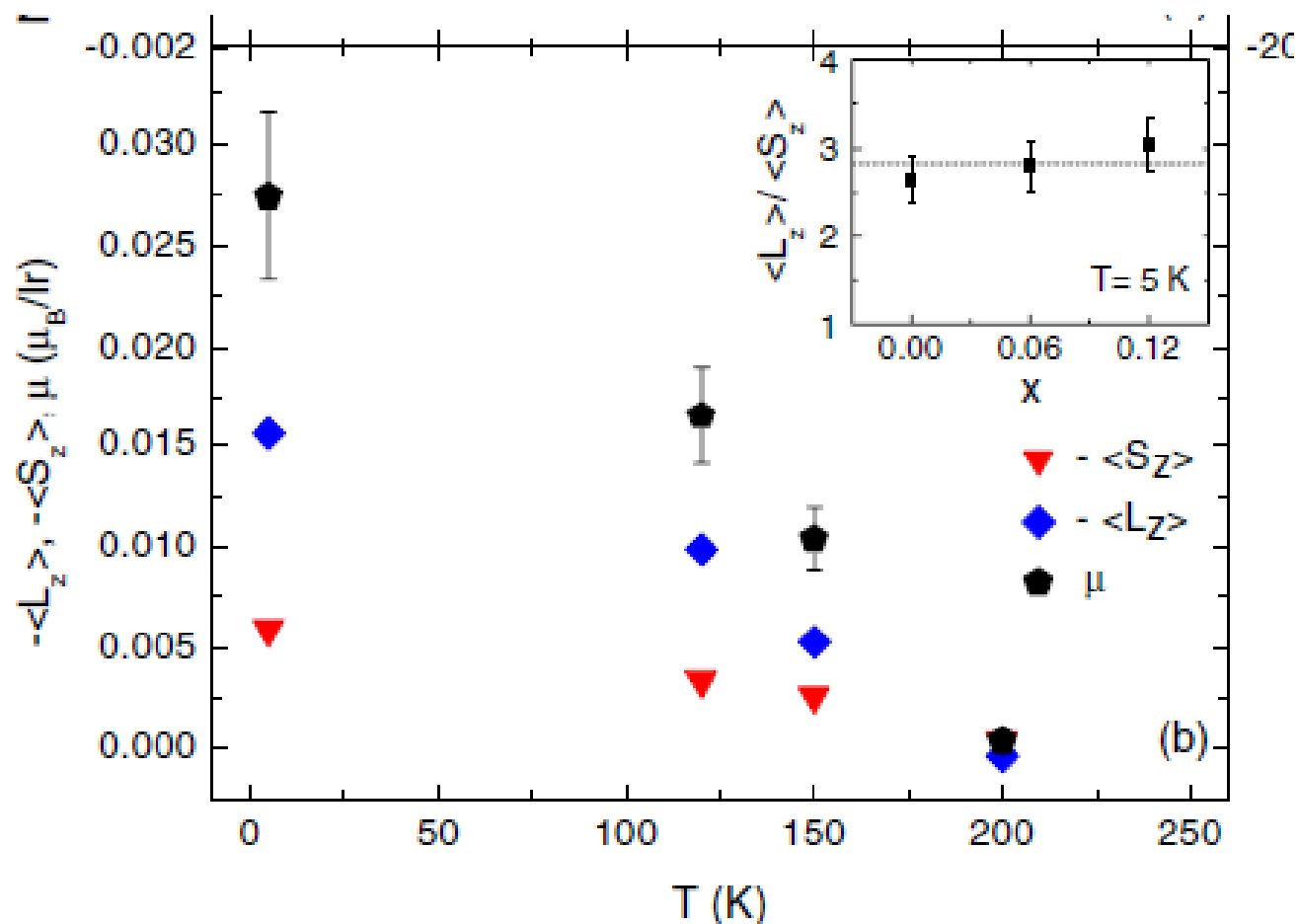
5d过渡元素氧化物的特点

Spin-Liquid State in the $S = 1/2$ Hyperkagome Antiferromagnet $Na_4Ir_3O_8$

1) 有着**hyperkagome** 结构
2) **Curie-Weiss** 温度**(大约为650K)**
3) **effective moment** 也较大（**1.96μ$_B$**）**??**
4) 在极低的温度下它都不表现任何磁有序。

三维的量子自旋液体**?**
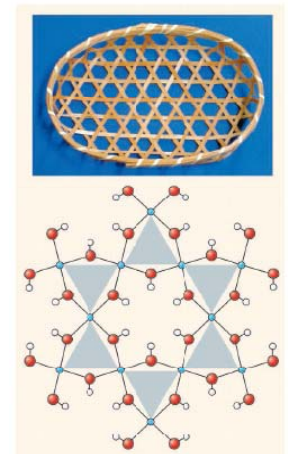
An End to the Drought of Quantum Spin Liquids

After decades of searching, several promising examples of a new quantum state of matter have now emerged.

Patrick A. Lee

Gapless Spin Liquids on the Three-Dimensional Hyperkagome Lattice of $Na_4Ir_3O_8$

Michael J. Lawler,[1] Arun Paramekanti,[1] Yong Baek Kim,[1] and Leon Balents[2]

Classical Antiferromagnet on a Hyperkagome Lattice

John M. Hopkinson,[1] Sergei V. Isakov,[1] Hae-Young Kee,[1] and Yong Baek Kim[1,2]

$Na_4Ir_3O_8$ as a 3D Spin Liquid with Fermionic Spinons

Yi Zhou,[1,2] Patrick A. Lee,[3] Tai-Kai Ng,[4] and Fu-Chun Zhang[1]

5d过渡元素氧化物的特点

PHYSICAL REVIEW LETTERS

Quantum Spin Hall Effect in a Transition Metal Oxide Na_2IrO_3

Atsuo Shitade,[1,*] Hosho Katsura,[2] Jan Kuneš,[3,4] Xiao-Liang Qi,[5] Shou-Cheng Zhang,[5] and Naoto Nagaosa[1,2]
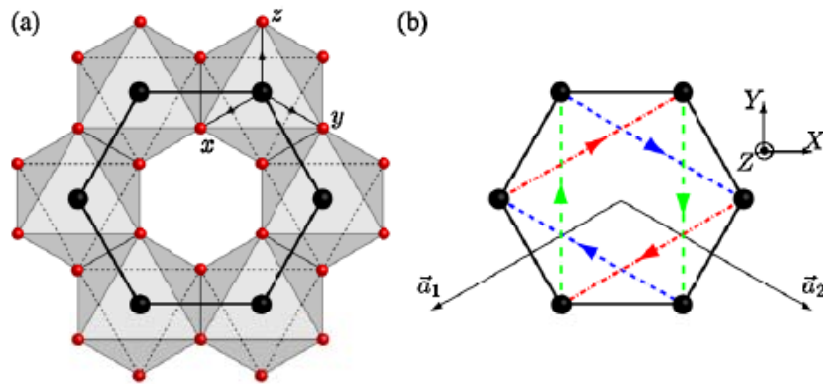
Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

G. Jackeli[1,*] and G. Khaliullin[1]

实验证实它有长程磁序（**Singh and Gegenwart 2010**）

烧绿石结构
磁阻错现象

烧绿石结构$A_2B_2O_7$；尖晶石结构AB_2O_4

A- Site
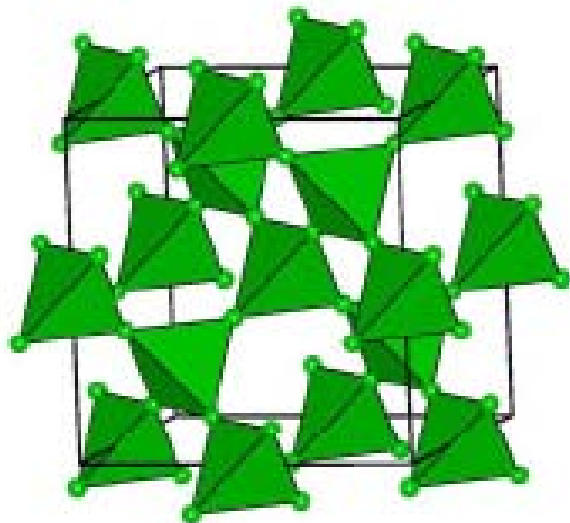
B- Site
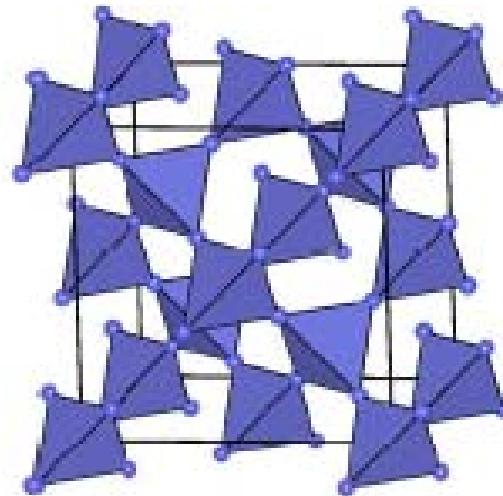
Spin ice

A$_2$B$_2$O$_7$,部分4f元素占据A位时表现出Ising-type的各向异性。

当**铁磁的**exchange interaction和Ising-type的各向异性结合可以导致出巨大的Geometrical frustration

Ho$_2$Ti$_2$O$_7$

A- Site   B- Site
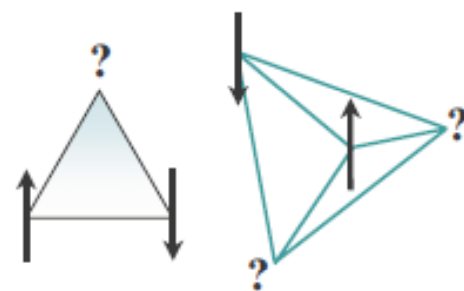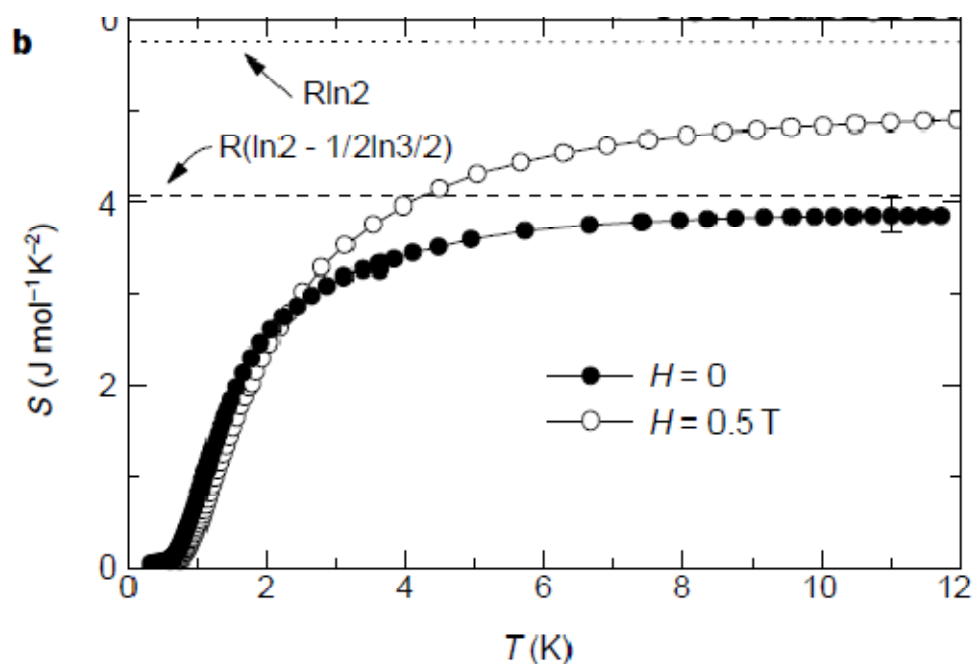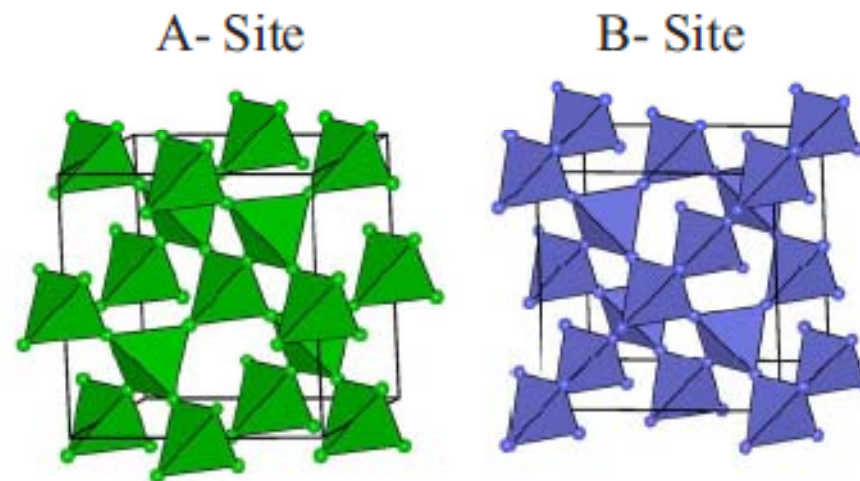
Magnetic Monopoles in Spin Ice

$$H = \frac{J}{3} \sum_{\langle ij \rangle} S_i S_j + Da^3 \sum_{(ij)} \left[\frac{\hat{e}_i \cdot \hat{e}_j}{|\mathbf{r}_{ij}|^3} - \frac{3 \left(\hat{e}_i \cdot \mathbf{r}_{ij} \right) \left(\hat{e}_j \cdot \mathbf{r}_{ij} \right)}{|\mathbf{r}_{ij}|^5} \right] S_i S_j$$

$$\mathcal{V}(r_{ij}) = \begin{cases} \frac{\mu_0}{4\pi} \frac{q_i q_j}{r_{ij}} & r_{ij} \neq 0 \\ v_0 q_i q_j & r_{ij} = 0, \end{cases}$$
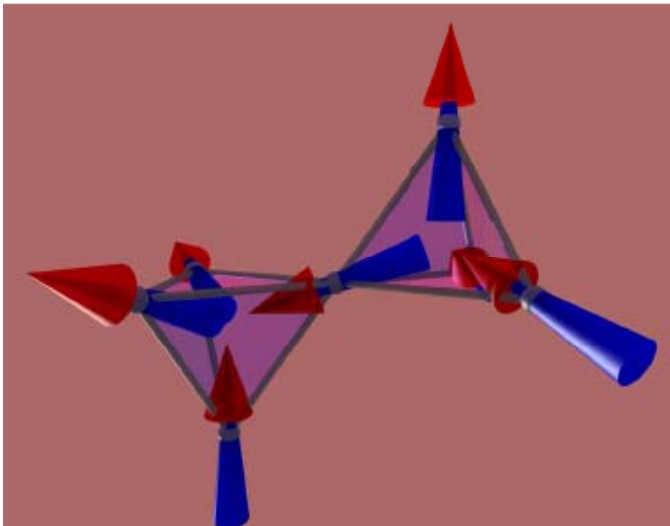
烧绿石结构$A_2Ir_2O_7$

这些材料表现强的磁响应

实验定磁结构不容易

基本没有能带计算的工作
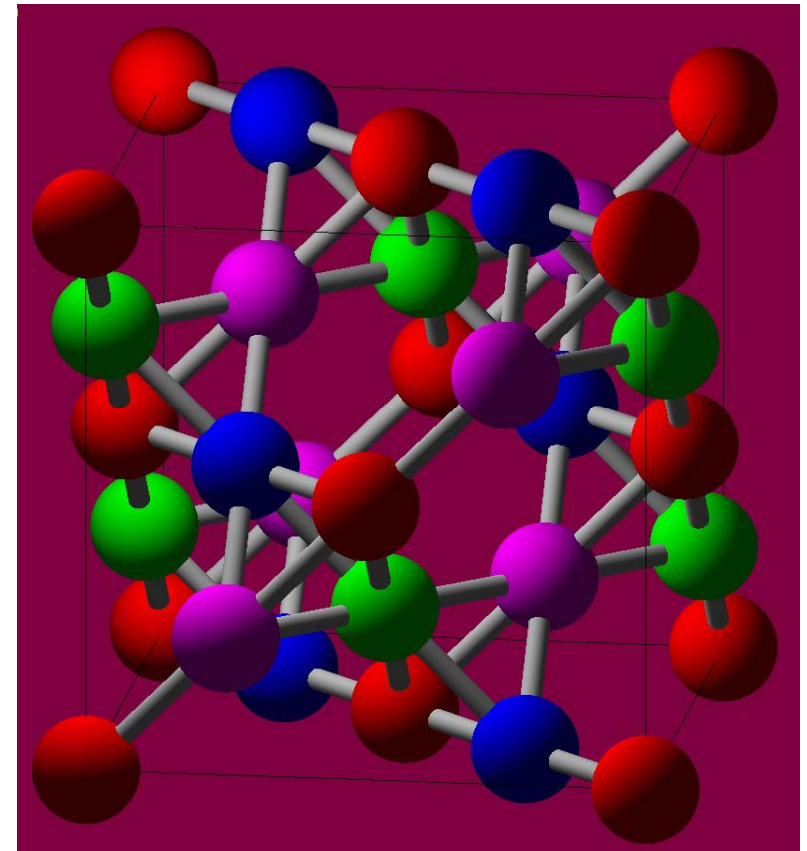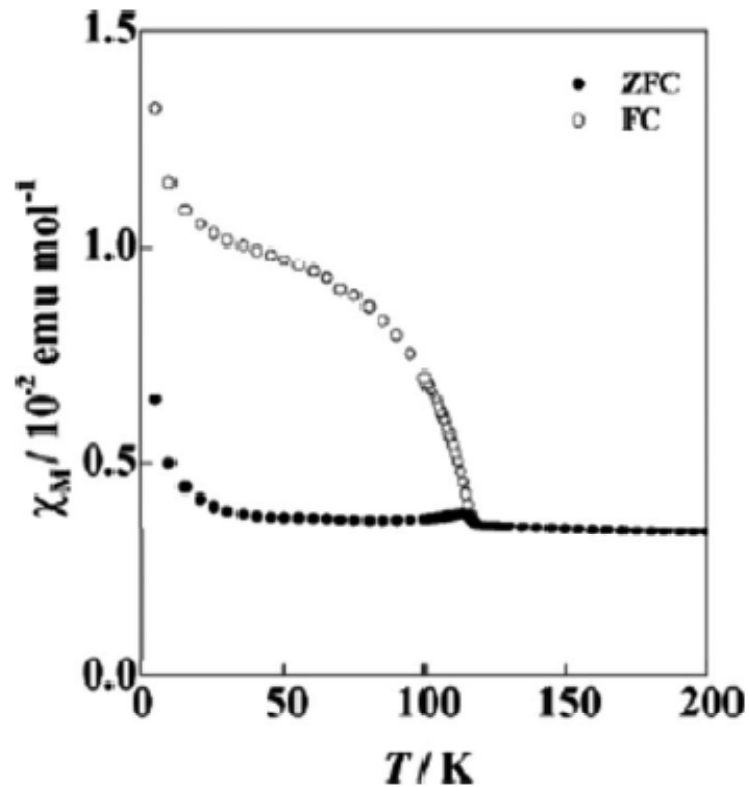
Magnetic susceptibility for $Sm_2Ir_2O_7$

烧绿石结构氧化物是强拓扑绝缘体?

Mott physics and band topology in materials with strong spin-orbit interaction

Dmytro Pesin[1,2]*† and Leon Balents[2]

Recent theory and experiment have revealed that strong spin-orbit coupling can have marked qualitative effects on the band structure of weakly interacting solids, leading to a distinct phase of matter, the topological band insulator. We show that spin-orbit interaction also has quantitative and qualitative effects on the correlation-driven Mott insulator transition. Taking Ir-based pyrochlores as a specific example, we predict that for weak electron–electron interaction Ir electrons are in metallic and topological band insulator phases at weak and strong spin-orbit interaction, respectively. We show that by increasing the electron–electron interaction strength, the effects of spin-orbit coupling are enhanced. With increasing interactions, the topological band insulator is transformed into a 'topological Mott insulator' phase having gapless surface spin-only excitations. The proposed phase diagram also includes a region of gapless Mott insulator with a spinon Fermi surface, and a magnetically ordered state at still larger electron–electron interaction.

内容

- **5d**过渡金属氧化物

- 烧绿石结构铱化合物
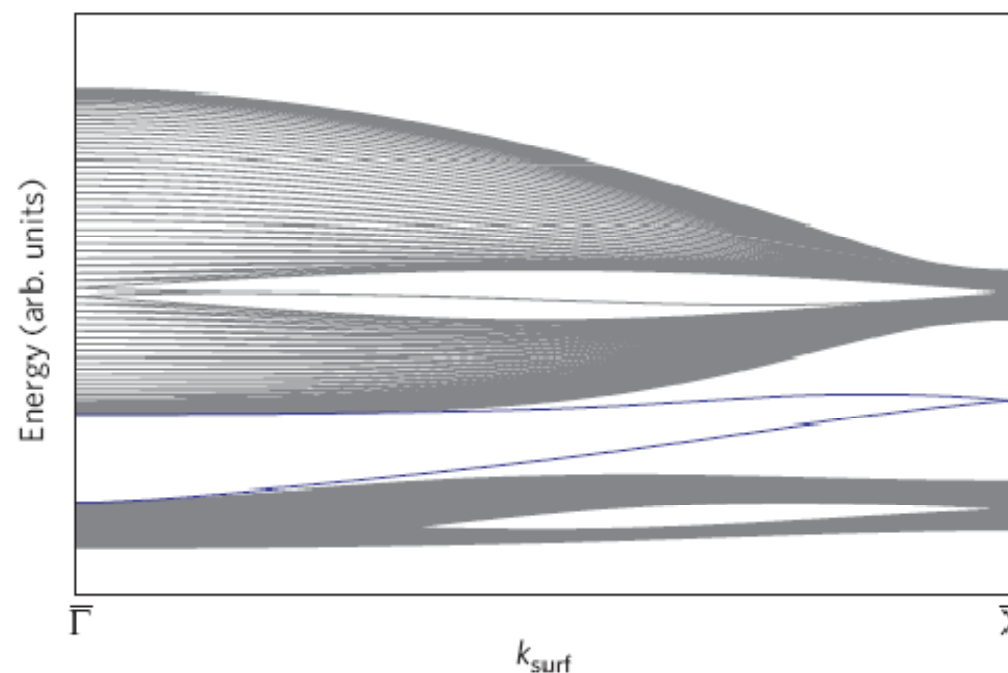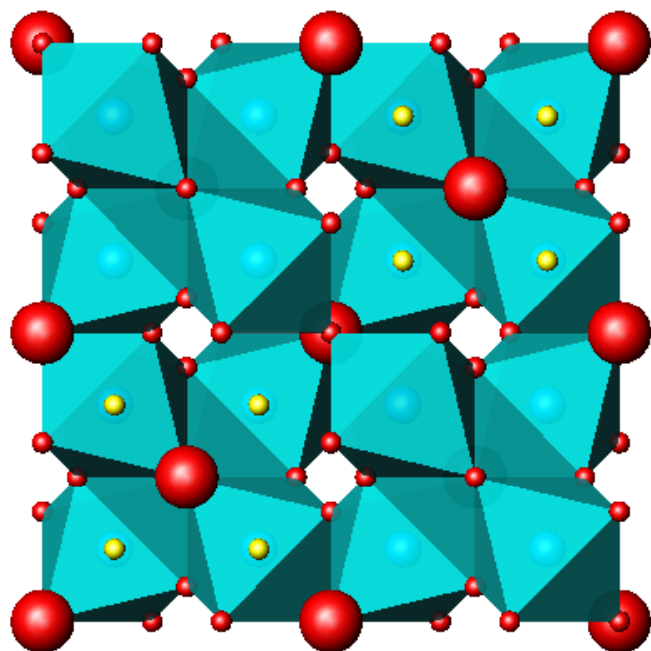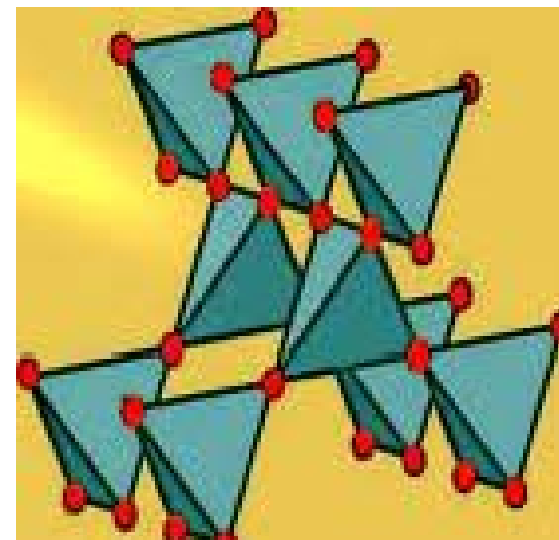
- 磁基态构型,**Weyl**半金属,**Fermi Arc**

- 设计**Axion**绝缘体

烧绿石结构铱氧化物$A_2Ir_2O_7$(A=Y,稀土元素)
实验事实
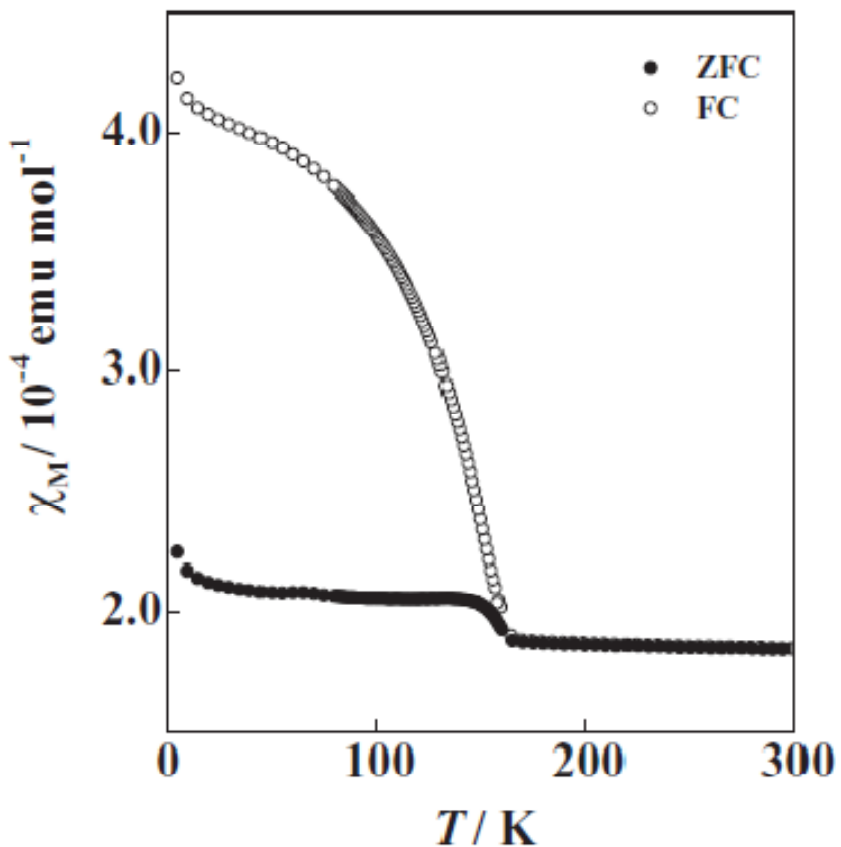
N. Taira, M. Wakeshima and Y. Hinatsu
(2001)
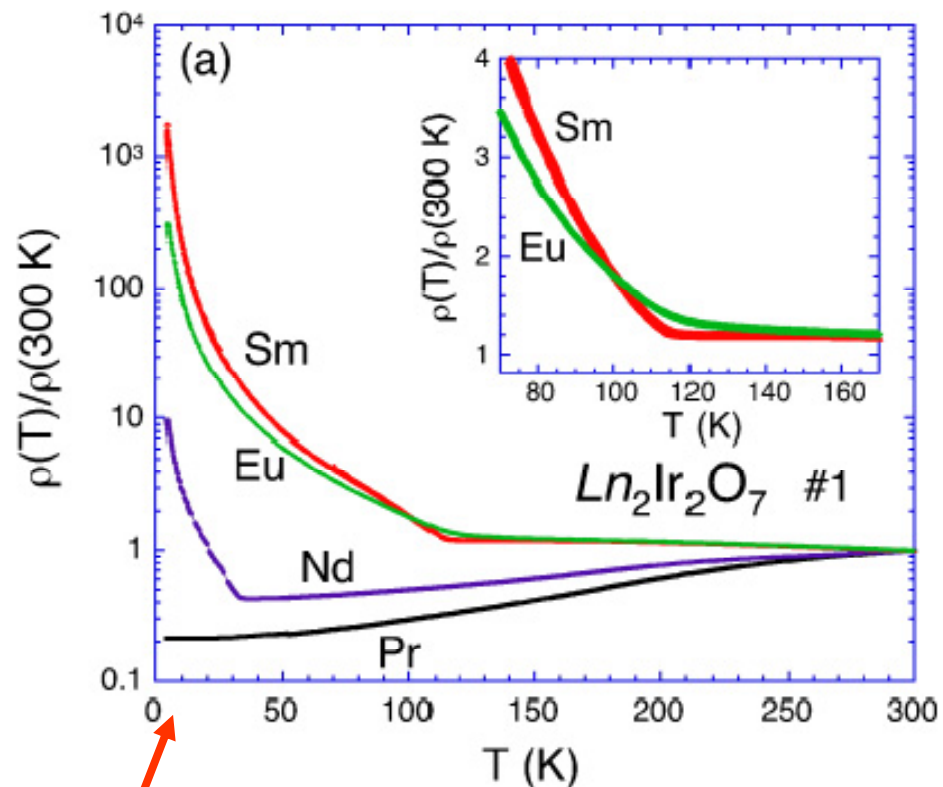
MATSUHIRA et al., (2007)

U !!!

局域密度近似+自旋轨道耦合计算
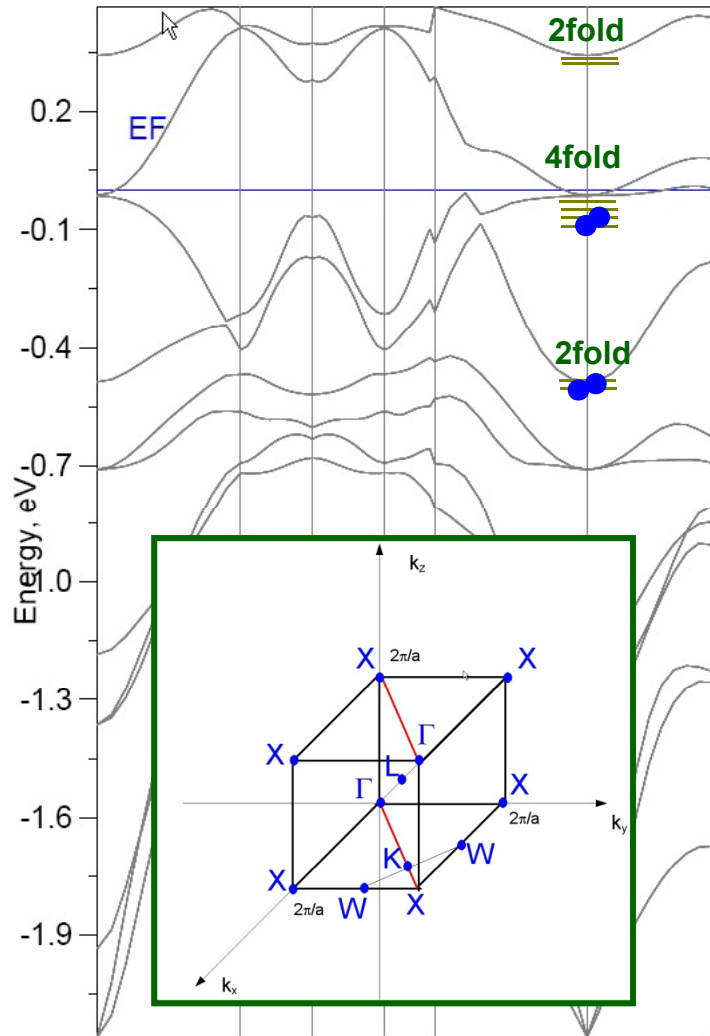
Fermi Level

> $Y_2Ir_2O_7$元胞里面有**4**个**Ir**原子，所以有**8**个相对论的**|Γ7>**态

> 每个**Ir**的**|Γ7>**带填一个电子(每个**J=3/2**带填**4**个电子，成为满带); 所以总的**|G7>**带填**4**个电子.

> 在Γ点的简并度为**2-4-2.** 填**4**个电子➔**metal!**

几何阻错结构磁性基态的找寻

$$J_{\tau R \tau' R'}^{\alpha\beta} = \sum_{\mathbf{q}} \sum_{\mathbf{k}jj'} \frac{f_{\mathbf{k}j} - f_{\mathbf{k+q}j'}}{\epsilon_{\mathbf{k}j} - \epsilon_{\mathbf{k+q}j'}} \langle \psi_{\mathbf{k}j} | [\sigma \times \mathbf{B}_\tau]_\alpha | \psi_{\mathbf{k+q}j'} \rangle \langle \psi_{\mathbf{k+q}j'} | [\sigma \times \mathbf{B}_{\tau'}]_\beta | \psi_{\mathbf{k}j} \rangle e^{i\mathbf{q}(\mathbf{R}-\mathbf{R}')}$$

X. Wan, Q. Yin, S.Y. Savrasov, PRL 97, 266403

X. Wan, T. A. Maier, and S. Y. Savrasov, PRB 79, 155114

X. Wan, J. Dong, and S. Y. Savrasov, PRB 83, 205201

X. Wan, M. Kohno, and X. Hu, PRL 94, 087205

X. Wan, M. Kohno, and X. Hu, PRL 95, 146602

磁性基态构型

All-in/all-out非共线磁结构
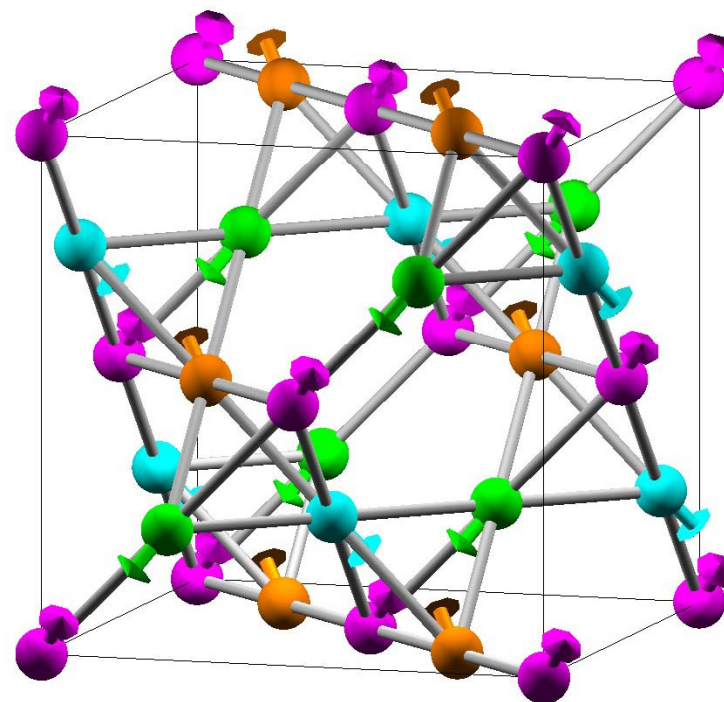
- 根据:

- 1) 有转过去的趋势
- 2) 此构型是我们计算的唯一稳定的磁构型
- 3) $J(q)$在$q=0$是极大
- 4) 没有Fermi surface nesting

实验证实

ॐ

Magnetic transition, long-range order, and moment fluctuations in the pyrochlore iridate $Eu_2Ir_2O_7$

Songrui Zhao,[1,*] J. M. Mackie,[1] D. E. MacLaughlin,[1] O. O. Bernal,[2] J. J. Ishikawa,[3] Y. Ohta,[3] and S. Nakatsuji[3]

Muon spin rotation and relaxation experiments in the pyrochlore iridate $Eu_2Ir_2O_7$ yield a well-defined muon spin precession frequency below the metal-insulator/antiferromagnetic transition temperature $T_M = 120$ K, indicative of long-range commensurate magnetic order and thus ruling out quantum spin liquid and spin-glass-like ground states. The dynamic muon spin relaxation rate is temperature-independent between 2 K and $\sim T_M$ and yields an

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Magnetic order in the pyrochlore iridates $A_2Ir_2O_7$ (A = Y, Yb)

S. M. Disseler,[1] Chetan Dhital,[1] A. Amato,[2] S. R. Giblin,[3] Clarina de la Cruz,[4] Stephen D. Wilson,[1] and M. J. Graf[1,*]
[1]Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA

We present results from muon spin relaxation/rotation, magnetization, neutron scattering, and transport measurements on polycrystalline samples of the pyrochlore iridates $Y_2Ir_2O_7$ (Y-227) and $Yb_2Ir_2O_7$ (Yb-227). Well-defined spontaneous oscillations of the muon asymmetry are observed together with hysteretic behavior in magnetization below 130 K in Yb-227, indicative of commensurate long-range magnetic order. Similar

实验证实

Magnetic order and the electronic ground state in the pyrochlore iridate $Nd_2Ir_2O_7$

S. M. Disseler,[1] Chetan Dhital,[1] T. C. Hogan,[1] A. Amato,[2] S. R. Giblin,[3] Clarina de la Cruz,[4] A. Daoud-Aladine,[3] Stephen D. Wilson,[1] and M. J. Graf[1]

We report a muon spin relaxation/rotation, bulk magnetization, neutron scattering, and transport study of the electronic properties of $Nd_2Ir_2O_7$. We observe the onset of strongly hysteretic behavior in the temperature-dependent magnetization below 120 K, and an abrupt increase in the temperature-dependent resistivity below 8 K. Muon spin relaxation measurements show that the hysteretic magnetization is driven by a transition to a magnetically disordered state, and below 8 K a magnetically ordered ground state sets in, as evidenced by the onset of spontaneous muon precession. Our measurements point toward the absence of a true metal-to-insulator

Continuous transition between antiferromagnetic insulator and paramagnetic metal in the pyrochlore iridate $Eu_2Ir_2O_7$

Jun J. Ishikawa,* Eoin C. T. O'Farrell, and Satoru Nakatsuji[†]

Our single crystal study of the magnetothermal and transport properties of the pyrochlore iridate $Eu_2Ir_2O_7$ reveals a continuous phase transition from a paramagnetic metal to an antiferromagnetic insulator for a sample with stoichiometry within ~1% resolution. The insulating phase has strong proximity to an antiferromagnetic semimetal, which is stabilized by several % level of the off-stoichiometry. Our observations suggest that in addition to electronic correlation and spin-orbit coupling the magnetic order is essential for opening the charge gap.

实验证实

Emergence of Magnetic Long-range Order in Frustrated Pyrochlore $Nd_2Ir_2O_7$ with Metal-insulator Transition

K. Tomiyasu,[1, *] K. Matsuhira,[2] K. Iwasa,[1] M. Watahiki,[1] S. Takagi,[2] M. Wakeshima,[3] Y. Hinatsu,[3] M. Yokoyama,[4] K. Ohoyama,[5] and K. Yamada[6]

In this study, we performed powder neutron diffraction and inelastic scattering measurements of frustrated pyrochlore $Nd_2Ir_2O_7$, which exhibits a metal-insulator transition at a temperature T_{MI} of 33 K. The diffraction measurements revealed that the pyrochlore has an antiferromagnetic long-range structure with propagation vector q_0 of (0,0,0) and that it grows with decreasing temperature below 15 K. This structure was analyzed to be of the all-in all-out type, consisting of highly anisotropic Nd^{3+} magnetic moments of magnitude $2.3 \pm 0.4\mu_B$, where μ_B is the Bohr magneton. The inelastic scattering measurements revealed that the Kramers ground doublet of Nd^{3+} splits below T_{MI}. This suggests the appearance of a static internal magnetic field at the Nd sites, which probably originates from a magnetic order consisting of Ir^{4+} magnetic moments. Here, we discuss a magnetic structure model for the Ir order and the relation of the order to the metal-insulator transition in terms of frustration.

理论方面

Topological and magnetic phases of interacting electrons in the pyrochlore iridates

William Witczak-Krempa[1] and Yong Baek Kim[1,2]

Mean field approximation

DCA
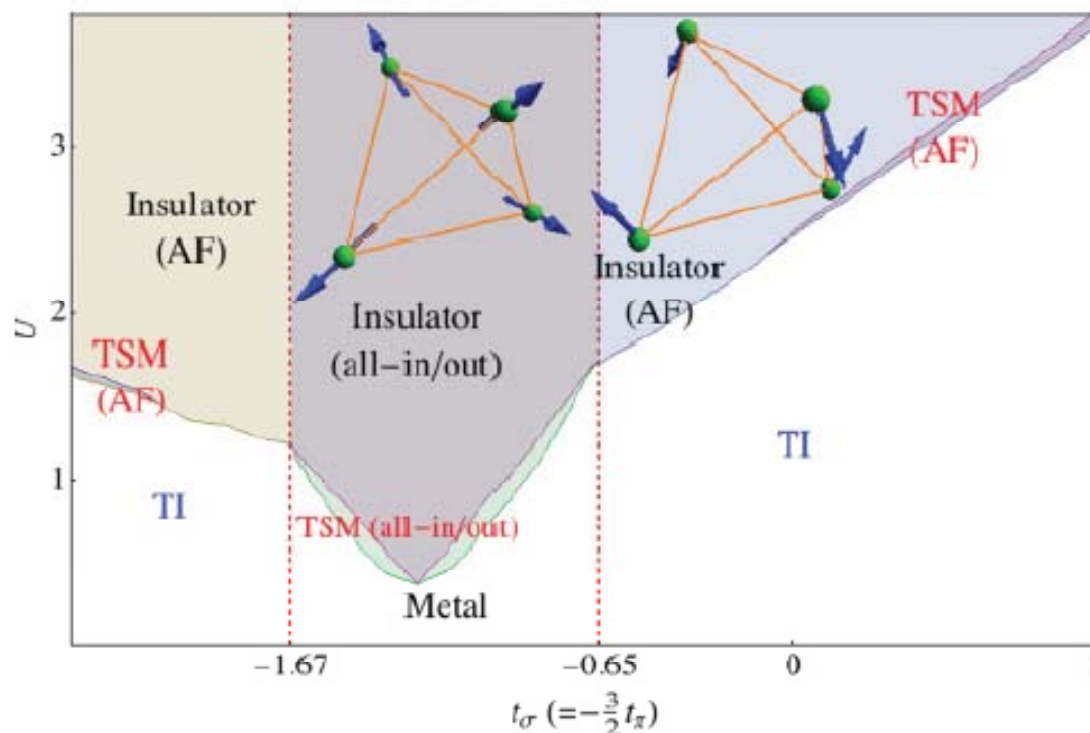
理论方面

Magnetic orders and topological phases from f-d exchange in pyrochlore iridates

Gang Chen and Michael Hermele

   We study theoretically the effects of f-d magnetic exchange interaction in the $R_2Ir_2O_7$ pyrochlore iridates. The R^{3+} f-electrons form localized magnetic doublets due to the crystal field environment, while the Ir^{4+} d-electrons are more itinerant and feel a strong spin-orbit coupling. We construct and analyze a minimal model capturing this physics, treating the Ir subsystem using a Hubbard-type model. First neglecting the Hubbard interaction, we find Weyl semi-metal and Axion insulator phases induced by the f-d exchange. Next, we find that f-d exchange can cooperate with the Hubbard interaction to stabilize the Weyl semi-metal over a larger region of parameter space than when it is induced by d-electron correlations alone. Applications to experiments are discussed.
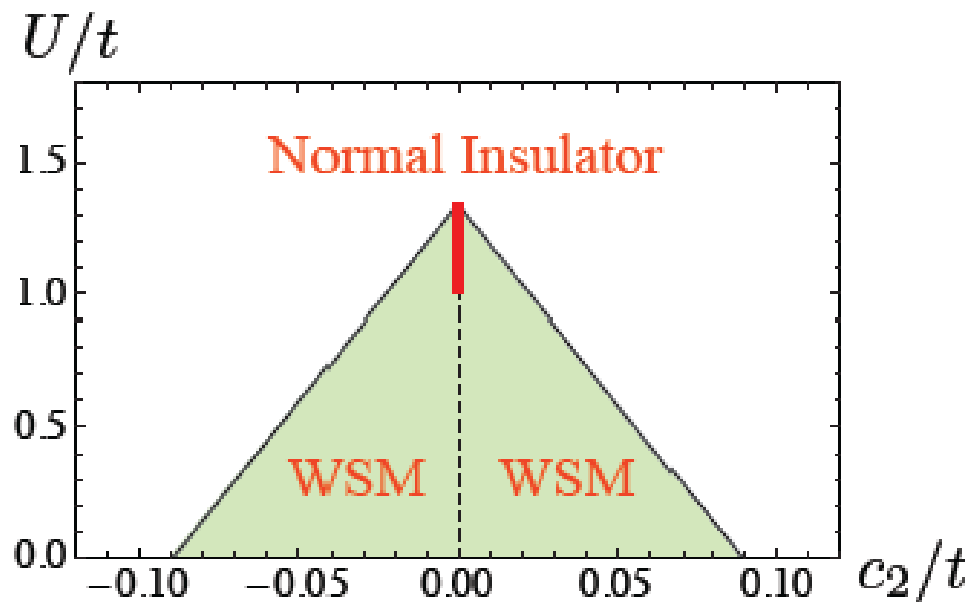
All-in/all-out非共线磁结构

$Cd_2Os_2O_7$

2001

Continuous metal-insulator transition in the pyrochlore $Cd_2Os_2O_7$

D. Mandrus,[1,2,*] J. R. Thompson,[2,1] R. Gaal,[3] L. Forro,[3] J. C. Bryan,[4] B. C. Chakoumakos,[1] L. M. Woods,[2,1] B. C. Sales,[1] R. S. Fishman,[1] and V. Keppens[1,†]

2002

Electronic structure of the pyrochlore metals $Cd_2Os_2O_7$ and $Cd_2Re_2O_7$

D. J. Singh

Code 6391, Naval Research Laboratory, Washington, DC 20375

P. Blaha and K. Schwarz

Institut für Physik und Theoretische Chemie, TU Wien, A-1060 Wien, Austria

J. O. Sofo

All-in/all-out非共线磁结构

Noncollinear Magnetism and Spin-Orbit Coupling in 5d Pyrochlore Oxide $Cd_2Os_2O_7$

We investigate the electronic and magnetic properties of the pyrochlore oxide $Cd_2Os_2O_7$ using the density-functional theory plus on-site repulsion (U) method, and depict the ground-state phase diagram with respect to U. We conclude that the all-in–all-out noncollinear magnetic order is stable in a wide range of U. We also show that the easy-axis anisotropy arising from the spin-orbit coupling plays a significant role in stabilizing the all-in–all-out magnetic order. A *pseudogap* was observed near the transition between

Tetrahedral Magnetic Order and the Metal-Insulator Transition in the Pyrochlore Lattice of $Cd_2Os_2O_7$

accompanied with any spatial symmetry breaking. We propose a noncollinear all-in–all-out spin arrangement on the tetrahedral network made of Os atoms. Based on this we suggest that the transition is not caused by the Slater mechanism as believed earlier but by an alternative mechanism related to the

内容

- **5d**过渡金属氧化物

- 烧绿石结构铱化合物

  磁基态构型, **Weyl**半金属, **Fermi Arc**

- 设计**Axion**绝缘体

电子关联+自旋轨道耦合➔新的物理?

这里是磁性打破了时间反演，所以这个体系不是**常规的**拓扑绝缘体。

是否有新的物理？

绝缘体 只要能隙没有闭合，其拓扑量子序不变。所以对于绝缘体可以定义拓扑性质。

对于金属呢？

反常的能带行为
宇称反转

U-0-all-in-SO-Y2Ir2O7   U-1-all-in-SO-U-Y2Ir2O7   U-1.5-all-in-SO-U-Y2Ir2O7   all-in-SO-U-Y2Ir2O7   U-2.2-all-in-SO-U-Y2Ir2O7

U=0 eV   U=1 eV   U=1.5 eV   U=2 eV   U=2.2 eV

100k points   **Parities change!**   **Mott Insulator**
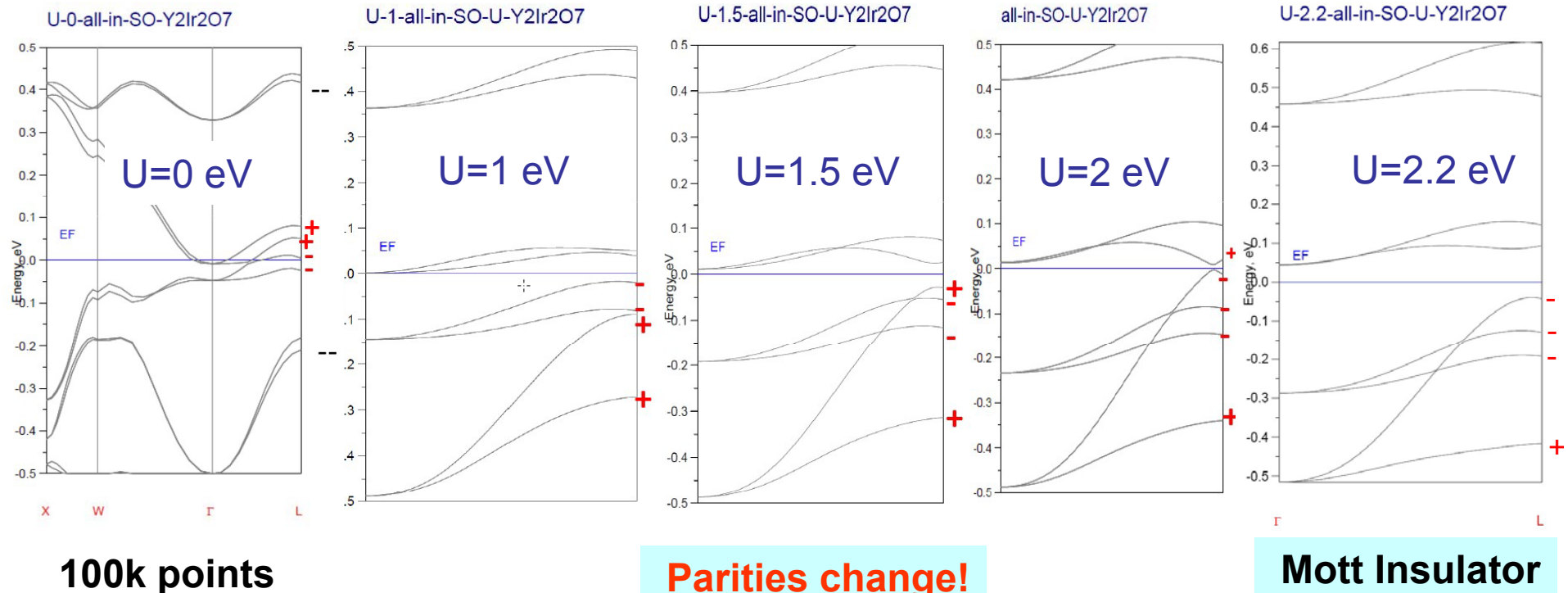
We study changes in band parities that may indicate a presence of topological insulator and also semi-metallic phase since topological insulators in 3D must be separated from trivial insulator by 3D Dirac (Weyl) points (Murakami, Kuga, 2008).

在合理的**U**的范围内（**1.0eV<U<1.8 eV**）是**Weyl semi–metal**

LEFT:within k_z=0 plane of BZ   RIGHT:for k_z=0.3 plane of BZ
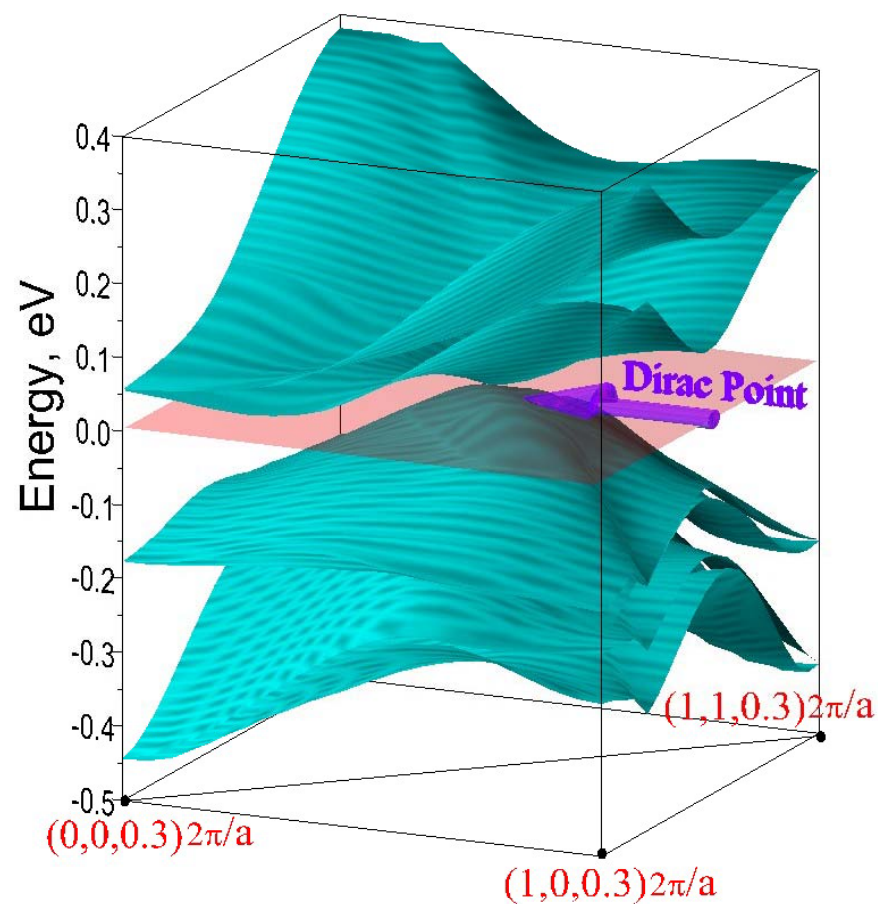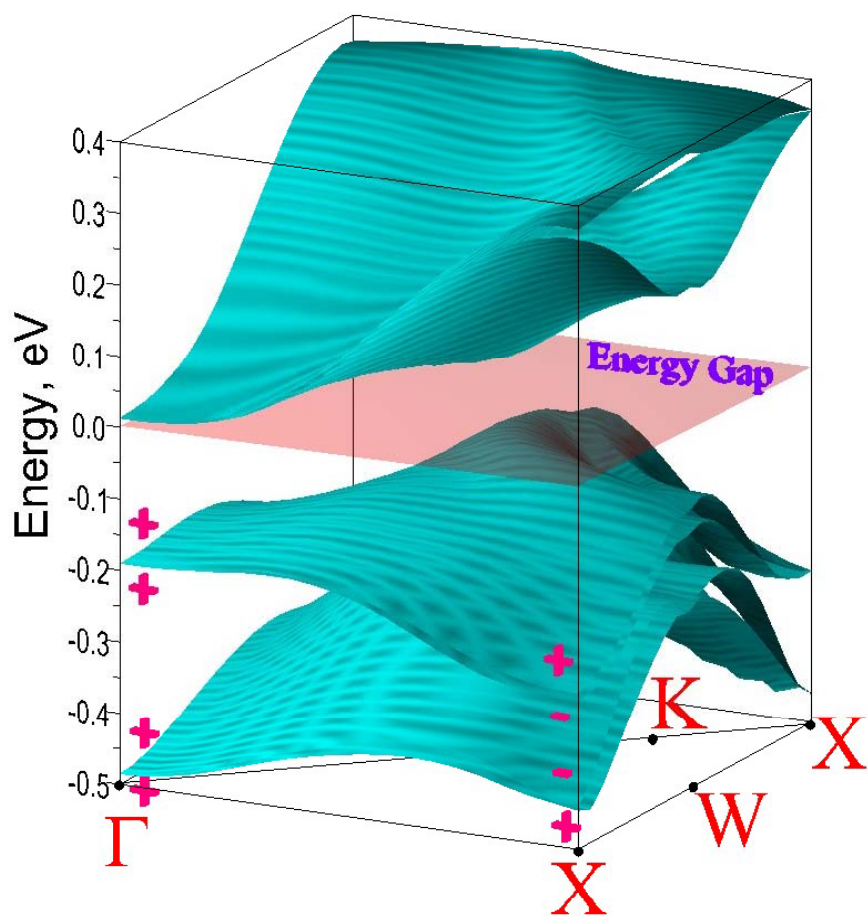
Arita *et al.*, PRL (2012)→ U在1.4→2.3 eV

Weyl-semimetal

- Graphene 里面的Dirac point 是4分量的)。

- Weyl点一旦产生，就非常稳定，小的扰动不能把它消灭。只有2个具有相反符号的Weyl点相遇，Weyl点才能消失，材料变为绝缘体。

- 要打破时间反演或空间反演不变。

$$\begin{pmatrix} A & C \\ C^* & B \end{pmatrix} \quad \odot \quad \begin{pmatrix} A & & B \\ \operatorname{Re} C & & 0 \\ \operatorname{Im} C & & 0 \end{pmatrix}, \quad k_x, k_y, k_z$$

金属 拓扑？

- 绝缘体 只要能隙没有闭合，其拓扑量子序不变。所以对于绝缘体可以定义拓扑性质。

- 对于金属呢？

Weyl-semimetal

In the vicinity of Weyl Point: $q = k - k_W$

$$H(q) = \sum_{i=xyz} v_i \bullet q \sigma_i \qquad E_{\pm}(q) = \pm \sqrt{\sum_{i=xyz} (v_i \bullet q)^2}$$

The Berry curvature is evaluated to be

$$\Omega(k) = i \sum_{n=1}^{N_{occ}} \langle \nabla_k u_{kn} | \times | \nabla_k u_{kn} \rangle \rightarrow \sum_{ijk} \frac{1}{2} \varepsilon_{ijk} (v_i \times v_j)(v_k \bullet q) \frac{1}{\left(\sum_i (v_i \bullet q)^2 \right)^{3/2}}$$

Integrating over small sphere surrounding Weyl point produces flux that is given by chiral charge c

$$c = \frac{1}{2\pi} \oiint_S dS \Omega(k) = \text{sign}(v_1 \bullet v_2 \times v_3)$$

Weyl point acts as a **magnetic monopole** at the origin:

$$\Omega(q) = c \frac{1}{2} \frac{q}{q^3}$$

"点电荷"

Charge determined in terms of electron velocities at this k_D point:

$$c = \text{sign}(v_1 \bullet v_2 \times v_3)$$
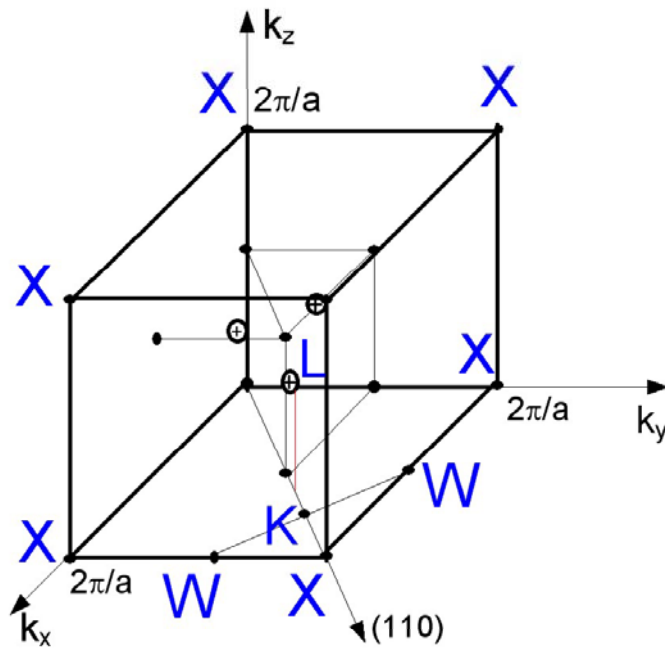
Three positive Weyl points around L
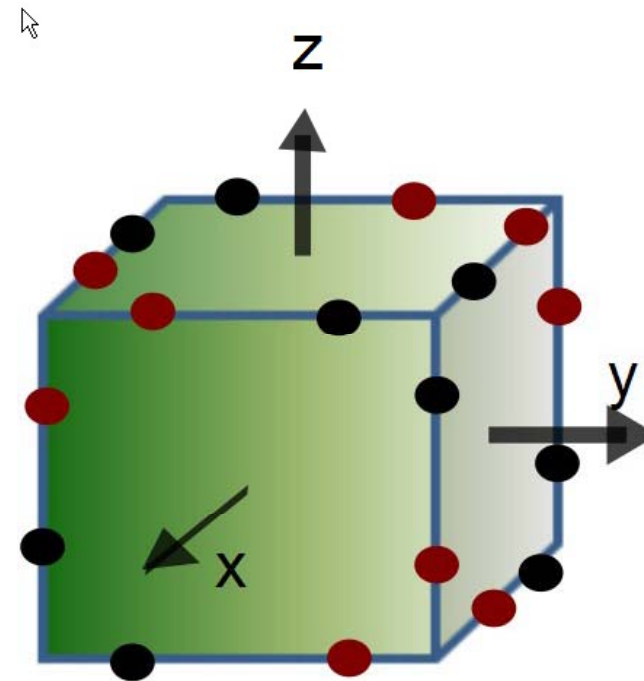
Positive and negative Weyl points in BZ

变化U的影响

增加U→Weyl Point朝L点移动,当
U=1.8eV时,2个相反符号的Weyl
Point在L点相遇→Mott insulator
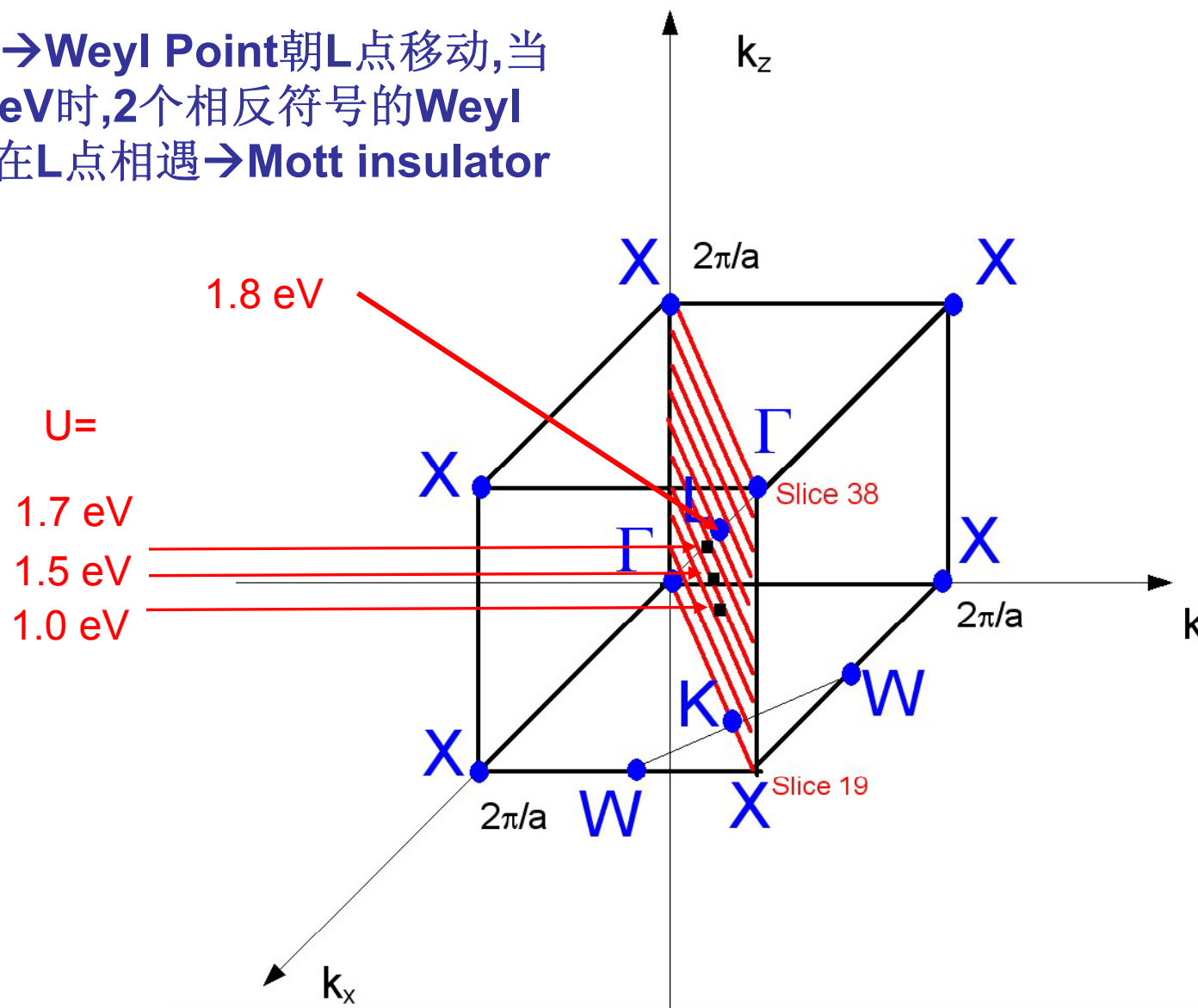
变化**U**的影响
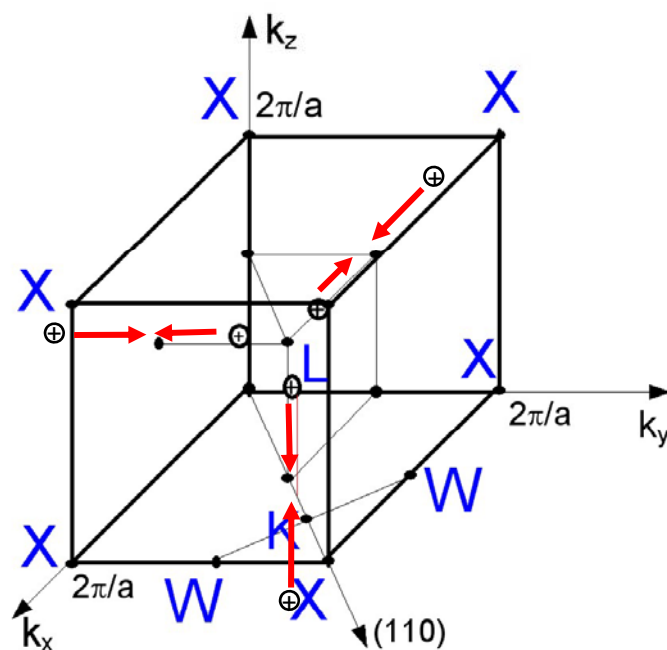
减小**U→Weyl Point**朝**X**点移动,当**U=1.0eV**时,**2**个相反符号的**Weyl Point**在**X**点相遇.如果材料是绝缘体的话这将是**Axion Insulator**
但是**LDA+SO+U**发现别处有能带通过**Fermi level**

内容

❑ **5d**过渡金属氧化物

❑ 烧绿石结构铱化合物

　　　　磁基态构型, **Weyl**半金属, **Fermi Arc**

❑ 设计**Axion**绝缘体

Fermi Arc (费米面是不连续的线段)
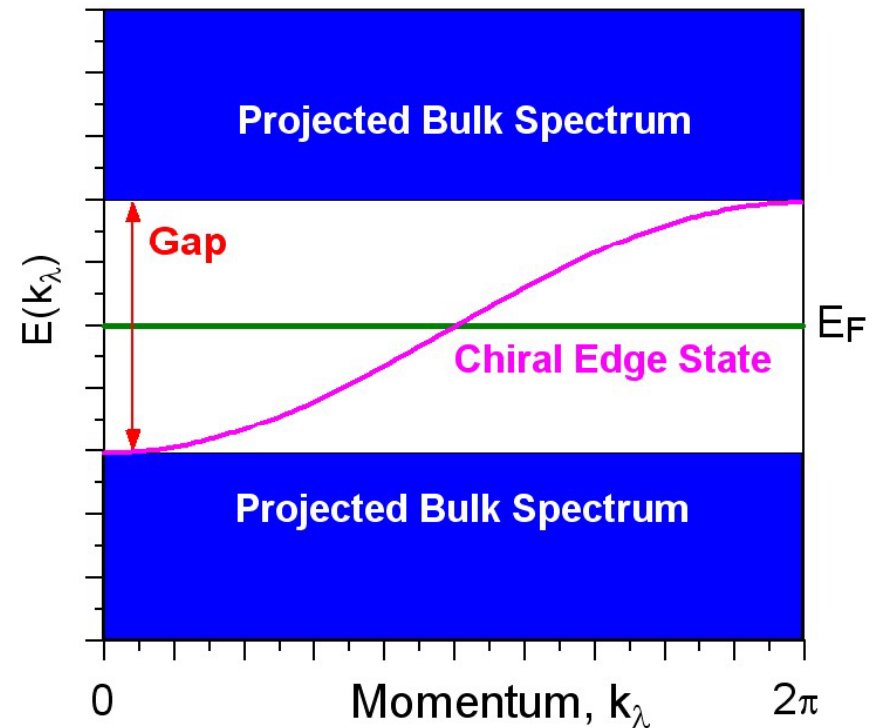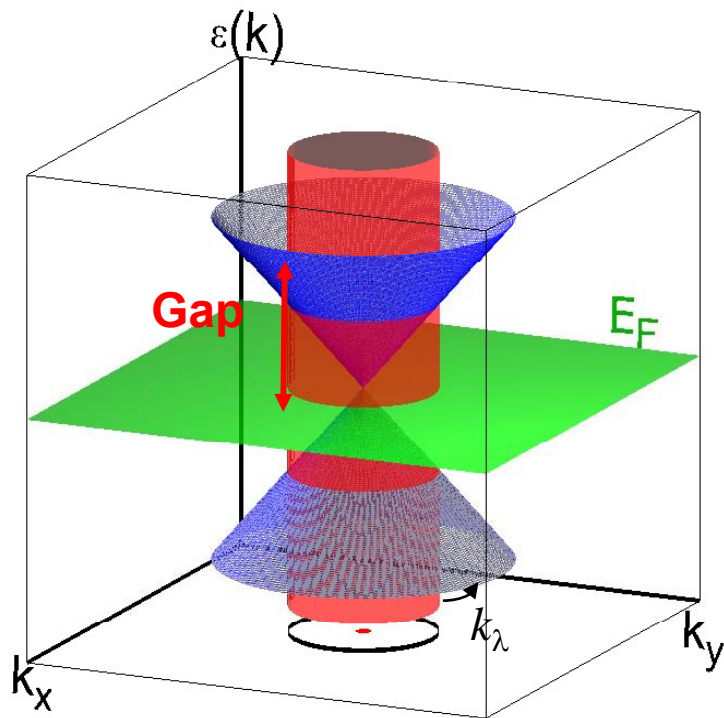
Fermi Arc (topo→费米面是不连续的线段)
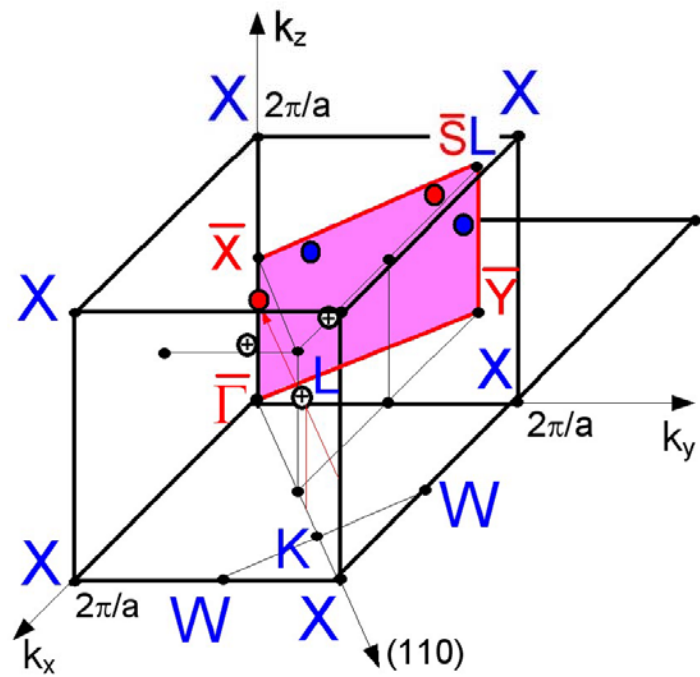
（110）面
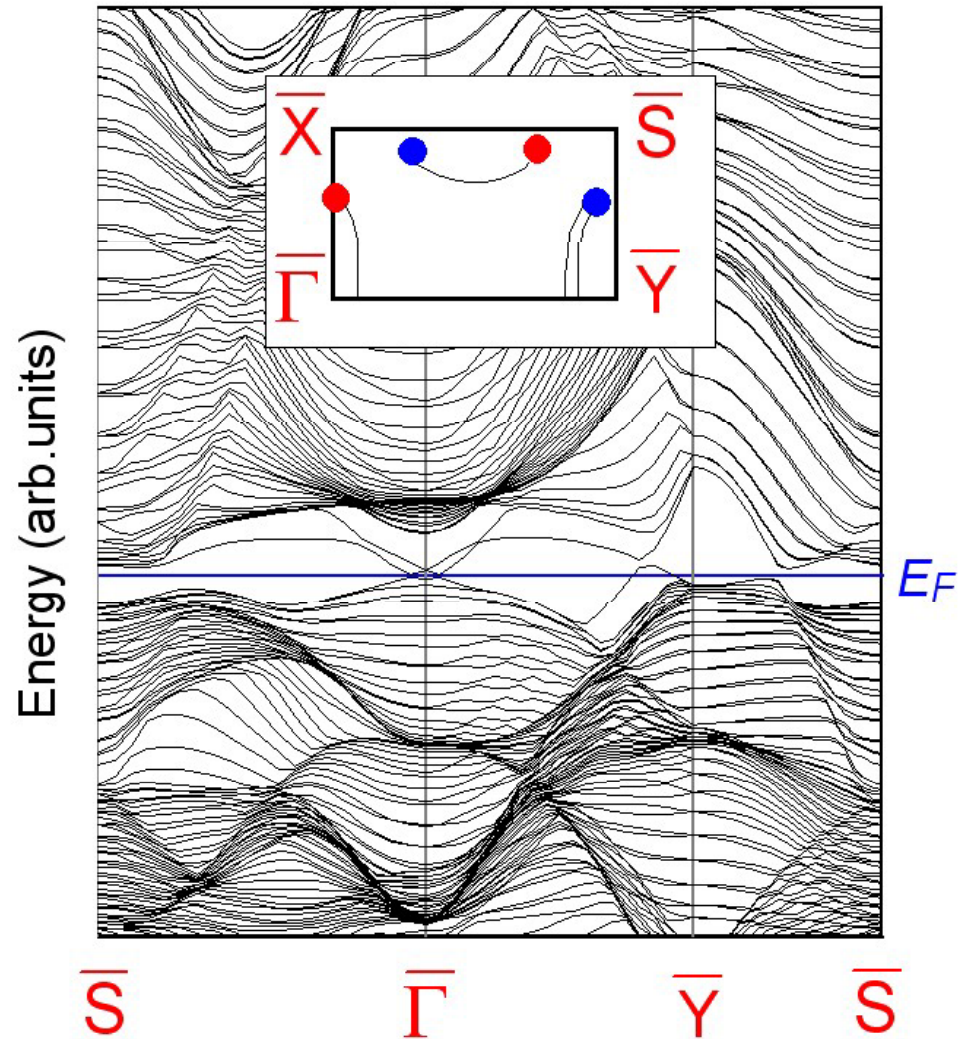
Fermi Arcs connecting Weyl points of opposite chirality can be directly observed

烧绿石结构Ir氧化物（$A_2Ir_2O_7$）相图
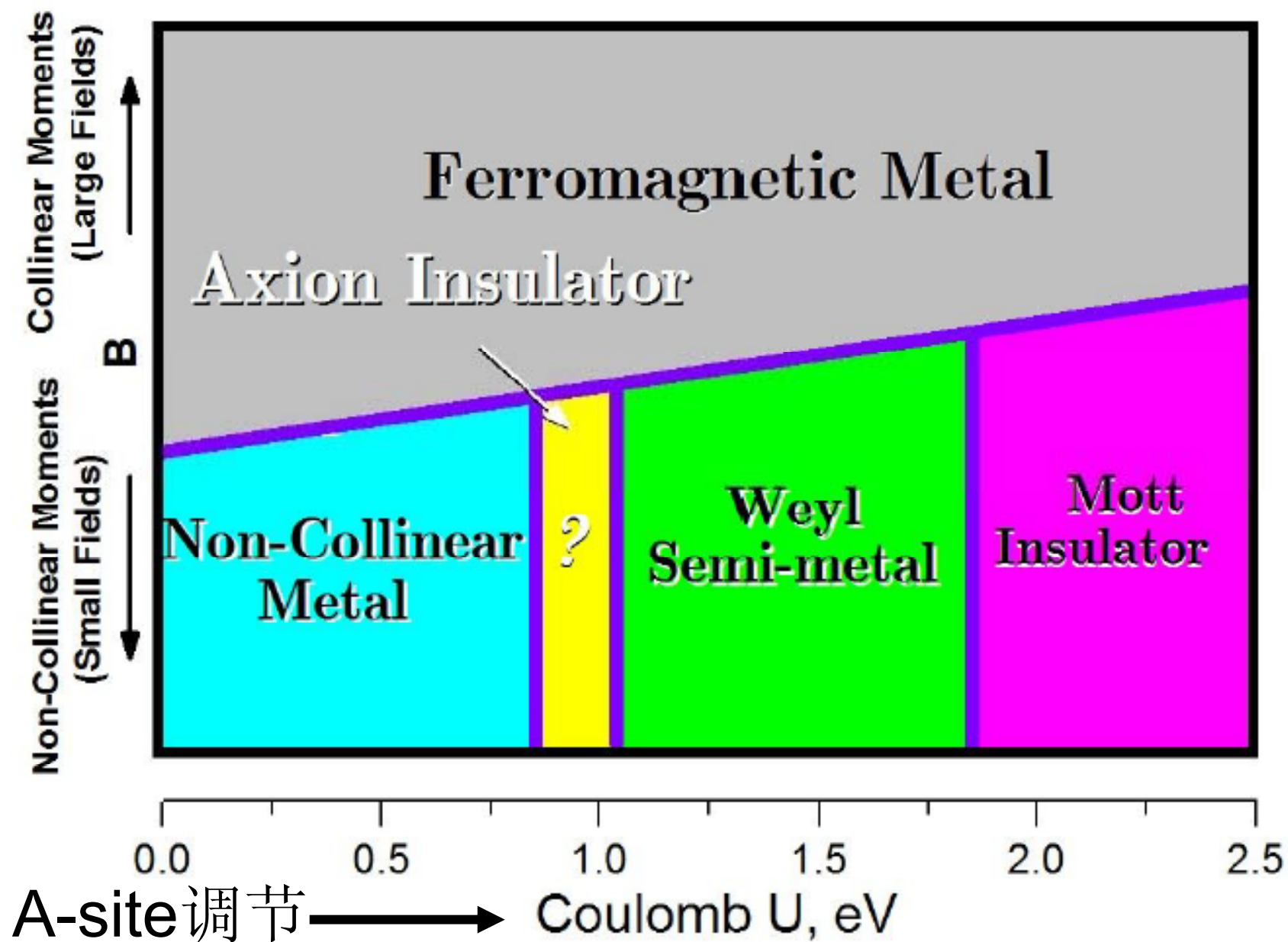
新型的拓扑量子态—Weyl半金属

- **a) Weyl点是稳定的**
- **b) 有受拓扑保护的表面态，即非闭合的费米面(Fermi arc)**
- **c) 它对外场的响应也由其拓扑性质决定(只与Weyl点的位置有关，和能带的细节无关)。**
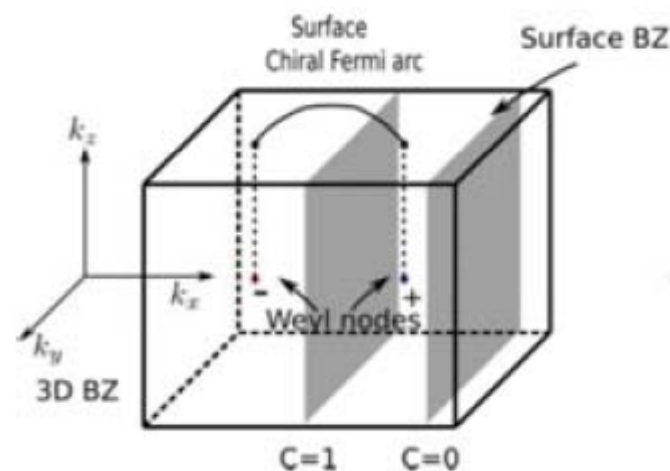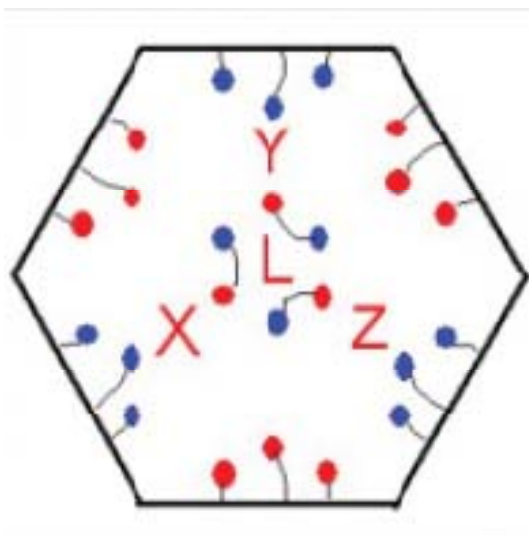
Variation of Charge Dynamics in the Course of Metal-Insulator Transition for Pyrochlore-Type $Nd_2Ir_2O_7$

K. Ueda,[1] J. Fujioka,[1] Y. Takahashi,[1] T. Suzuki,[2] S. Ishiwata,[1] Y. Taguchi,[2] and Y. Tokura[1,2]
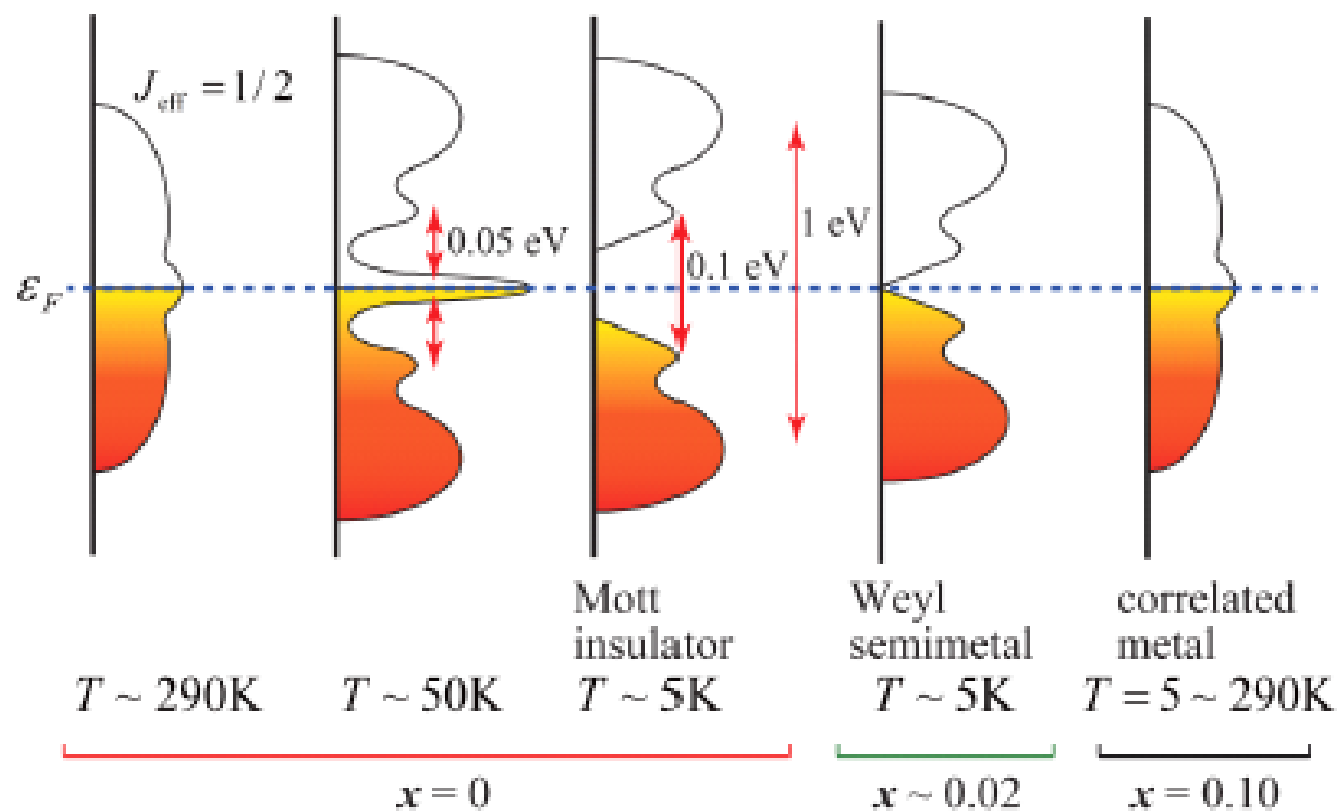
相关实验

Linear magnetoresistance and time reversal symmetry breaking of pyrochlore iridates $Bi_2Ir_2O_7$

Jiun-Haw Chu,[1,2,*] Scott. C. Riggs,[3,4] Maxwell Shapiro,[3,4] Jian Liu,[1,2] Claudy Ryan Serero,[5] Di Yi,[5] M. Melissa,[1] S. J. Suresha,[2] C. Frontera,[6] Ashvin Vishwanath,[1,2] Xavi Marti,[5] I. R. Fisher,[3,4] and R. Ramesh[1,5,2]

内容

□ **5d**过渡金属氧化物

□ 烧绿石结构铱化合物
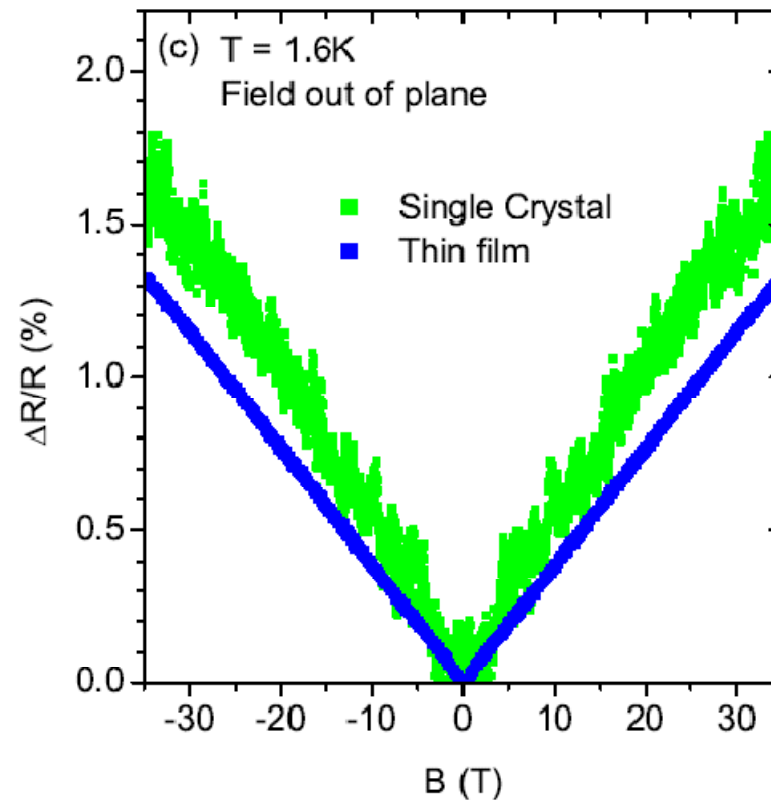
　　　　磁基态构型**,Weyl**半金属**,Fermi Arc**

□ 设计**Axion**绝缘体

Axion Insulators

Dynamical axion field in topological magnetic insulators

Rundong Li[1], Jing Wang[1,2], Xiao-Liang Qi[1] and Shou-Cheng Zhang[1]★

$$S_0 = \frac{8}{\pi} \int d^3 x dt \left(\varepsilon E^2 - B^2 / \mu \right)$$

$$S_\theta = \frac{\theta}{2\pi} \frac{e^2}{2\pi \hbar c} \int d^3 x dt \, \vec{E} \vec{B}$$

时间反演对称➔θ=0,π

空间反演对称➔θ=0,π

没有时间空间反演对称➔θ不再量子化，但是都很小BFO, 10^{-4}

磁+拓扑

- The simplest way is to coat a topological insulator with magnetic material to get rid of surface states. that will also have

  theta = pi, but there are technical problems there. (Y.L. Chen et al., Science (2010))

- Combine band topology with intrinsic magnetic order.

设计大的磁电响应材料

- 磁需要电子关联
- 拓扑量子序需要自旋轨道耦合

- Bi_2Se_3等已知的不好
- 3d,4d不好
- 4f,5f不好

- **5d！**

计算θ

Turner, Zhang, Vishwanath, arXiv:1010.4335
Hughes, Prodan and Bernevig, PRB (2011)

$$P \quad \blacksquare \quad \blacklozenge \frac{e^2}{2\pi} B$$

$$\theta = \pi \cdot M (\mathrm{mod}\ 2)$$

where $M = (\sum_k N_i)/2$, and N_i is the number of occupied states at the TRIM points i with odd parity.

TABLE III: Calculated parities of states at Time Reversal Invariant Momenta (TRIMs) of $CaOs_2O_4$. Only the 4 empty t_{2g} bands are shown in order of increasing energy. Lx $2\pi/a$(-0.5,0.5,0.5), Ly $2\pi/a$(0.5,-0.5,0.5), Lz $2\pi/a$(-0.5,0.5,0.5) and L $2\pi/a$(0.5,0.5,0.5)).

	Lx	Ly	Lz	L
U=0.5 eV	++++	++++	++++	- - - -
U=1.5 eV	-+++	-+++	-+++	+ - - -

$CaOs_2O_4$

$SrOs_2O_4$

Xiangang Wan,[1] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[4]

设计**Axion insulator**
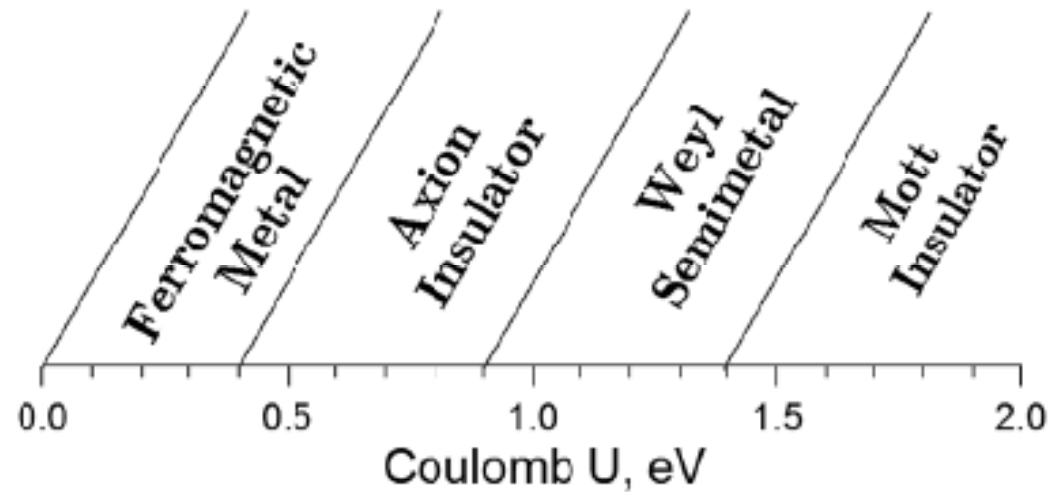
FIG. 3. Sketch of the predicted phase diagram for spinel osmates.

Xiangang Wan,[1] Ashvin Vishwanath,[2,3] and Sergey Y. Savrasov[4]

汇报内容

❑ **5d**过渡金属氧化物

❑ 烧绿石结构铱化合物

      磁基态构型, **Weyl**半金属, **Fermi Arc**

❑ 设计**Axion**绝缘体

❑ **Slater insulator**

Slater Insulator

- 金属➔绝缘体转变
- Mott (1940s电子关联)
- Anderson (1970s localization via disorder)
- Slater (1951) antiferromagnetic AF order alone can open a gap regardless of the magnitude of the Coulomb interaction.

- Generally, a 3D conductor causes only a small fraction of changes in its electronic structure through the AF ordering所以 Slater insulator很少受到关注。

Slater Insulator $Cd_2Os_2O_7$

(2001)

Continuous metal-insulator transition in the pyrochlore $Cd_2Os_2O_7$

D. Mandrus,[1,2,*] J. R. Thompson,[2,1] R. Gaal,[3] L. Forro,[3] J. C. Bryan,[4] B. C. Chakoumakos,[1] L. M. Woods,[2,1] B. C. Sales, R. S. Fishman,[1] and V. Keppens[1,†]

All-in/all-out非共线磁结构

PHYSICAL REVIEW LETTERS

Noncollinear Magnetism and Spin-Orbit Coupling in 5d Pyrochlore Oxide $Cd_2Os_2O_7$

We investigate the electronic and magnetic properties of the pyrochlore oxide $Cd_2Os_2O_7$ using the density-functional theory plus on-site repulsion (U) method, and depict the ground-state phase diagram with respect to U. We conclude that the all-in–all-out noncollinear magnetic order is stable in a wide range of U. We also show that the easy-axis anisotropy arising from the spin-orbit coupling plays a significant role in stabilizing the all-in–all-out magnetic order. A *pseudogap* was observed near the transition between

PHYSICAL REVIEW LETTERS

Tetrahedral Magnetic Order and the Metal-Insulator Transition in the Pyrochlore Lattice of $Cd_2Os_2O_7$

accompanied with any spatial symmetry breaking. We propose a noncollinear all-in–all-out spin arrangement on the tetrahedral network made of Os atoms. Based on this we suggest that the transition is not caused by the Slater mechanism as believed earlier but by an alternative mechanism related to the

NaOsO$_3$

Continuous metal-insulator transition of the antiferromagnetic perovskite NaOsO$_3$

Y. G. Shi,[1,2] Y. F. Guo,[1,2] S. Yu,[3] M. Arai,[4] A. A. Belik,[1,2] A. Sato,[5] K. Yamaura,[2,3,*] E. Takayama-Muromachi,[1,2,3] H. F. Tian,[6] H. X. Yang,[6] J. Q. Li,[6] T. Varga,[7] J. F. Mitchell,[7] and S. Okamoto[8]
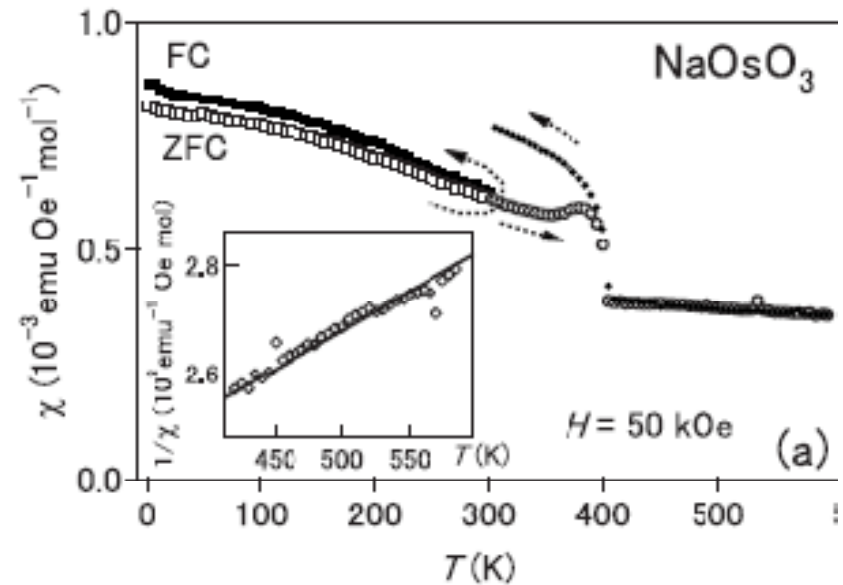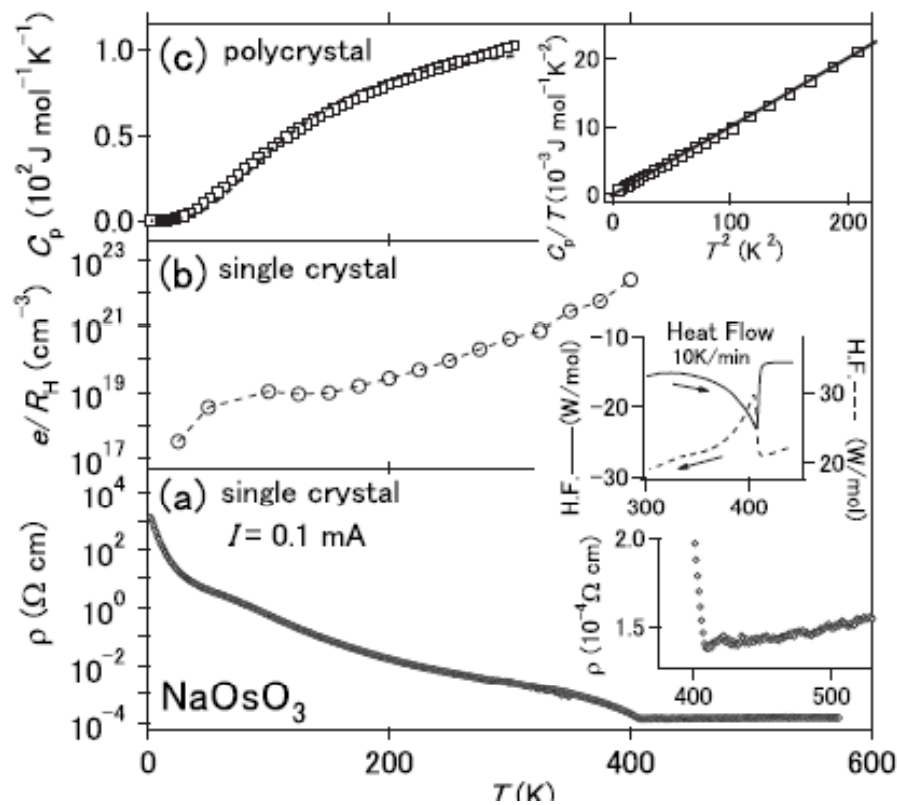
Electronic structure and magnetic properties of NaOsO$_3$

Yongping Du,[1] Xiangang Wan,[1,2,*] Li Sheng,[1] Jinming Dong,[1] and Sergey Y. Savrasov[2]

1) Despite its big value the SOC has only weak effect on the band structure and magnetic moment.

2) The electronic correlations alone cannot open the band gap, and the low-temperature phase of NaOsO$_3$ is not a Mott-type insulator.

3) The magnetic configuration has an important effect on the conductivity, and the ground state is a G-type AFM insulator.

4) magnetic ordering→insulating behavior of NaOsO$_3$.

5) 磁化率曲线要小心

Magnetically Driven Metal-Insulator Transition in NaOsO₃

S. Calder,[1,*] V. O. Garlea,[1] D. F. McMorrow,[2] M. D. Lumsden,[1] M. B. Stone,[1] J. C. Lang,[3] J.-W. Kim,[3] J. A. Schlueter,[4] Y. G. Shi,[5,6] K. Yamaura,[6] Y. S. Sun,[7] Y. Tsujimoto,[7] and A. D. Christianson[1]
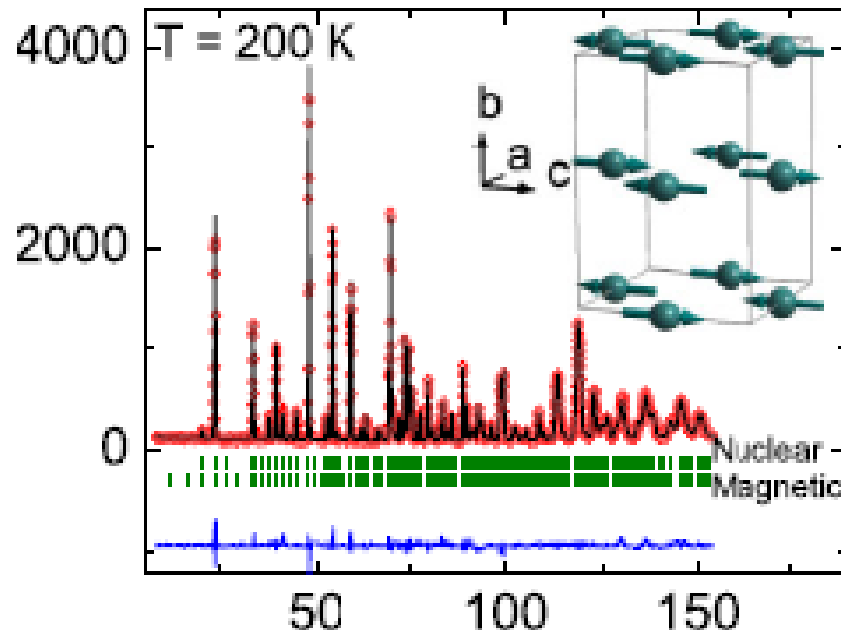
我们的理论结果被这篇实验很好的证实

磁矩大小，磁结构，SOC影响不大

主要的内容

- **1）烧绿石结构过渡金属Ir氧化物的磁结构**

- **2）对于金属也是可以对其拓扑分类的**

- **3）Axion insulator**

- **4）确定了NaOsO$_3$是Slater insulator**

BiS$_2$层状超导体 (2012-07)

- Bi$_4$O$_4$S$_3$
- LaO$_{1-x}$F$_x$BiS$_2$
- NdOBiS$_2$
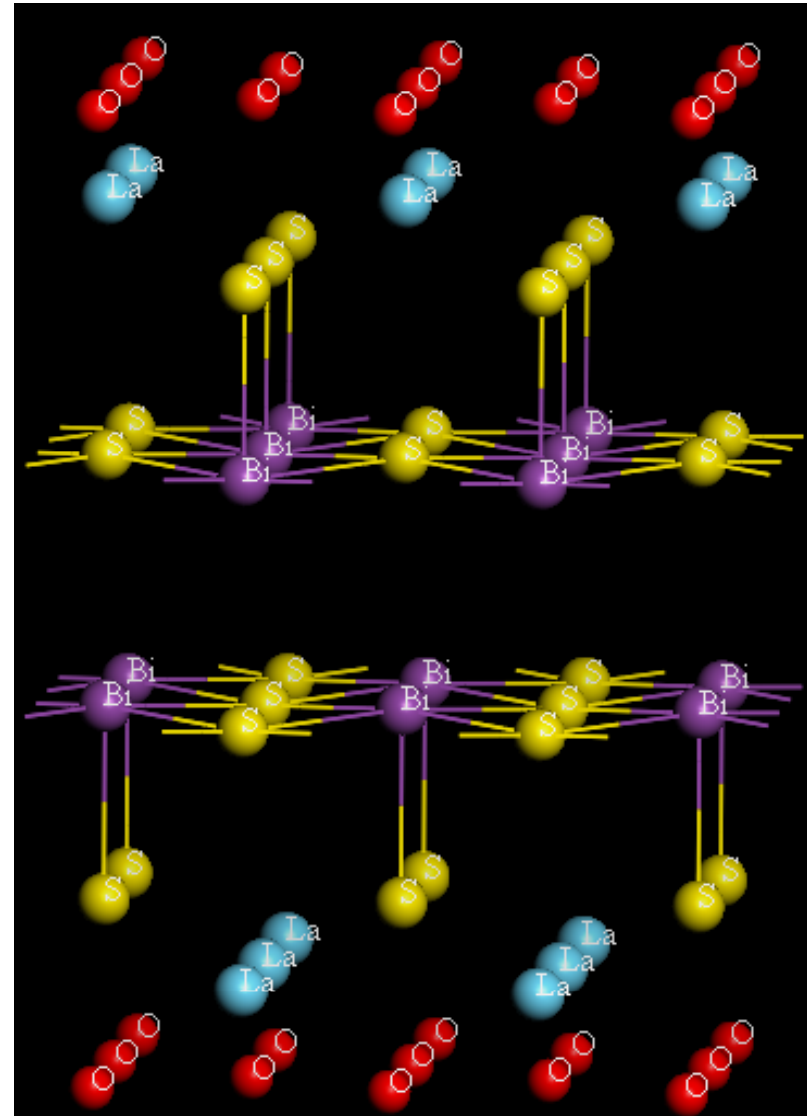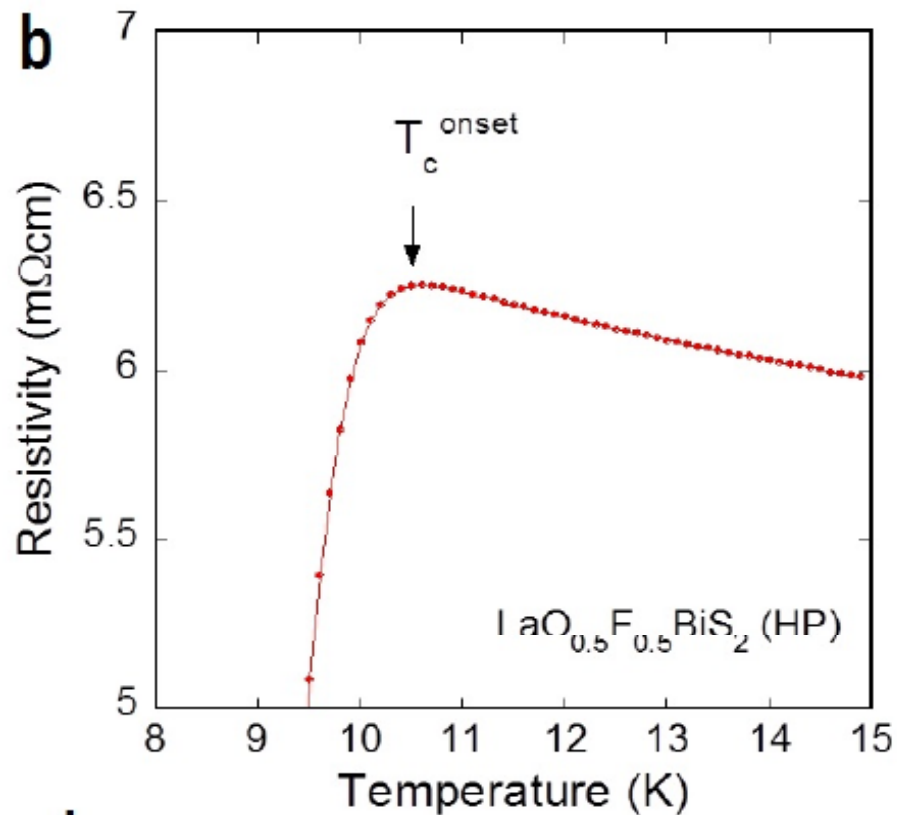
LaO$_{0.5}$F$_{0.5}$BiS$_2$的Fermi surface
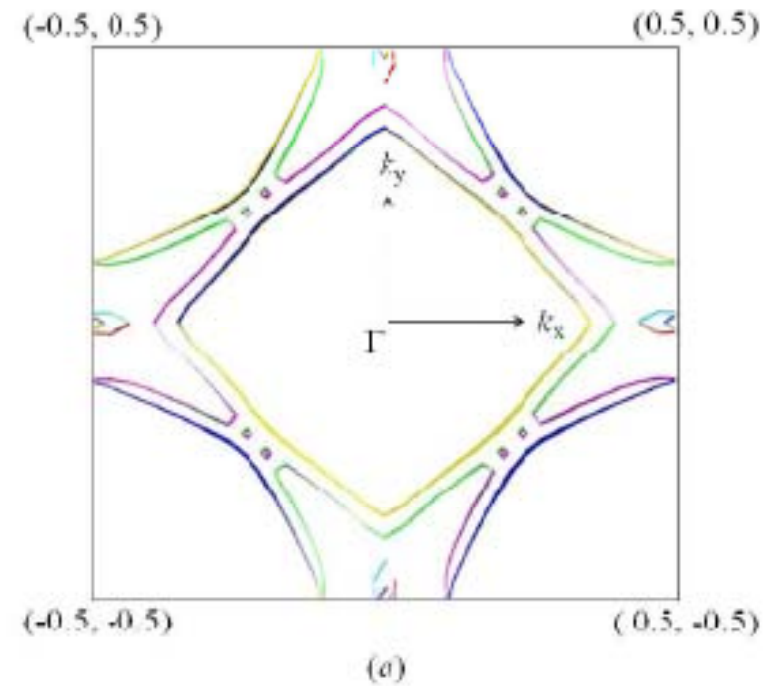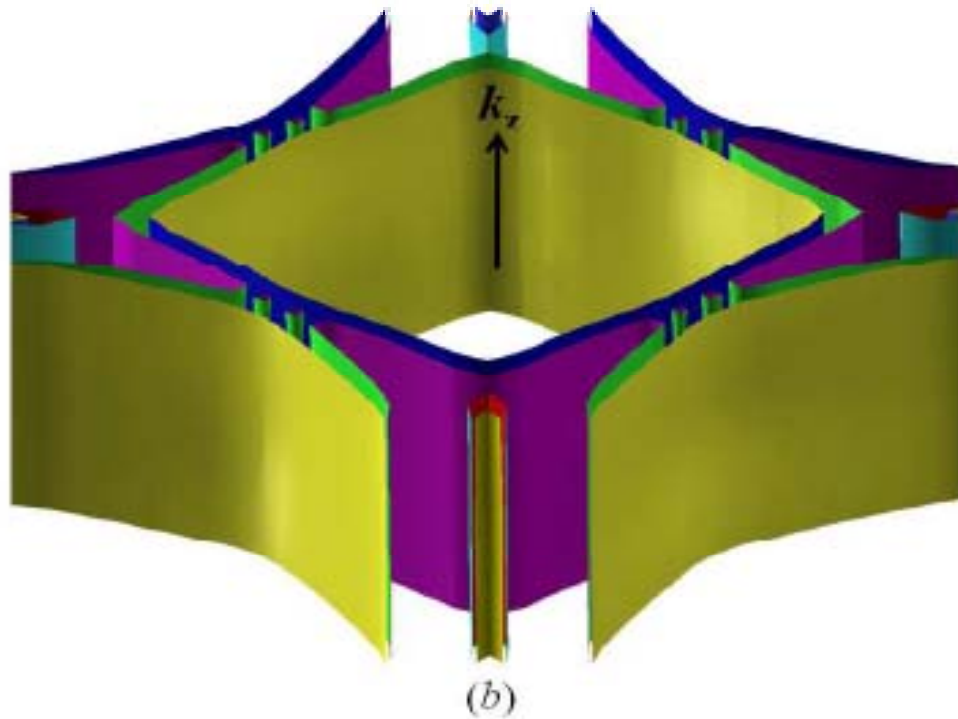
strong Fermi surface nesting at wavevectors near k =(π, π, 0).

CDW?

Sun et al.,
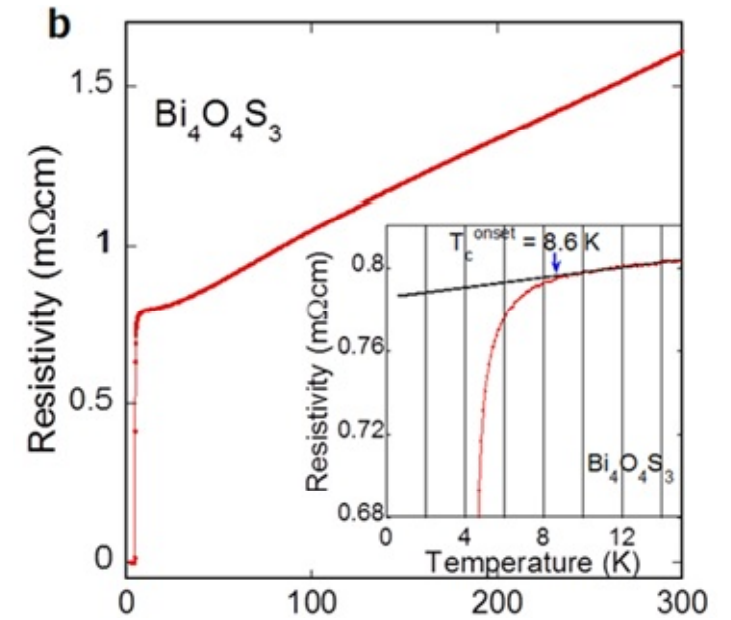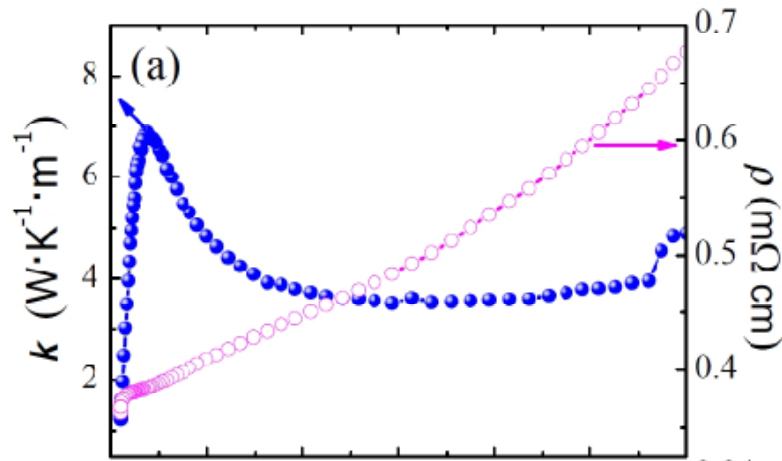
Wen et al.,
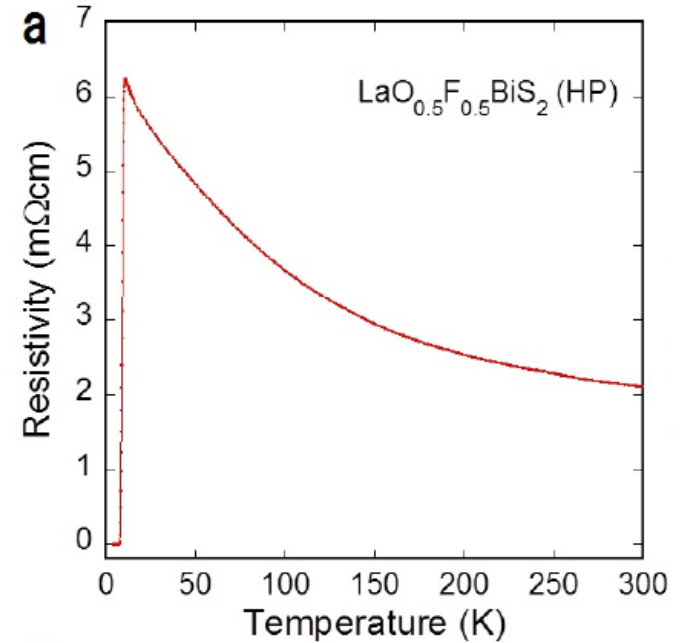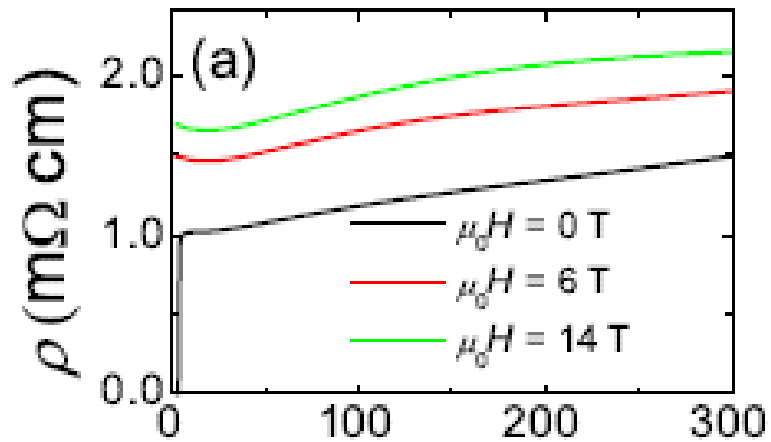
LaO$_{0.5}$F$_{0.5}$BiS$_2$的声子谱

linear response phonon calculation
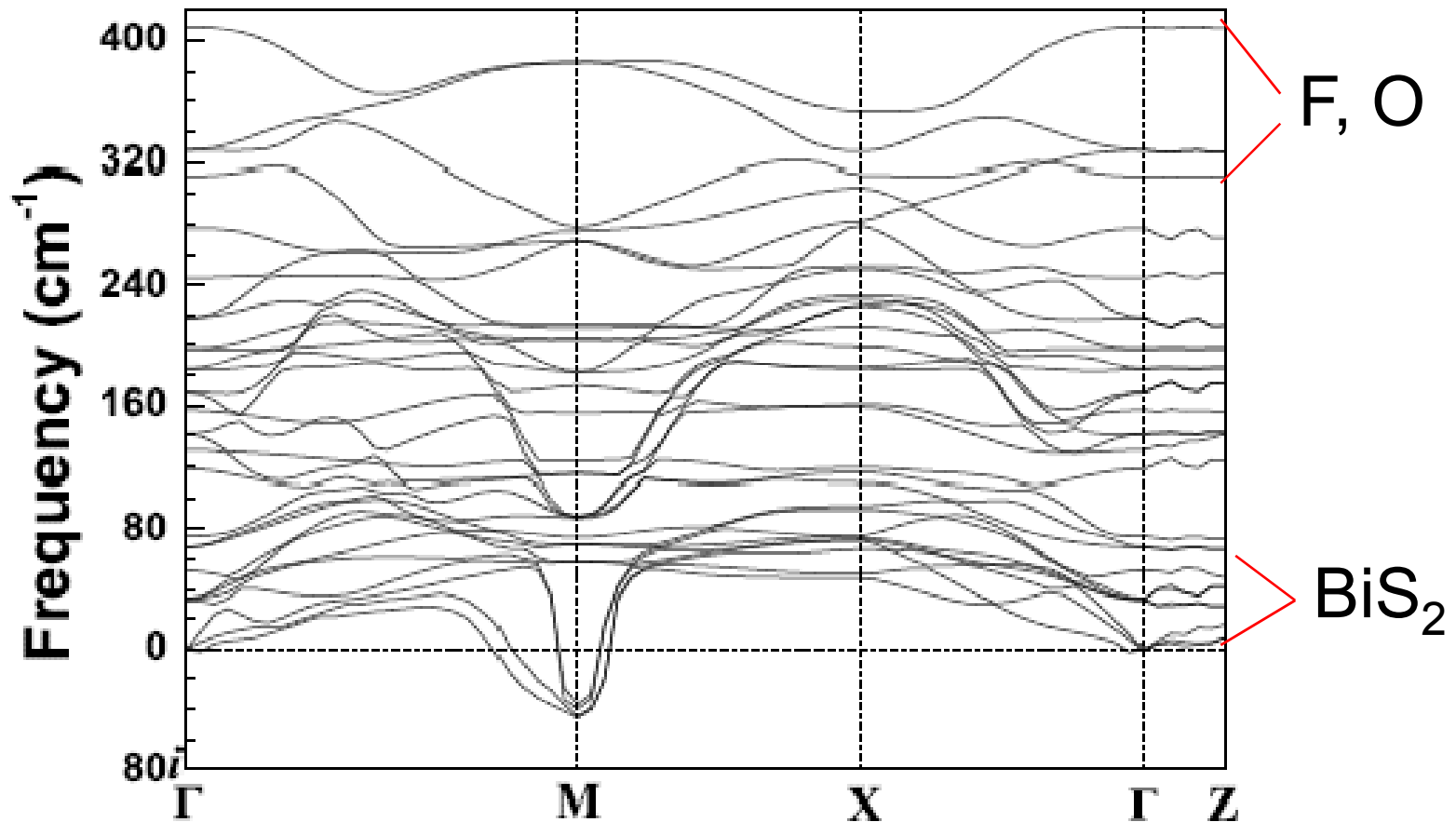
Frozen phonon calculation
Nesting→CDW?
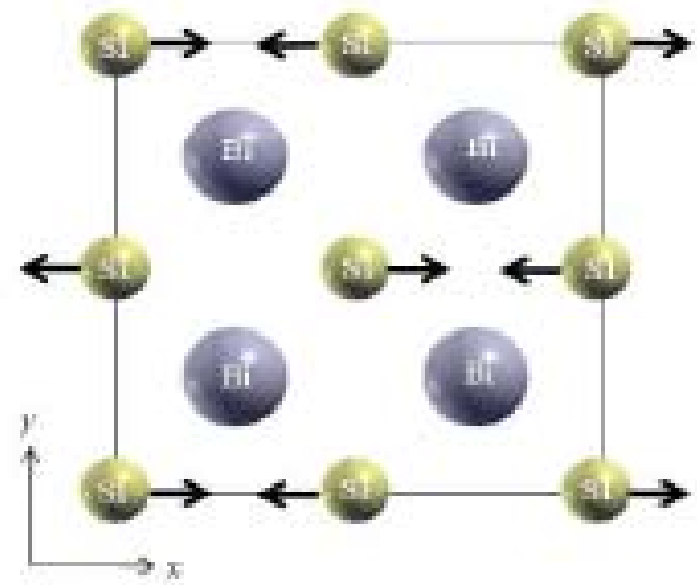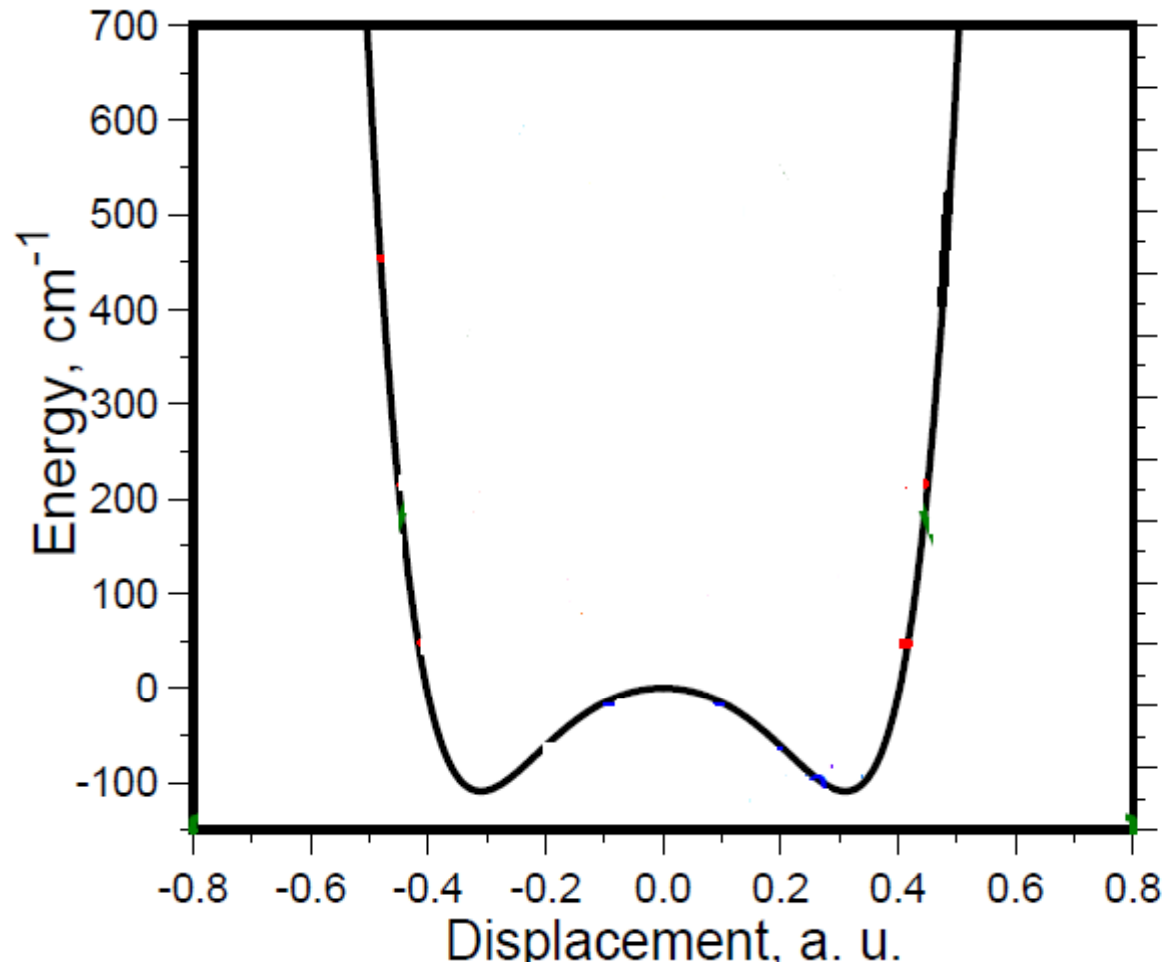
2套程序都得到了
double well

anharmonic problem

非谐的贡献

$$\gamma = \frac{1}{N} \sum_{kk',n} \frac{|\langle n|M_{kk'}|0\rangle|^2}{(E_n - E_0)}$$
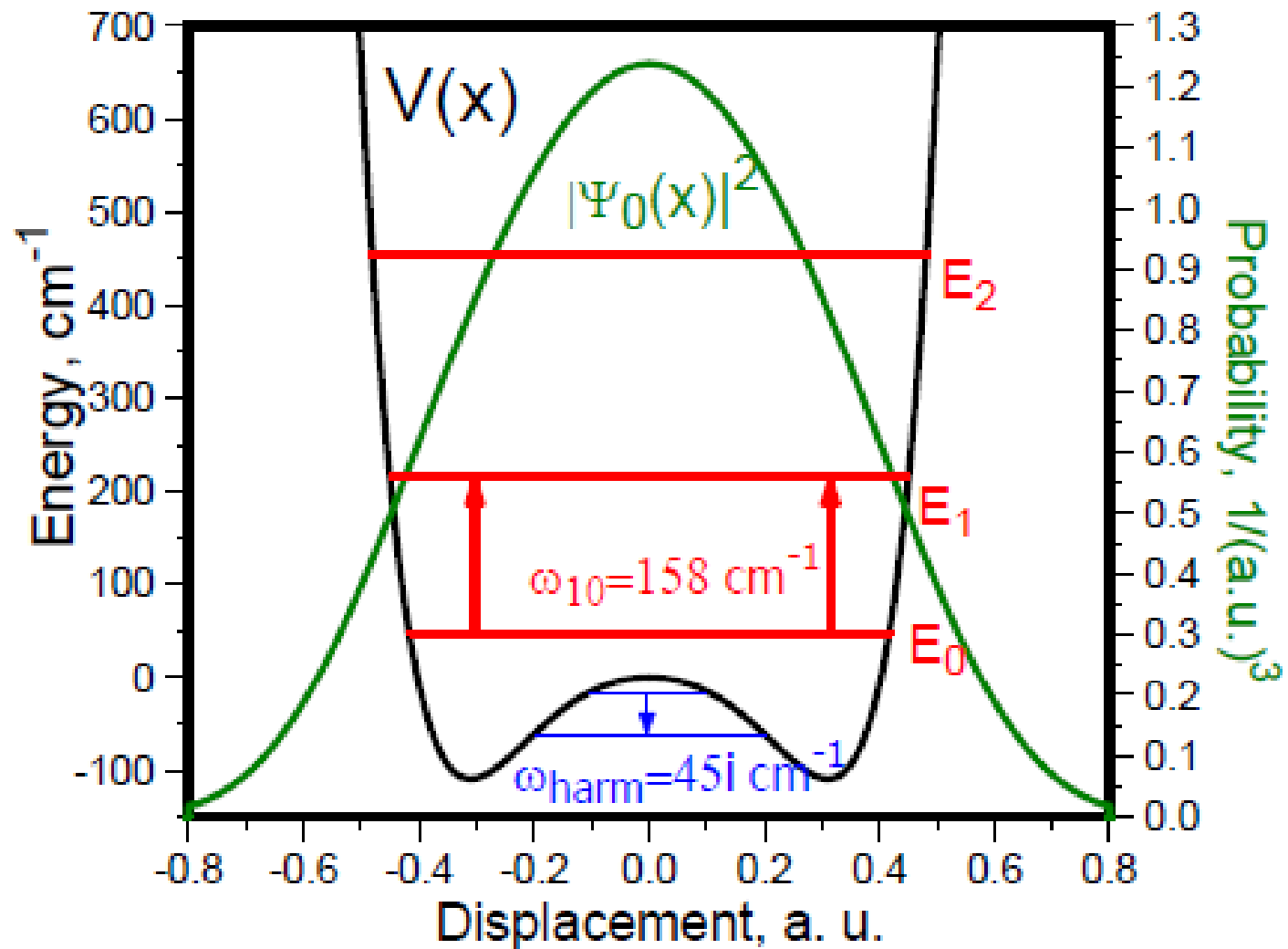
$|0\rangle$ 是基态, $|n\rangle$ 是激发态

在谐波近视下 $E_n - E_0 = \frac{1}{N} n \cdot \eta_q$, η_q 是声子能量

在非谐下 E_n 就不是 evenly spaced

Hui, Allen (1974)

electron-phonon interaction

- Four anharmonic modes

$$\lambda_{total} = 0.85$$

McMillan formula for T_c:

$$T_c = \frac{\Theta_D}{1.45} \exp\left[\frac{-1.04(1+\lambda)}{\lambda(1-0.62\mu^*)-\mu^*}\right]$$

Coulomb parameter $\mu^* = 0.1$

$\Theta_D = 260K$

calculated $T_c = 11.3K$

拓扑超导

Fu and Berg (PRL 2010)判据: **odd-parity pairing symmetry** and its Fermi surface encloses an odd number of time reversal invariant moments

已知的拓扑+超导的材料都是*s/p*电子体系

对于实际的材料体系 电声子耦合可能导致非常规超导吗?

BCS with General Pairing Symmetry

BCS gap equation

$$\Delta(\mathbf{k}) = -\sum_{\mathbf{k}'} W(\mathbf{k}\mathbf{k}')\Delta(\mathbf{k}')\tanh\left(\frac{\epsilon_{\mathbf{k}'}}{2T_c}\right)/2\epsilon_{\mathbf{k}'}$$

对于电声子耦合:

$$W(\mathbf{k}j\mathbf{k}+\mathbf{q}j') = |\langle\psi_{\mathbf{k}j}|\delta^{\mathbf{q}\nu}V_{eff}|\psi_{\mathbf{k}+\mathbf{q}j'}\rangle|^2$$

线性响应密度泛函

$$V_{ext} = \sum_{R,t} \frac{Ze^2}{|r-R-t_R|}$$

$$\delta V_{eff} = \delta V_{ext} + \int e^2 \frac{\delta \rho}{|r-r'|} + \int \frac{dV_{xc}}{d\rho}\, \delta\rho$$

$$\delta^2 = \int V_{eff}\, \delta\rho_{kj}\, \psi_{kj} + \int \delta V_{eff}\, \psi_{kj} = 0$$

$$\delta\rho = \sum_{kj} f_{kj}\, \delta\psi_{kj}\, \psi_{kj} + h.c.$$

Orthonormalize polynomials at a given energy surface (such, e.g., as spherical harmonics in case of a sphere)

$$\frac{1}{N(\varepsilon)} \sum_{\mathbf{k}} \eta_a(\mathbf{k})\eta_b(\mathbf{k})\delta(\epsilon_{\mathbf{k}} - \varepsilon) = \delta_{ab}$$

Expanding superconducting energy gap and pairing interaction

$$\Delta(\mathbf{k}) = \sum_{\alpha} \Delta_a(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k}) \qquad \Delta_a(\varepsilon) = \frac{1}{N(\varepsilon)} \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}} - \varepsilon)\Delta(\mathbf{k})\eta_b^*(\mathbf{k})$$

$$W(\mathbf{k}\mathbf{k}') = \sum_{\alpha\beta} W_{ab}(\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}'})\eta_a(\mathbf{k})\eta_b(\mathbf{k}')$$

$$W_{ab}(\varepsilon\varepsilon') = \frac{1}{N(\varepsilon)N(\varepsilon')} \sum_{\mathbf{k}\mathbf{k}'} \delta(\epsilon_{\mathbf{k}} - \varepsilon)\eta_a^*(\mathbf{k})W(\mathbf{k}\mathbf{k}')\eta_b(\mathbf{k}')\delta(\epsilon_{\mathbf{k}'} - \varepsilon')$$

The gap equation becomes

$$\Delta_a(\varepsilon) = -\int d\varepsilon' \sum_{b} W_{ab}(\varepsilon\varepsilon')\Delta_b(\varepsilon')N(\varepsilon')\tanh\left(\frac{\varepsilon'}{2T_c}\right)/2\varepsilon'$$

pairing occurs for the electrons within a thin layer near E_f

$$\Delta_a(\varepsilon) = \begin{cases} \Delta_a & \text{for } -\omega_D < \varepsilon < +\omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$W_a(\varepsilon\varepsilon') = \begin{cases} W_a & \text{for } -\omega_D < \varepsilon < +\omega_D \\ 0 & \text{otherwise} \end{cases}$$

This reduces the gap equation to (integral is extended over Debye frequency range)

$$\Delta_a = -N(0) \sum_b W_{ab}\Delta_b \int_{-\omega_D}^{+\omega_D} d\varepsilon' \frac{1}{2\varepsilon'} \tanh\left(\frac{\varepsilon'}{2T_c}\right)$$

Assuming crystal symmetry makes $W_{ab} - W_a\delta_{ab}$ and evaluating the integral gives

$$T_c = 1.134\omega_D e^{-1/\lambda_a} \qquad\qquad \lambda_a = -N(0)W_a$$

where the average electron-phonon coupling in a given a channel is given by the Fermi surface average of the electron-phonon coupling

$$W_a = \frac{1}{N(0)N(0)} \sum_{kk'} \delta(\epsilon_k)\eta_a(k)W(kk')\eta_a(k')\delta(\epsilon_{k'})$$

Finally, the superconducting state with largest λ_a will be realized.

为何实际材料电声子耦合总是s-wave like?

电声子耦合往往是实空间局域的 $W(\mathbf{k}, \mathbf{k}')$ 基本与k无关

$$\lambda_a = -\frac{1}{N(0)} \sum_{\mathbf{k}\mathbf{k}'} \delta(\epsilon_{\mathbf{k}}) \eta_a(\mathbf{k}) W(\mathbf{k}\mathbf{k}') \eta_a(\mathbf{k}') \delta(\epsilon_{\mathbf{k}'})$$

In the extreme case $W(\mathbf{k}, \mathbf{k}') = W_0$ we obtain:

$$\lambda_a = -W_0 N(0) \delta_{a=s-wave}$$

所以只有s-wave!

另外一个极限：电声子耦合在**k**空间局域

$$W(\mathbf{k}, \mathbf{k}') = W_1 \delta(\mathbf{k} - \mathbf{k}' - \mathbf{q}_0) = W_1 \sum_a \eta_a(\mathbf{k})\eta_a(\mathbf{k}' + \mathbf{q}_0)$$

$$\lambda_a = -W_1 \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k})\eta_a(\mathbf{k} + \mathbf{q}_0) = -W_1 N(0) O_a(\mathbf{q}_0)$$

where the overlap matrix between two polynomials shows up

$$O_a(\mathbf{q}_0) = \frac{1}{N(0)} \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}})\eta_a(\mathbf{k})\eta_a(\mathbf{k} + \mathbf{q}_0)$$

It would be less than unity for non-zero angular momentum index a unless

$$\mathbf{q}_0 \Rightarrow 0$$

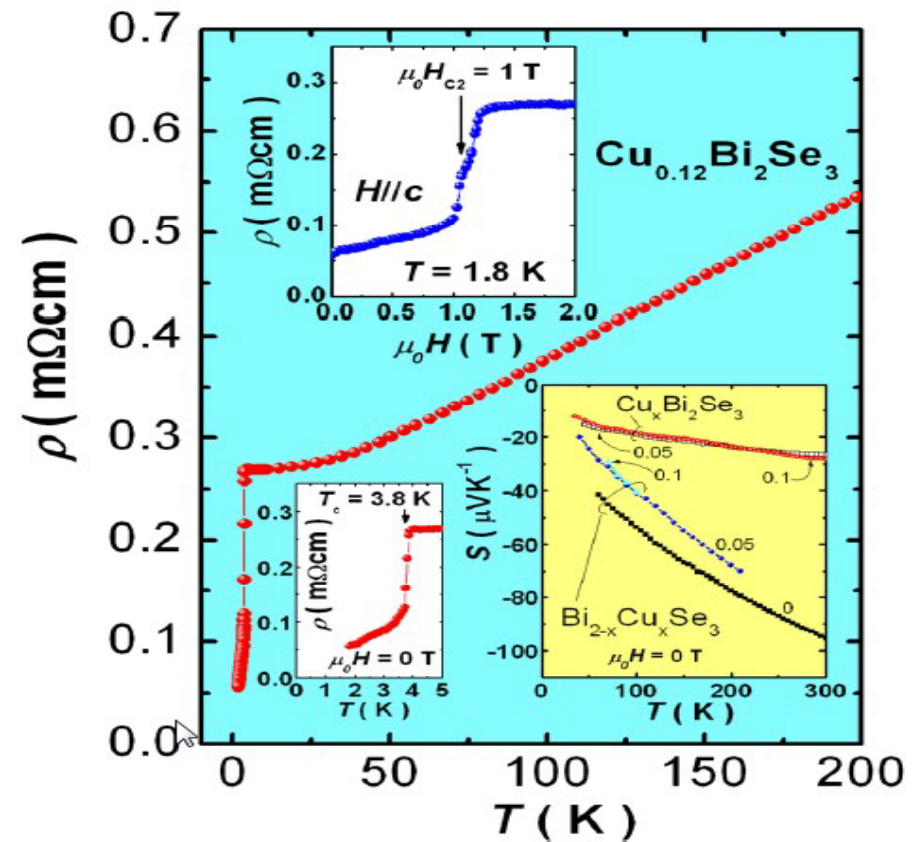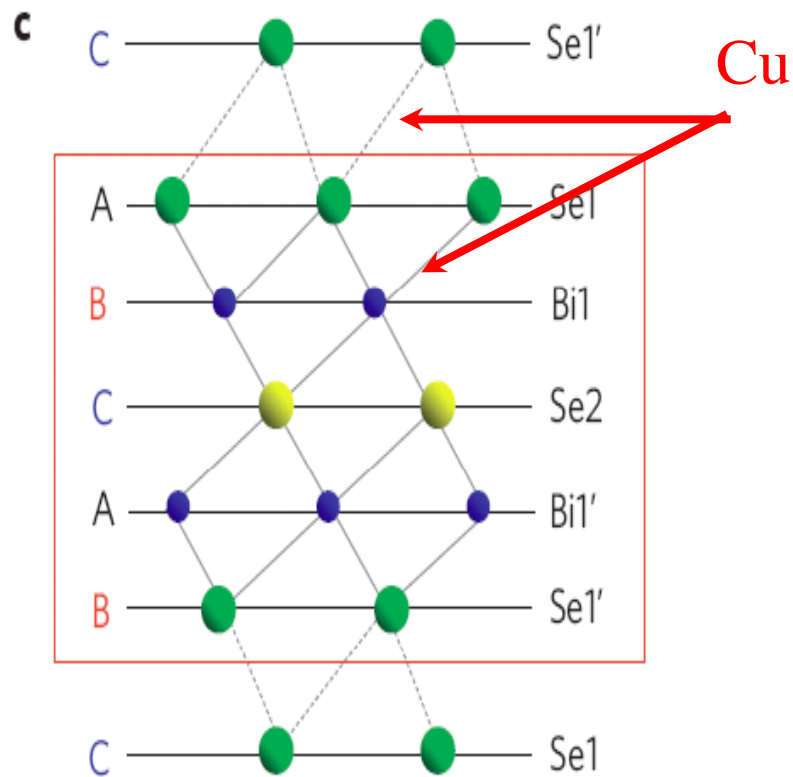$$\lim_{q_0 \to 0} O_a(\mathbf{q}_0) = 1$$

实际材料电声子耦合只能s-wave吗?

要找电声子耦合在倒空间局域

需要

LDA+SO → Bi_2Se_3!

Superconductivity in $Cu_xBi_2Se_3$

Hor et al, PRL 104, 057001 (2010)

Tc up to 3.8K

Symmetry of Pairing State

- Point-contact spectroscopy: odd-parity pairing in $Cu_xBi_2Se_3$ (Sasaki et.al, PRL 2011) via observed zero-bias conductance

PHYSICAL REVIEW LETTERS

### Topological Superconductivity in $Cu_xBi_2Se_3$

Satoshi Sasaki,[1] M. Kriener,[1] Kouji Segawa,[1] Keiji Yada,[2] Yukio Tanaka,[2] Masatoshi Sato,[3] and Yoichi Ando[1,*]

[1]Institute of Scientific and Industrial Research, Osaka University, Ibaraki, Osaka 567-0047, Japan
[2]Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan
[3]Instituite for Solid State Physics, University of Tokyo, Chiba 277-8581, Japan
(Received 2 August 2011; published 14 November 2011)
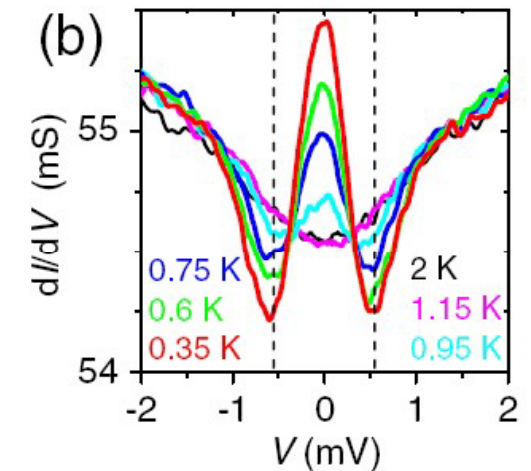
- Scanning-tunneling spectroscopy: fully gapped state in $Cu_xBi_2Se_3$

PHYSICAL REVIEW LETTERS

Experimental Evidence for s-Wave Pairing Symmetry in Superconducting $Cu_xBi_2Se_3$ Single Crystals Using a Scanning Tunneling Microscope

Niv Levy,[1,2] Tong Zhang,[1,2] Jeonghoon Ha,[1,2,3] Fred Sharifi,[1] A. Alec Talin,[1] Young Kuk,[3] and Joseph A. Stroscio[1,*]

[1]Center for Nanoscale Science and Technology, NIST, Gaithersburg, Maryland 20899, USA
[2]Maryland NanoCenter, University of Maryland, College Park, Maryland 20742, USA
[3]Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea
(Received 1 November 2012; published 12 March 2013)
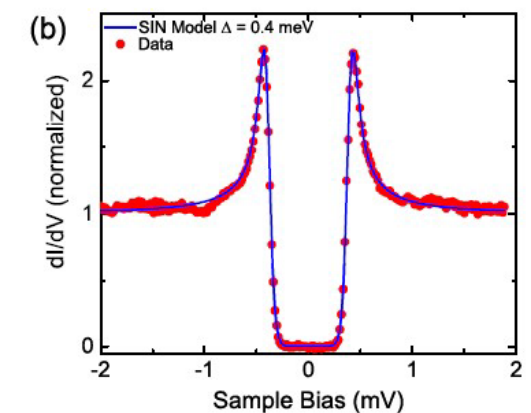
Pressure-Induced Unconventional Superconducting Phase in the Topological Insulator Bi_2Se_3

Kevin Kirshenbaum,[1] P. S. Syers,[1] A. P. Hope,[1] N. P. Butch,[2] J. R. Jeffries,[2] S. T. Weir,[2] J. J. Hamlin,[3]
M. B. Maple,[3] Y. K. Vohra,[4] and J. Paglione[1,*]

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College Park, Maryland 20742, USA*
[2]*Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, Livermore, California 94550, USA*
[3]*Department of Physics, University of California, San Diego, La Jolla, California 92093, USA*
[4]*Department of Physics, University of Alabama at Birmingham, Birmingham, Alabama 35294, USA*
(Received 26 February 2013; published 20 August 2013)

Simultaneous low-temperature electrical resistivity and Hall effect measurements were performed
on single-crystalline Bi_2Se_3 under applied pressures up to 50 GPa. As a function of pressure, super-
conductivity is observed to onset above 11 GPa with a transition temperature T_c and upper critical field
H_{c2} that both increase with pressure up to 30 GPa, where they reach maximum values of 7 K and 4 T,
respectively. Upon further pressure increase, T_c remains anomalously constant up to the highest achieved
pressure. Conversely, the carrier concentration increases continuously with pressure, including a tenfold
increase over the pressure range where T_c remains constant. Together with a quasilinear temperature
dependence of H_{c2} that exceeds the orbital and Pauli limits, the anomalously stagnant pressure
dependence of T_c points to an unconventional pressure-induced pairing state in Bi_2Se_3 that is unique
among the superconducting topological insulators.

Phonon Spectrum for Bi_2Se_3
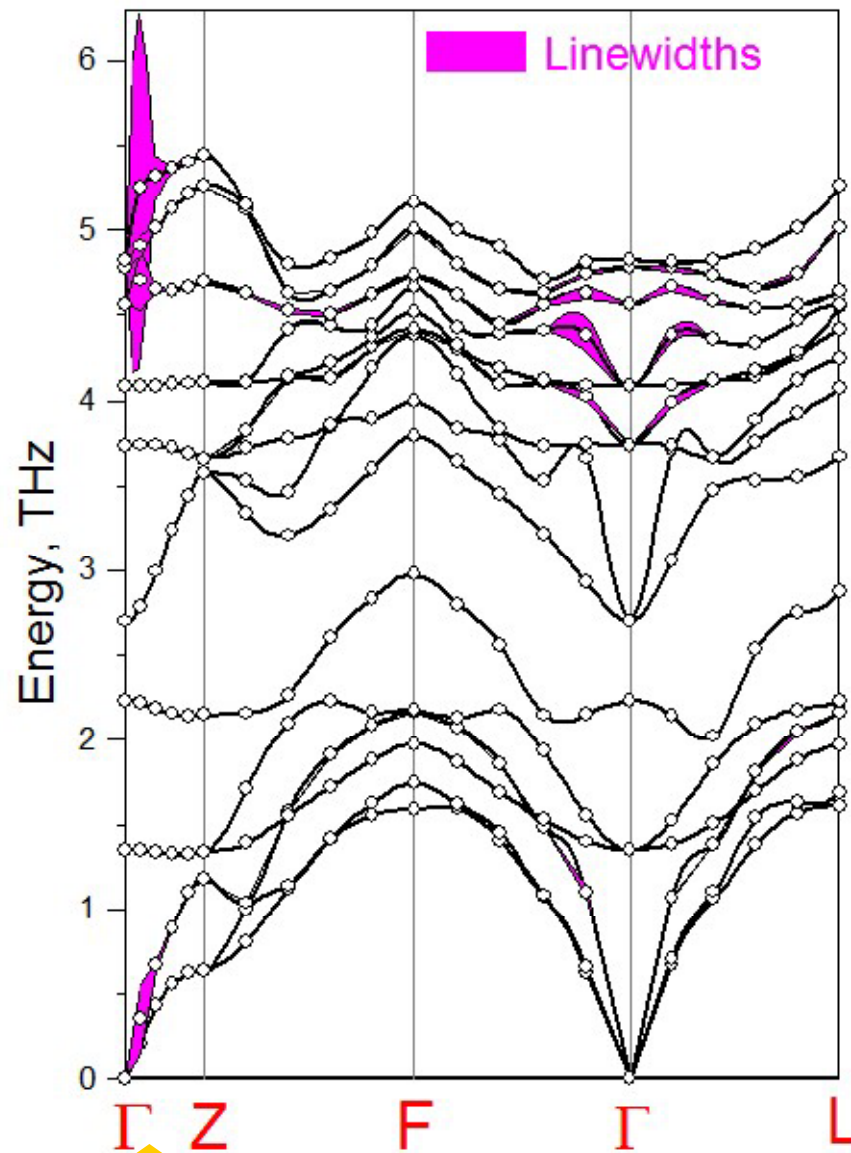
Density functional linear response approach

LDA+SO

Prior VASP calculations in
Appl. Phys. Lett. **100**, 082109 (2012)
reported some instabilities which
we did not confirm
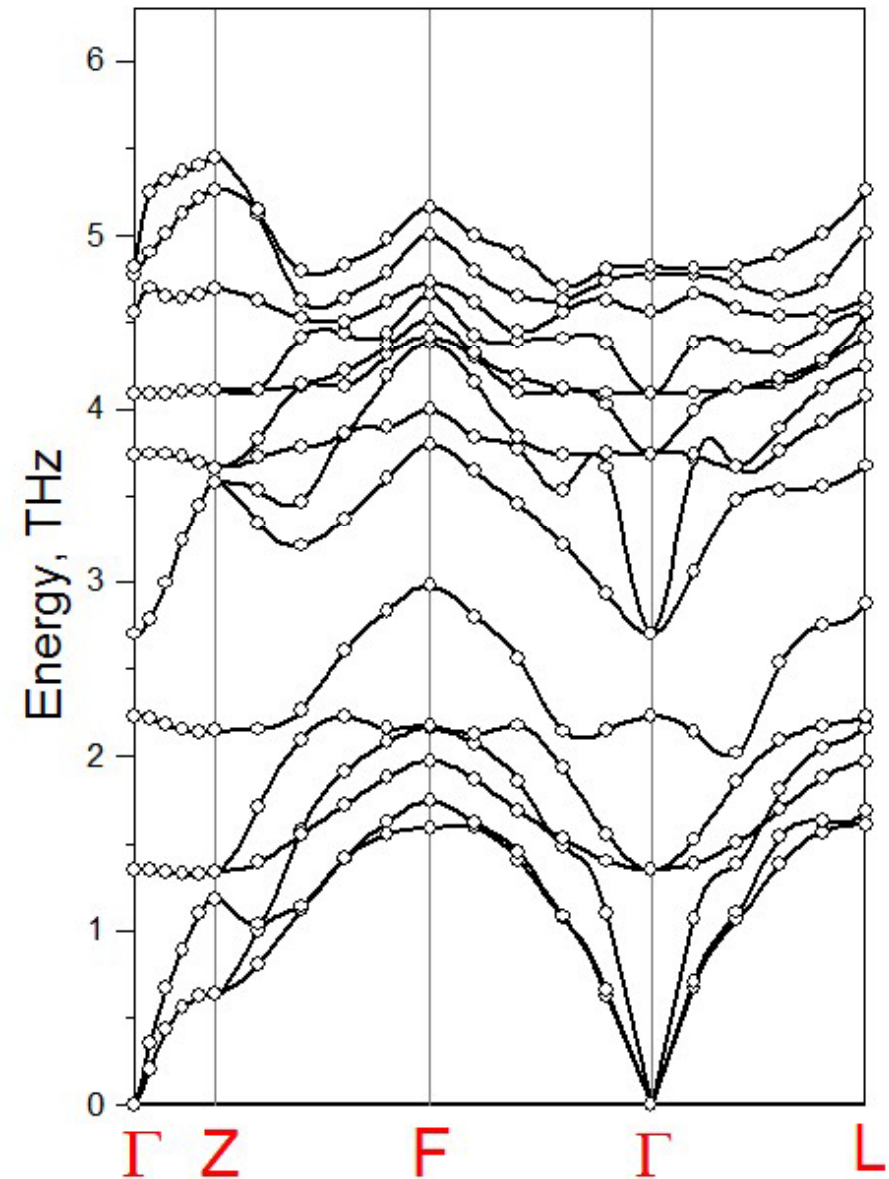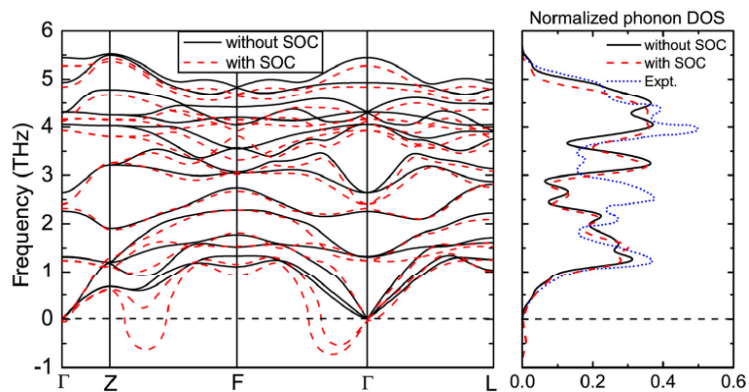
Calculated phonon linewidths in doped Bi_2Se_3

Electron-phonon coupling is enormous at $q_0 \sim (0,0,0.04)2\pi/c$

Nesting Function

$$\chi(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k+q}})$$

Doping 0.16 el.
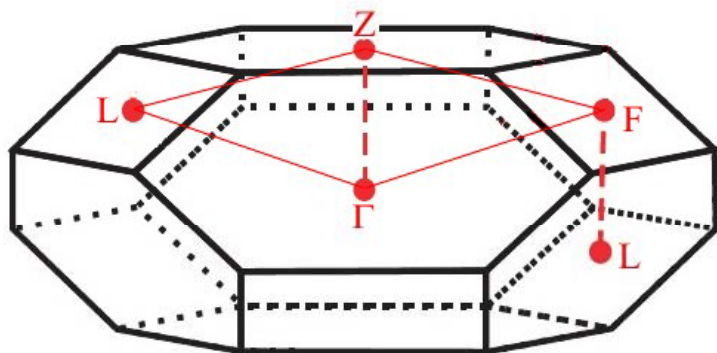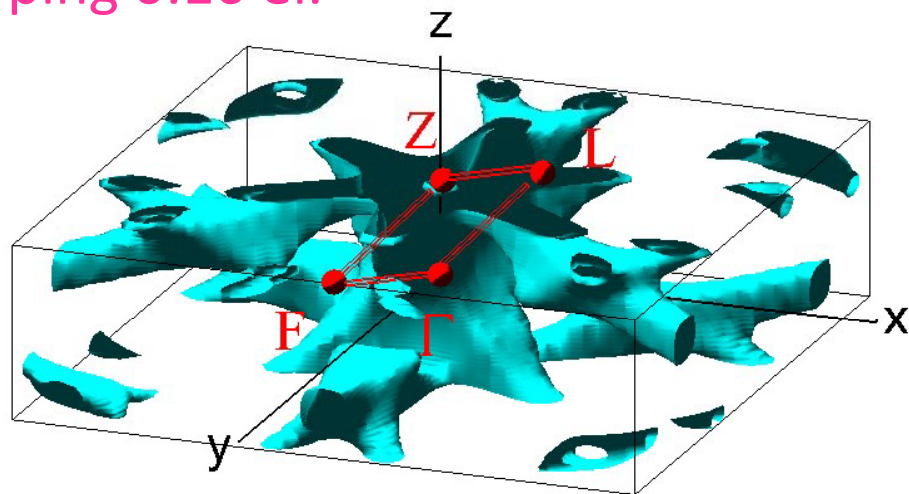
Basal area is rhombus

$\lim_{\omega \to 0} \mathrm{Im}\chi(q,\omega)/\omega$, a.u.

$L(\pi 0 0)$

$\Gamma(000)$

$F(\pi\pi 0)$

$Z(\pi\pi\pi)$

Shows a strong ridge-like structure along ΓZ line at small q's due to quasi 2D features of the Fermi surface.

Calculated electron-phonon matrix elements

Define average electron-phonon matrix element (squared) as follows

$$\langle W(\mathbf{q}) \rangle = \frac{\sum_{\mathbf{k}} W(\mathbf{k}, \mathbf{k}+\mathbf{q}) \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}})}{\sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}})}$$
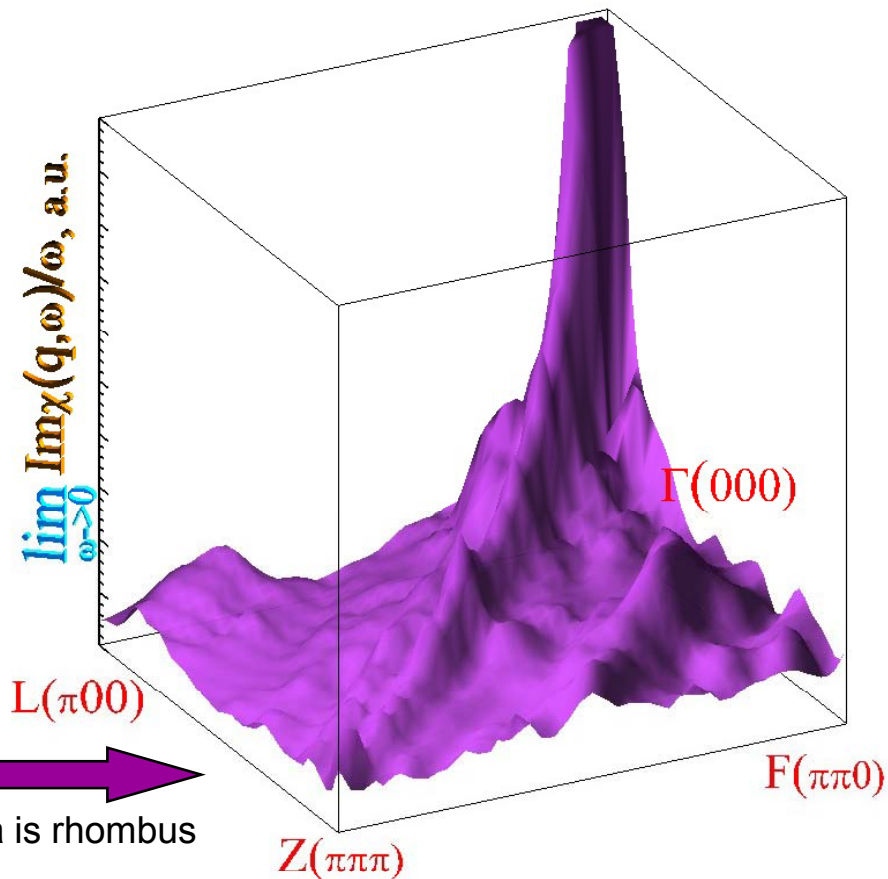
This eliminates all nesting-like features of $\chi(\mathbf{q}) = \sum_{\mathbf{k}} \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}+\mathbf{q}})$
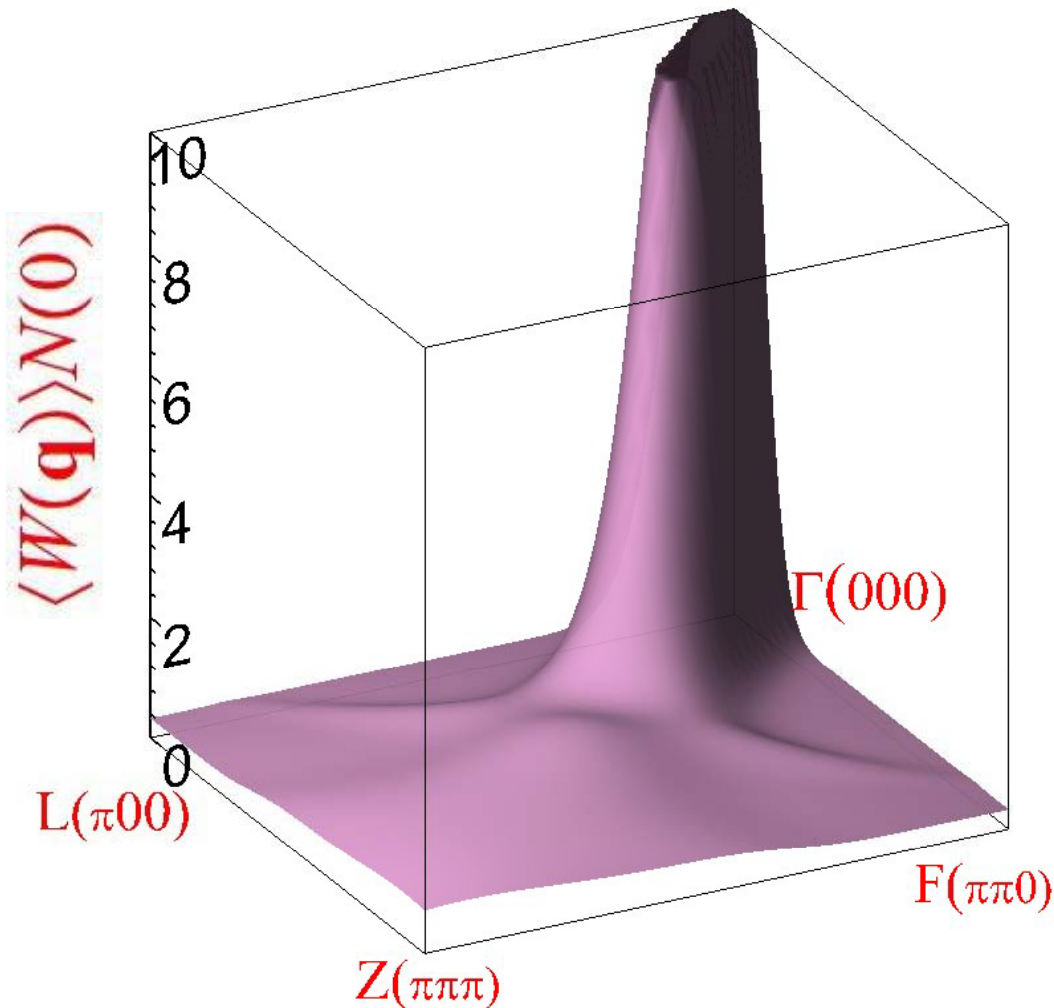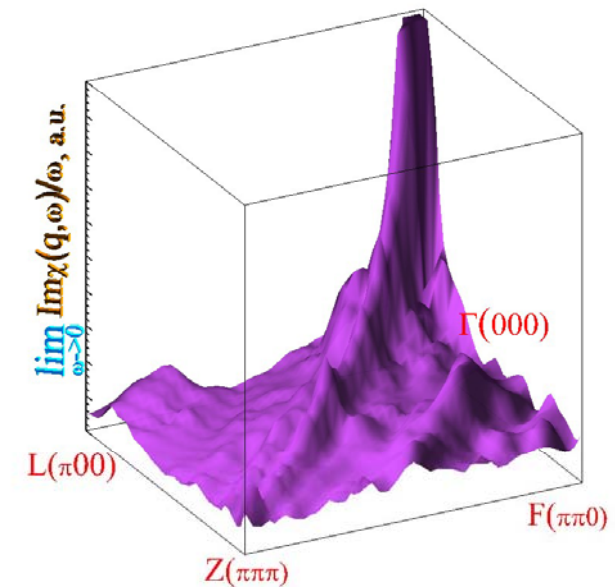

Still $\langle W(q) \rangle$ shows almost singular behavior for $q_0 \sim (0,0,0.04) 2\pi/c$

Calculated deformation potentials at long wavelengths

自旋轨道耦合

中心反演对称

打破中心反演对称

强的自旋轨道耦合在此很重要

Basis function for hexagonal lattices

Stability of anisotropic superconducting phases in UPt₃

W. Putikka and Robert Joynt

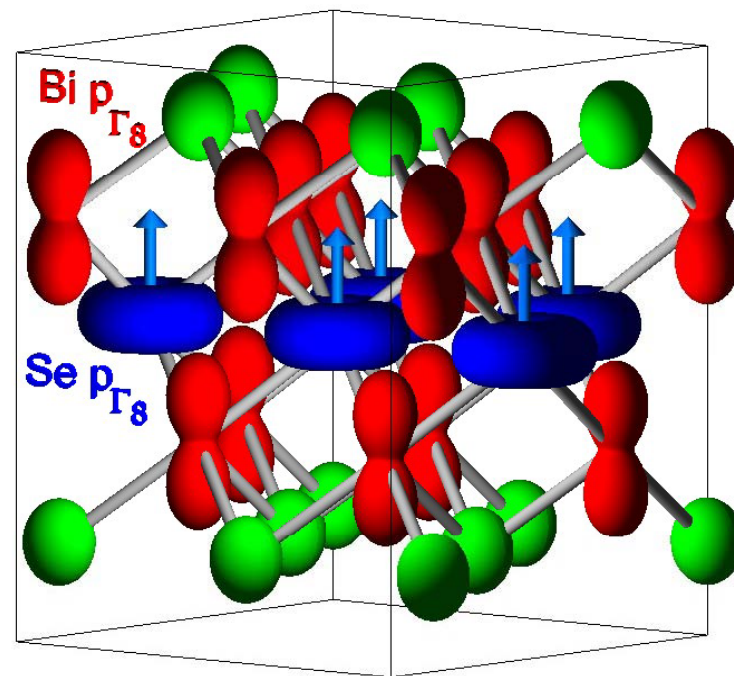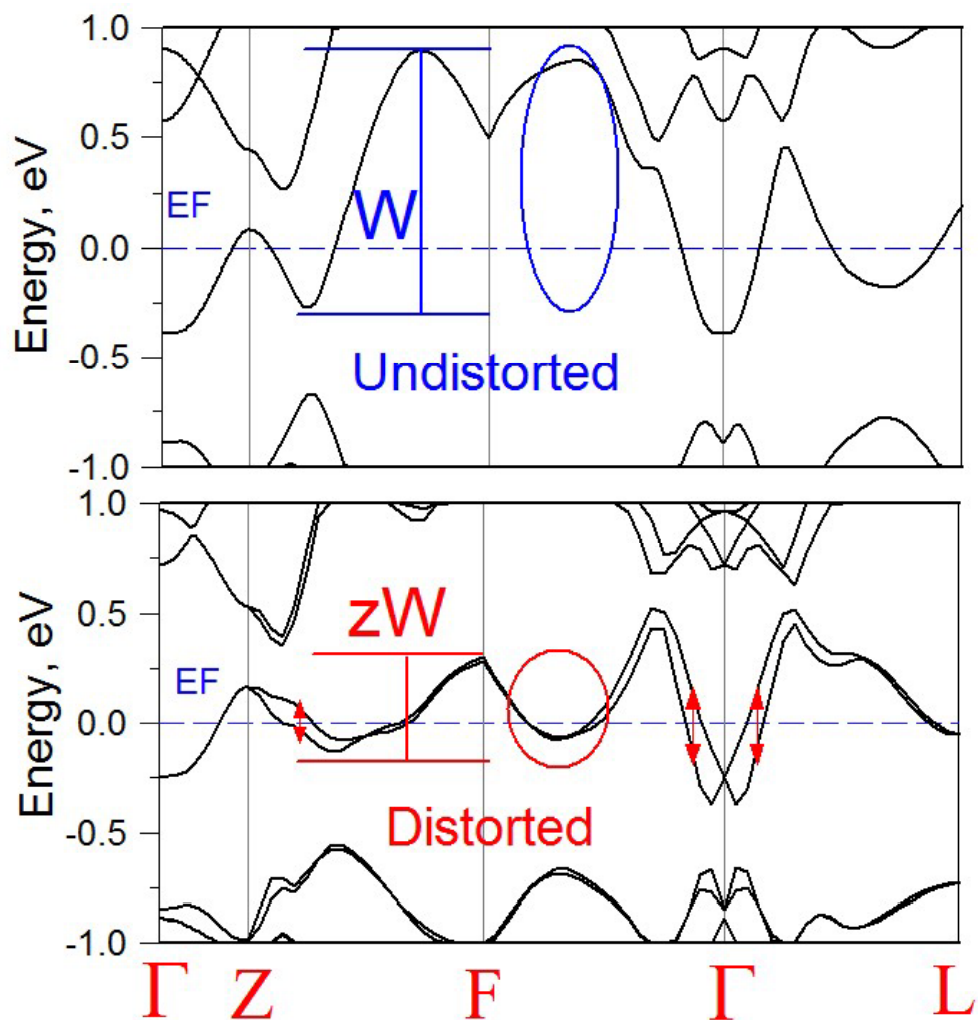*Physics Department, 1150 University Avenue, University of Wisconsin-Madison, Madison, Wisconsin 53706*
(Received 26 October 1987)

TABLE I. Basis functions for the various representations of D_6. The interaction can be decomposed into sums of products of these functions.

Representation	Function
A_{1g}	$\phi_k = \dfrac{1}{\sqrt{3}}\cos\left(\dfrac{ck_z}{2}\right)\left[\cos\left(\dfrac{\sqrt{3}ak_y}{3}\right)+\cos\left(\dfrac{ak_x}{2}+\dfrac{\sqrt{3}ak_y}{6}\right)+\cos\left(\dfrac{ak_x}{2}-\dfrac{\sqrt{3}ak_y}{6}\right)\right]$
B_{1g}	$\psi_k = \dfrac{1}{\sqrt{3}}\sin\left(\dfrac{ck_z}{2}\right)\left[\sin\left(\dfrac{\sqrt{3}ak_y}{3}\right)+\sin\left(\dfrac{ak_x}{2}-\dfrac{\sqrt{3}ak_y}{6}\right)-\sin\left(\dfrac{ak_x}{2}+\dfrac{\sqrt{3}ak_y}{6}\right)\right]$
E_{1g}	$\theta_k = \dfrac{1}{\sqrt{2}}\sin\left(\dfrac{ck_z}{2}\right)\left[\sin\left(\dfrac{ak_x}{2}+\dfrac{\sqrt{3}ak_y}{6}\right)+\sin\left(\dfrac{ak_x}{2}-\dfrac{\sqrt{3}ak_y}{6}\right)\right]$
	$\xi_k = \dfrac{1}{\sqrt{6}}\sin\left(\dfrac{ck_z}{2}\right)\left[2\sin\left(\dfrac{\sqrt{3}ak_y}{3}\right)+\sin\left(\dfrac{ak_x}{2}+\dfrac{\sqrt{3}ak_y}{6}\right)-\sin\left(\dfrac{ak_x}{2}-\dfrac{\sqrt{3}ak_y}{6}\right)\right]$

Large Electron-Phonon Interaction in $Cu_xBi_2Se_3$
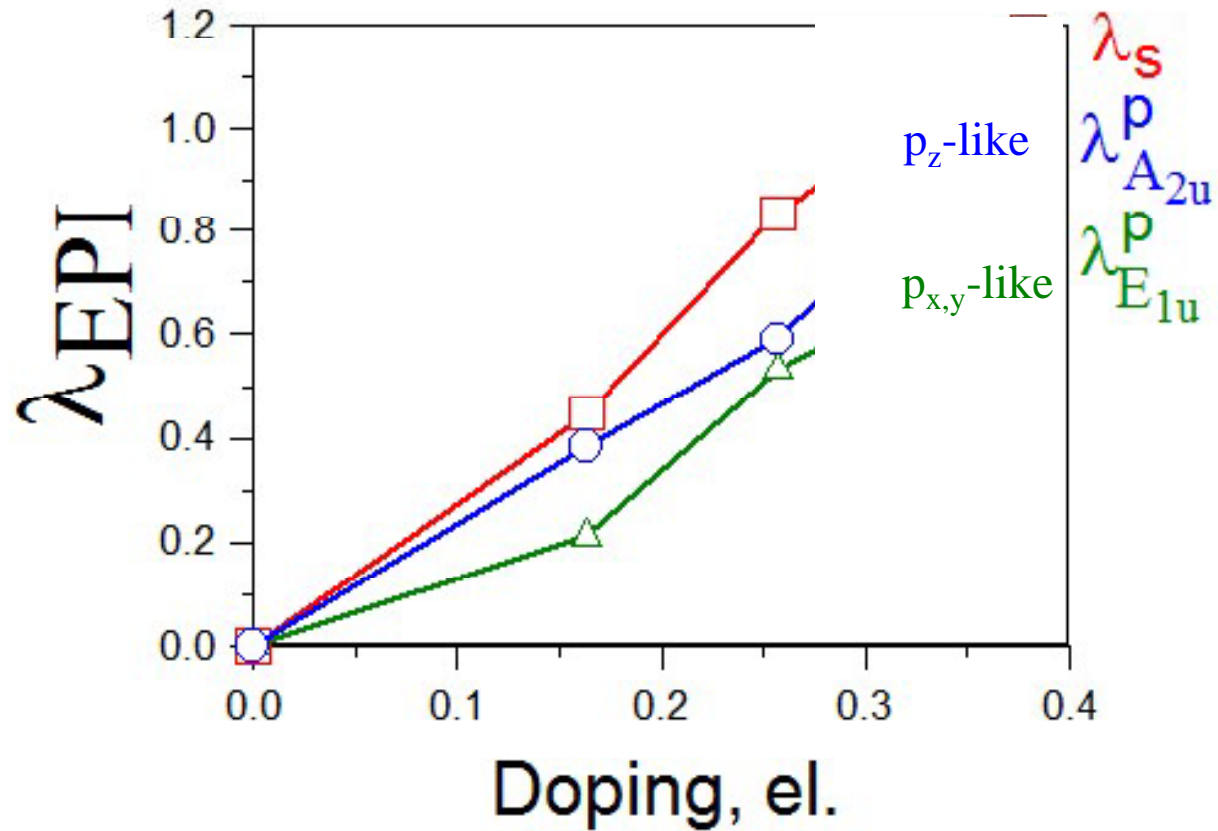
S-wave shows largest coupling. P-wave is also very large!

Coulomb pseudopotential μ^* 压制 s-wave

$$T_c^{(l)} = 1.14 \omega_D \exp\left(-\frac{1}{\lambda_l^{eff}}\right)$$

$$\lambda_l^{eff} = \frac{\lambda_l - \mu_l^*}{1 + \lambda_{s-h}} \qquad \mu_l^* = \frac{\mu_l}{1 + \mu_l \ln \epsilon_F/\omega_D}$$

where μ_l is the Fermi surface average of the screened Coulomb interaction

$$\mu_l = \frac{1}{N(0)} \sum_{\mathbf{kk'}} \langle \mathbf{k} - \mathbf{k}|U|\mathbf{k}' - \mathbf{k}'\rangle \delta(\epsilon_{\mathbf{k}}) \delta(\epsilon_{\mathbf{k}'}) \eta_l(\mathbf{k}) \eta_l(\mathbf{k}')$$

Assuming Hubbard like on-site Coulomb repulsion

$$\langle \mathbf{k} - \mathbf{k}|U|\mathbf{k}' - \mathbf{k}'\rangle = U$$

μ^* will affect s-wave pairing only

$$\mu_{l=s} = UN(0) \qquad \mu_{l>s} = 0$$

Estimates with μ^*

For doped Bi_2Se_3 we obtain the estimate

$$\omega_D \sim 100K$$

$$\varepsilon_F \sim 2000 - 5000K$$

and

$$\mu_s^* = 0.1$$

For doping by 0.16 electrons we get the estimates

S-wave

$$\lambda_s^{EPI} = 0.45$$

$$\mu_s^* = 0.1$$

P-wave

$$\lambda_{A_{2u}}^{EPI} = 0.39$$

$$\mu_{l>s}^* \sim 0$$

Effective coupling λ-μ^* for p-wave pairing channel wins!

Other Compounds

Bi_2Te_3

$TlBiTe_2$

Doped-SnTe

Conclusion

❑ Large electron-phonon coupling is found for $Cu_xBi_2Se_3$

❑ Not only s-wave but also p-wave pairing is found to be large due to strong anisotropy and quasi-2D Fermi surfaces. $\lambda_s \sim \lambda_p$

❑ Coulomb interaction and spin fluctuations will reduce λ_s and make $\lambda_p > \lambda_p$ therefore unconventional superconductivity may indeed be realized here.

❑ Discussed effects have nothing to do with topological aspect of the problem, may be found in other doped band insulators.

谢　　谢