Weyl Metal States and Surface Fermi Arcs in Iridates

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3D Topological Insulators

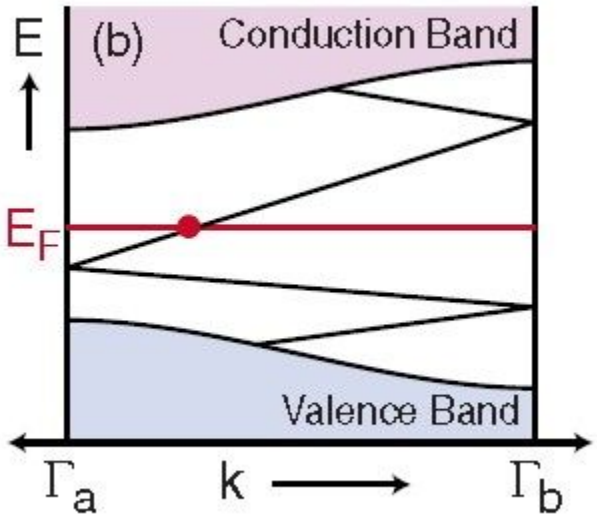
PHYSICS

A New Spin on the Insulating State

Charles L. Kane and Eugene J. Mele

Theory suggests a practical method for producing a novel insulating state of matter.

15 DECEMBER 2006 VOL 314 SCIENCE www.sciencemag.org



So far topological insulators with active p-electrons ($Bi_{1-x}Sb_x$, Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3) have been found experimentally.

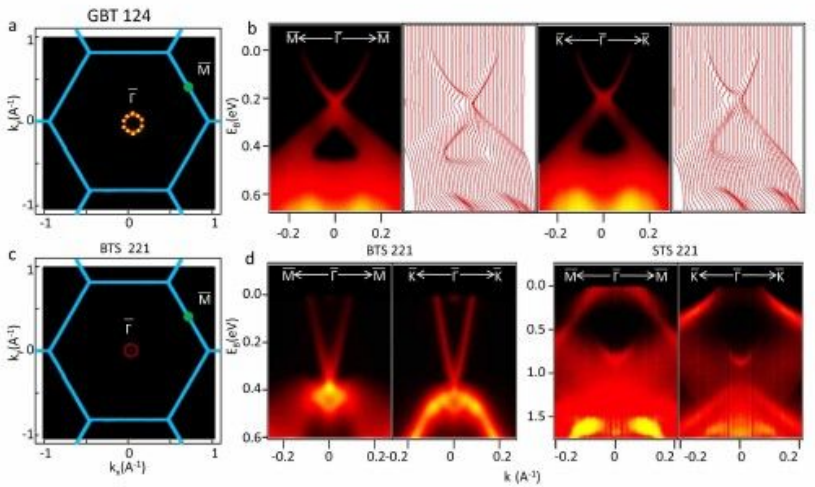
Letter

Nature Physics **5**, 398 - 402 (2009)
Published online: 10 May 2009 | doi:10.1038/nphys1274

Subject Categories: Condensed-matter physics | Materials physics

Observation of a large-gap topological-insulator class with a single Dirac cone on the surface

Y. Xia[1,2], D. Qian[1,3], D. Hsieh[1,2], L. Wray[1], A. Pal[1], H. Lin[4], A. Bansil[4], D. Grauer[5], Y. S. Hor[5], R. J. Cava[5] & M. Z. Hasan[1,2,6]



Coupled Spin Orbit and Hubbard Physics in 5d Iridates

5d electrons – interplay between spin-orbit, band structure and correlation effects

Iridates as frustrated magnets with exotic quantum ground states (*quantum spin liquids*) relevant for topological quantum computations. **$Na_4Ir_3O_8$ -** a candidate for a quantum spin liquid, (*Okamoto, et.al, PRL 2007*.)

Science

AAAS

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 5*d* 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.

Phys. Rev. Lett. 106, 136402 (2011) [4 pages]

Twisted Hubbard Model for Sr_2IrO_4: Magnetism and Possible High Temperature Superconductivity

Abstract | References | Citing Articles (5)

Download: PDF (130 kB) Export: BibTeX or EndNote (RIS)

Fa Wang and T. Senthil

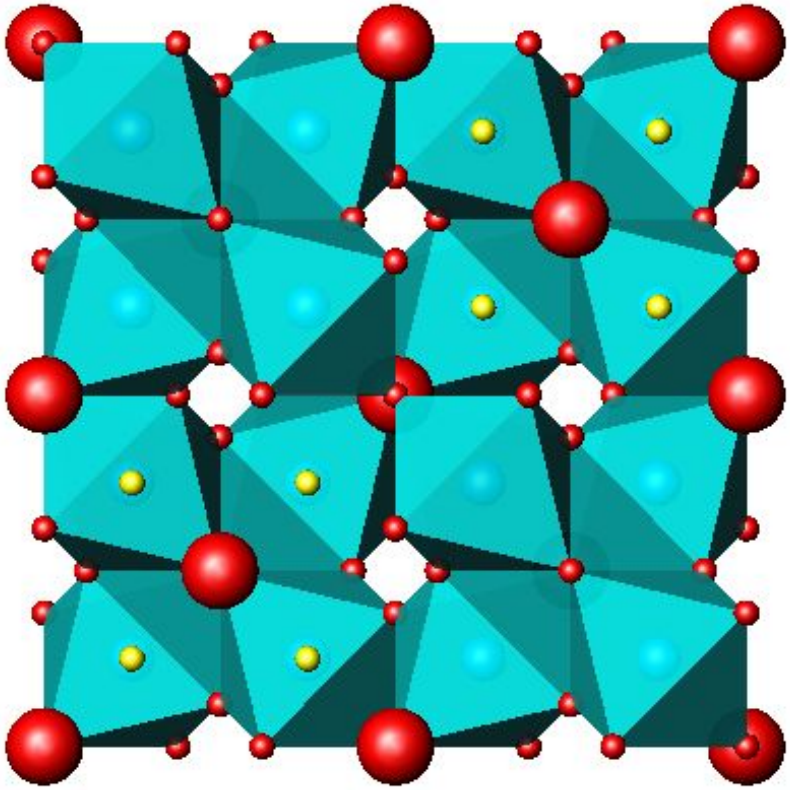
Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Pyrochlore Iridates as Novel Topological Insulators – a Proposal

Geometrically Frustrated Pyrochlore Lattice

$A_2Ir_2O_7$

where A is Yttrium or RE



ARTICLES
PUBLISHED ONLINE: 21 MARCH 2010 | DOI: 10.1038/NPHYS1606
nature physics

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

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

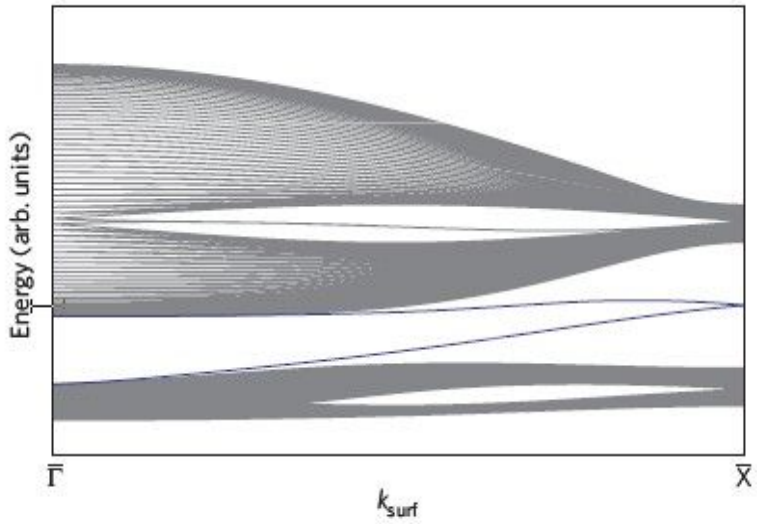


Figure 4 | Surface-state spectrum. The projected bulk spectrum (grey) and the surface spectrum (solid blue line) for a (010) surface are shown. The spectrum is plotted as a function of the dimensionless surface wavevector $k_{surf} \equiv (k_x, k_z)$ running from $\bar{\Gamma} = (0,0)$ to $\bar{X} = (0,2\pi)$. As it must be for a strong TBI, there are two more pairs of surface time-reversal-invariant momenta in the surface Brillouin zone with analogous surface-state spectra along the paths connecting these pairs in the k-space: $(0,0)$ and $(-\pi,\pi)$, and $(0,0)$ and (π,π).

Content

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- Band Topology, Weyl Semimetal States
- Surface States and Fermi Arcs
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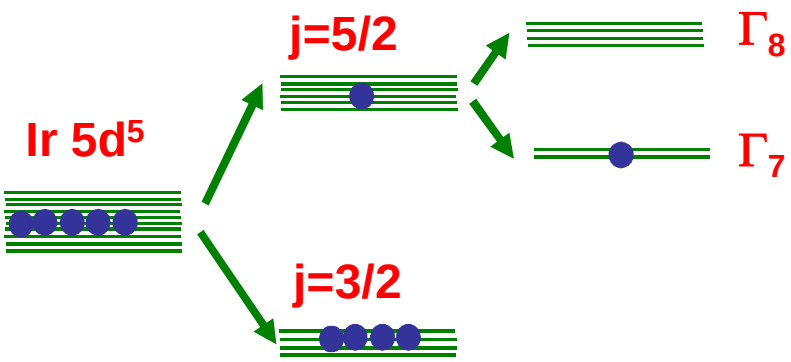
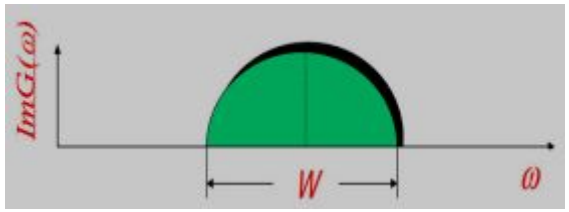
Electronic Structure Studies of $Y_2Ir_2O_7$ and Rare Earth Pyrochlore Iridates

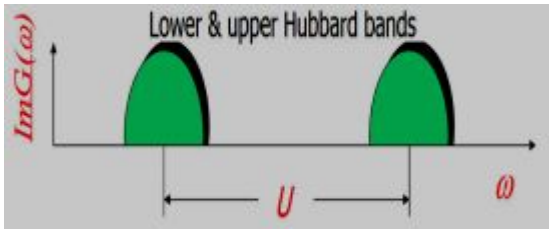
- LDA+U studies using full potential LMTO method.
  Ir 5d electrons: $0 < U < 4$ eV; Rare Earth 4f electrons: $U = 6$eV
- Spin Orbit Coupling
- Various Magnetic (Collinear and Non-Collinear) Configurations explored for frustrated pyrochlore lattice

Strong Spin Orbit Coupling in 5d orbitals



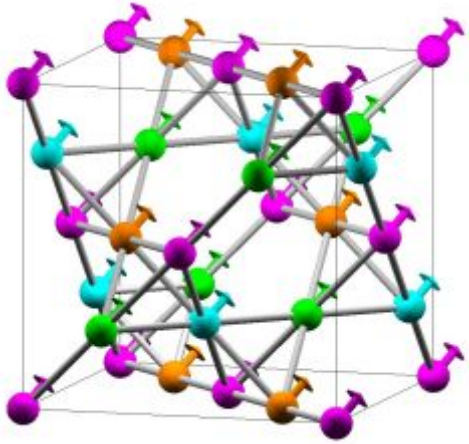
A small Hubbard U produces Mott insulating behavior for Γ_7 band at half feeling



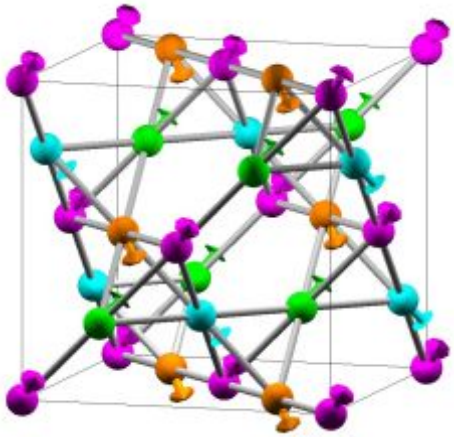


Studies of Magnetic Configurations in $Y_2Ir_2O_7$

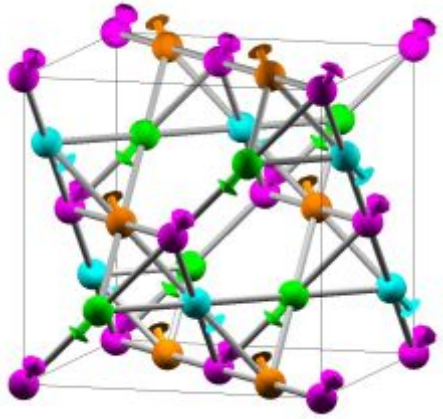
Collinear (111)



Non-Collinear 2-in/2-out



Non-Collinear All-in/out



Collinear (001)

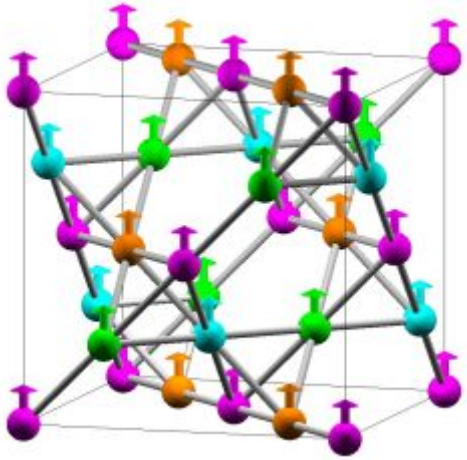


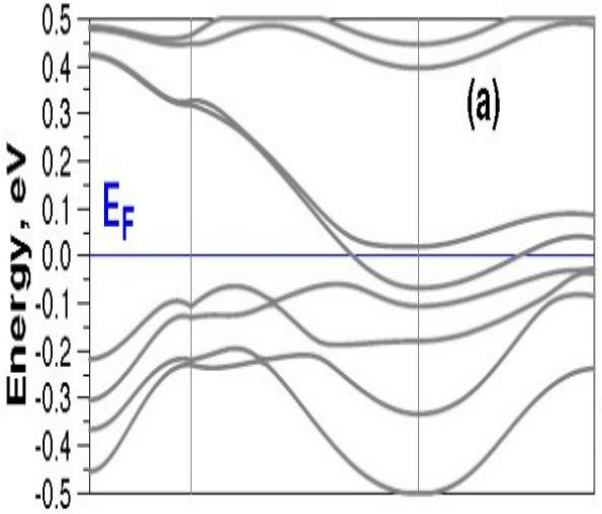
TABLE I: The spin $\langle S \rangle$ and orbital $\langle O \rangle$ moment (in μ_B), the total energy E_{tot} (in meV) as well as the band gap E_{gap}(in meV) for several selected magnetic configurations of $Y_2Ir_2O_7$.

Configuration:	(001)	(111)	2–in/2–out	all–in/out
$\langle S \rangle$	0.13	0.17	0.14	0.13
$\langle O \rangle$	0.13	0.13	0.15	0.17
E_{tot}(meV)	4.47	0.69	3.21	0.00
E_{gap}(meV)	0	0	0	30

Magnetic Non-Collinear All-In/Out Configuration has lowest energy!

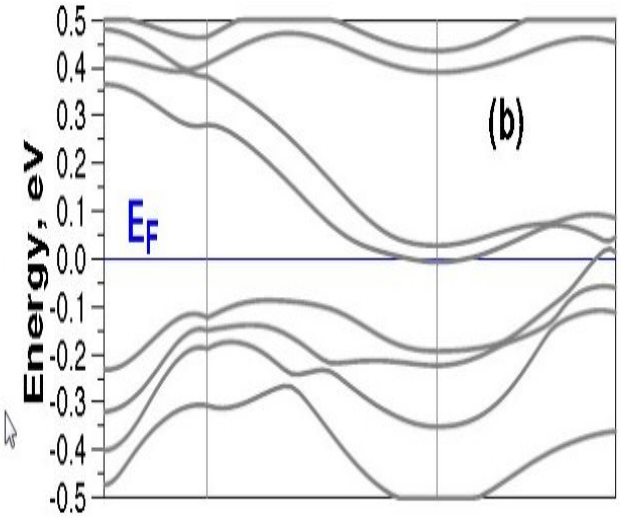
Electronic Structure as Function of Moments Orientations: LDA+U=1.5 eV

Collinear (001)



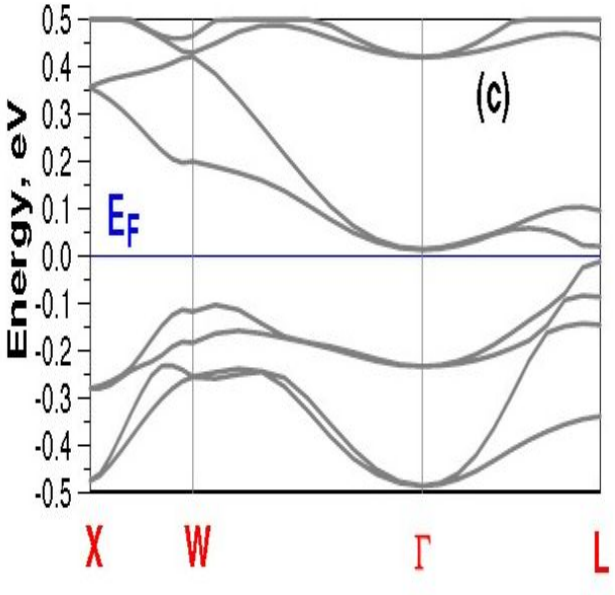
Large Fermi Surface
Normal Metal!

Collinear (111)



Small Fermi Surface
Bad Metal

Non-Collinear All-in/out



Looks Like Insulator!
(in fact depends on U)

Metallic behavior appears when moments are aligned collinearly, easy to switch with applied magnetic field – **Magnetic Field Induced Insulator to Metal Transition!**

Searching for Magnetic Topological Insulators

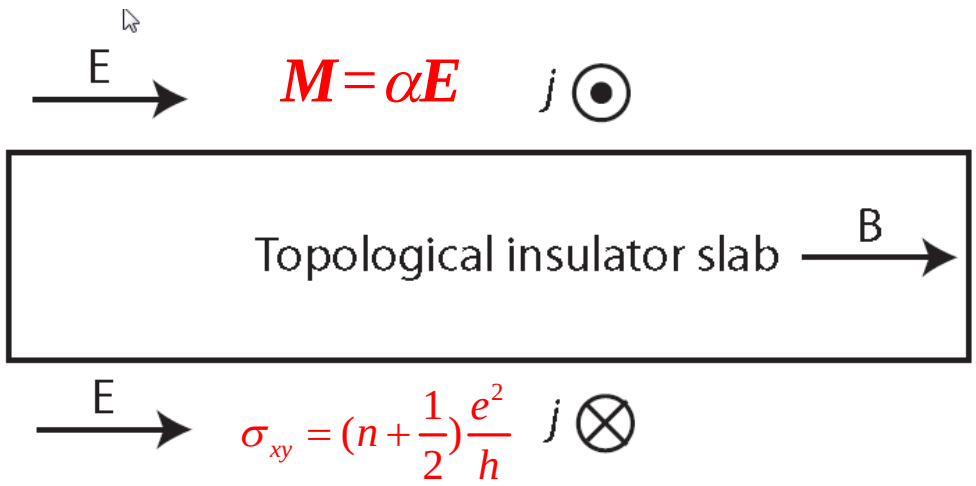
It follows that the ground state of Pyrochlore Iridates is magnetic non-collinear state.

Original proposal by Pesin and Balents (Nature Physics, 2010) on their topological insulating behavior does not work.

Magnetic topological insulators – time reversal symmetry is broken - aka Axion insulators – as a new theoretical proposal

Topological Magnetoelectric Effect

Adding a magnetic perturbation to topological insulator: Azimuthal surface Hall current $e^2/2h\mathbf{E}$ leads to a magnetic-dipole moment associated with a magnetization $\mathbf{M}=\alpha\mathbf{E}$, where the magnetoelectric polarizability is given by $\alpha=e^2/2h$. (Qi et al.)



Discussed in 1980s as "axion electrodynamics" (Wilczek, 1987).

ARTICLES
PUBLISHED ONLINE: 7 MARCH 2010 | DOI: 10.1038/NPHYS1534
nature physics

Dynamical axion field in topological magnetic insulators

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

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

$$M = \alpha E, \alpha = \frac{\theta}{2\pi}\frac{e^2}{h}$$

θ – **Axion field** – can be 0 or π in non-magnetic topological insulators due to time reversal and inversion symmetries. It can take any value (dynamic axion field) for magnetic topological insulators. In most known materials θ is small (10^{-3},in Cr_2O_3) **Highly interesting to study for Pyrochlore Iridates!** Here, due to inversion symmetry it still only can be 0 or π.

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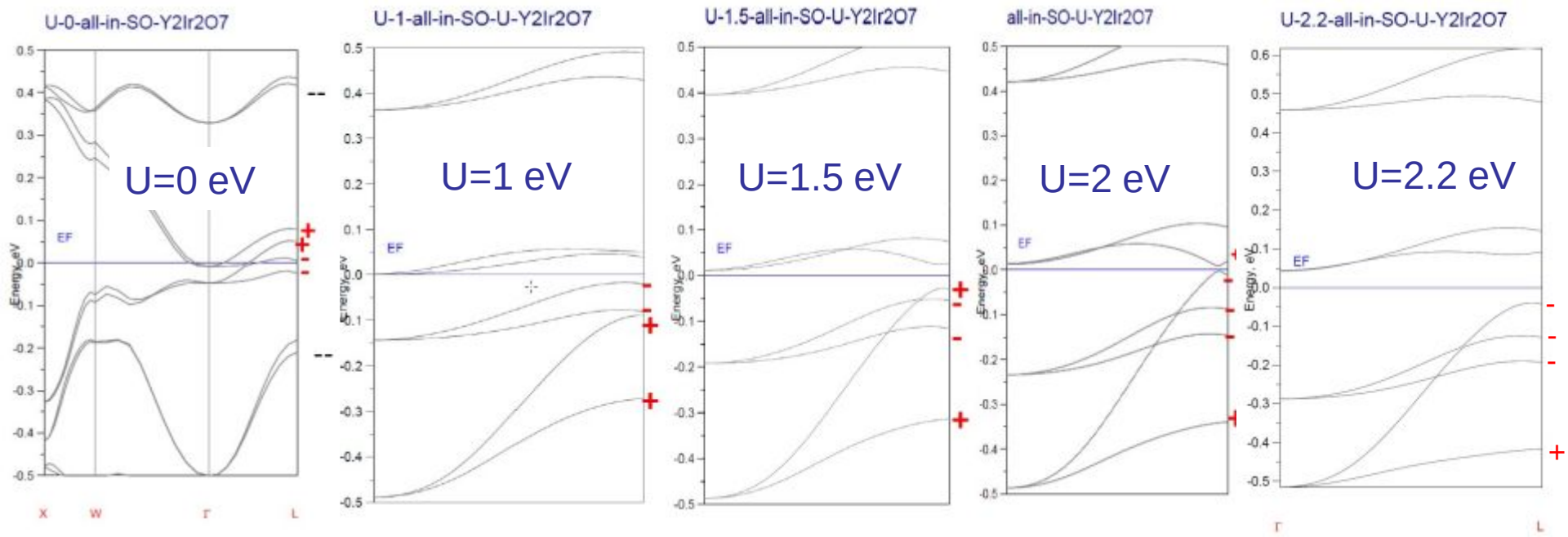
We study changes in band parities that may indicate a presence of topological insulator and also semi-metallic phase since topological insulators in 3D must be separated from trivial insulator by 3D Dirac (Weyl) points (Murakami, Kuga, 2008).

We have performed analysis of band parities to see if they change as we move from large U phase which is likely a trivial Mott insulator to smaller Us:



Parities change!

Mott Insulator

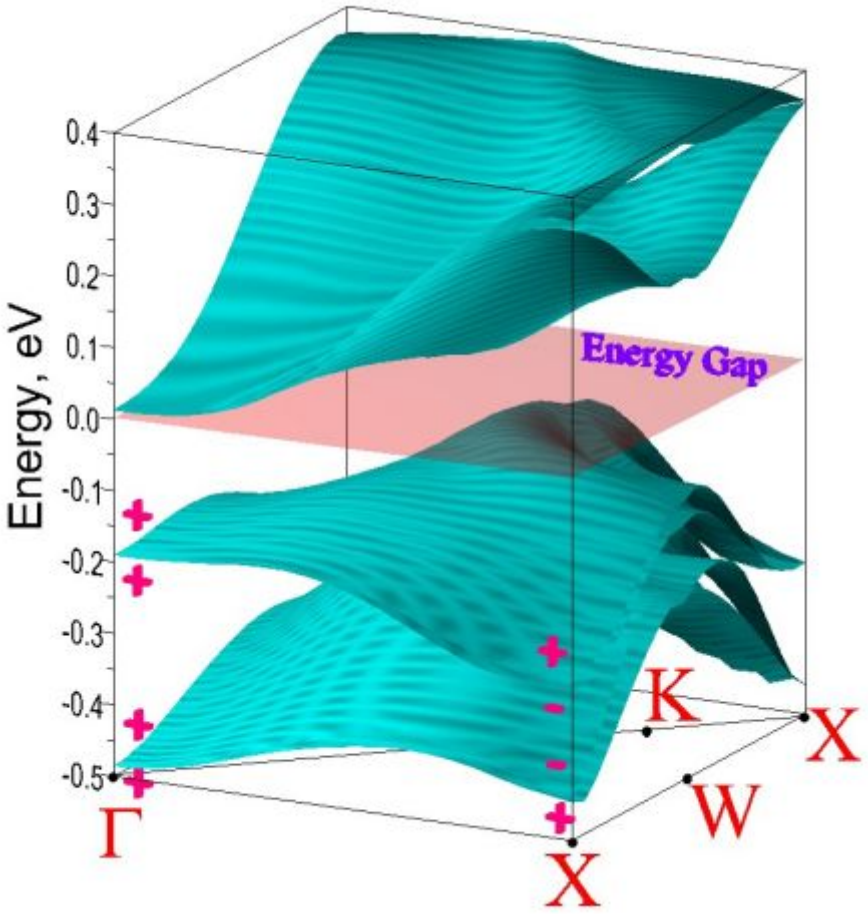
Decreasing U

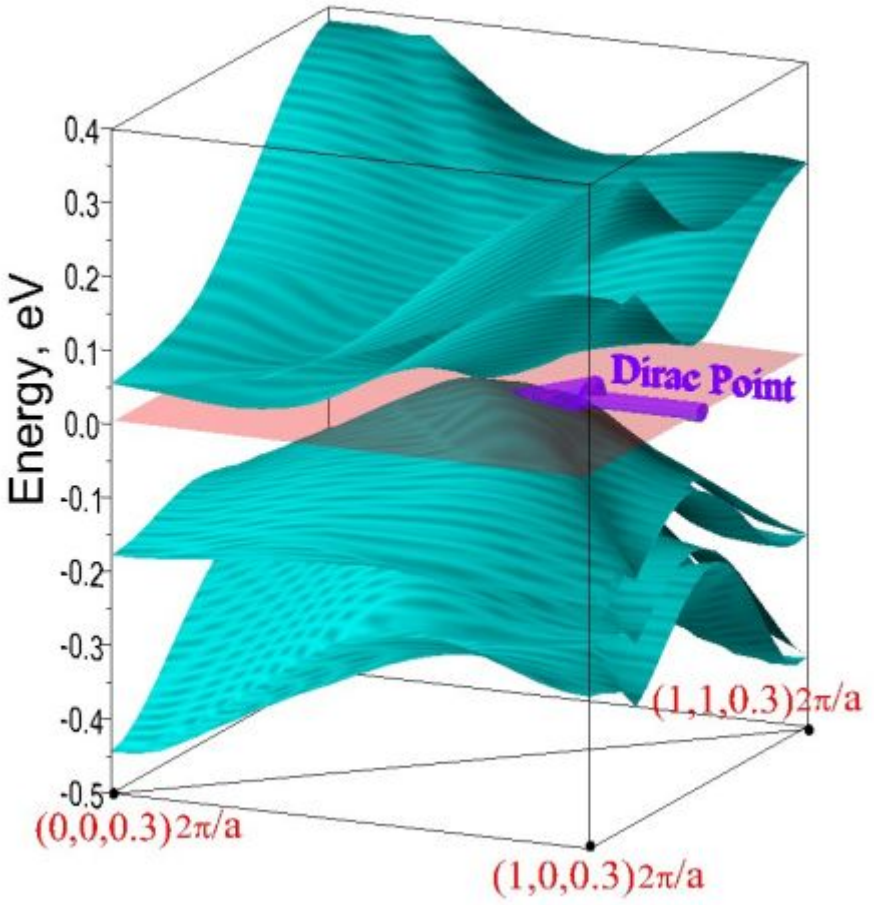
Birth of Weyl semi–metal phase at intermediate values of 1.0 eV<U<1.8 eV

Calculated energy bands using LDA+SO+U=1.5 eV

LEFT:within k_z=0 plane of BZ

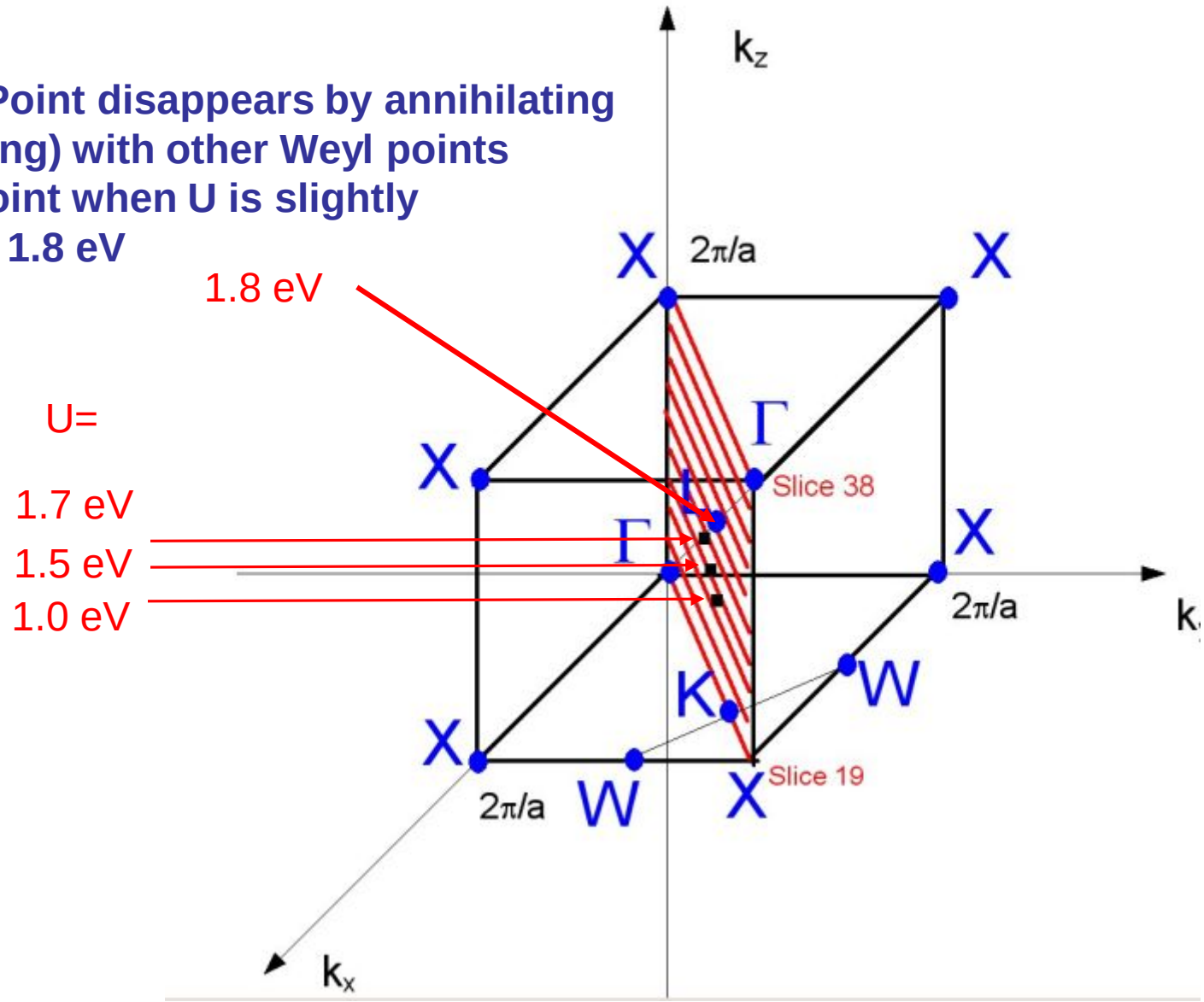
RIGHT:for k_z=0.3 plane of BZ





Weyl(Dirac) Point Location as a function of U

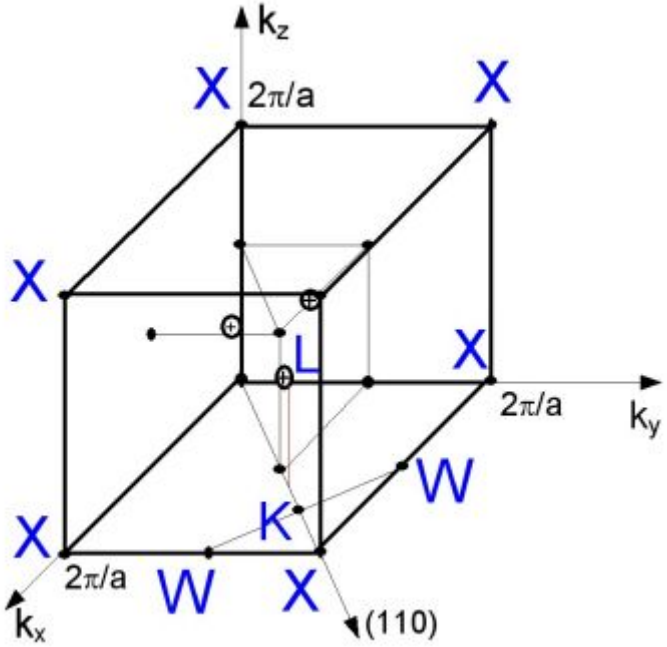
Weyl Point disappears by annihilating (meeting) with other Weyl points at L point when U is slightly above 1.8 eV

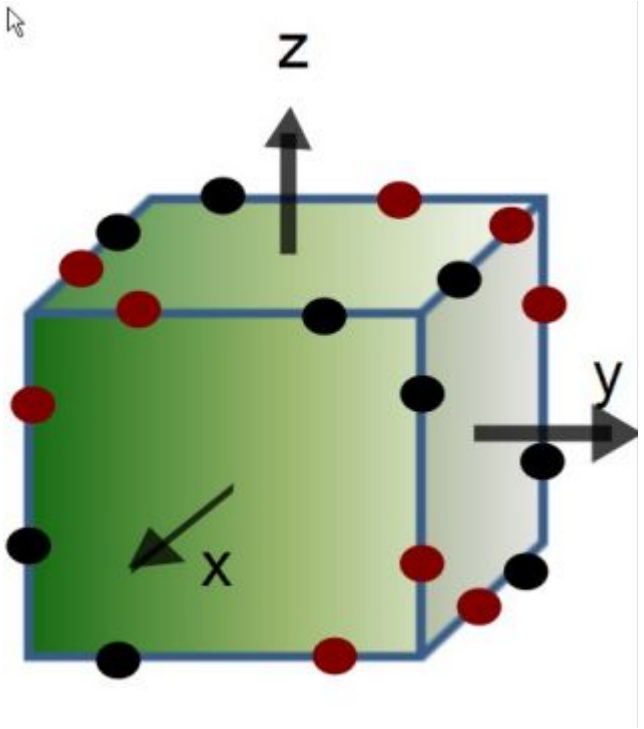


Annihilation of Weyl Points and Change in Band Topology

Our Weyl points are topological: they can only be eliminated by recombining with each other! Here is electrostatic analogy: each Weyl point can be characterized by **chiral charge** determined in terms of electron velocities at this k_W point: $c = sign(v_1 \bullet v_2 \times v_3)$

Thus there are "positive" Weyl points at locations k_W and "negative" Weyl points at locations $-k_W$ Here is our case:

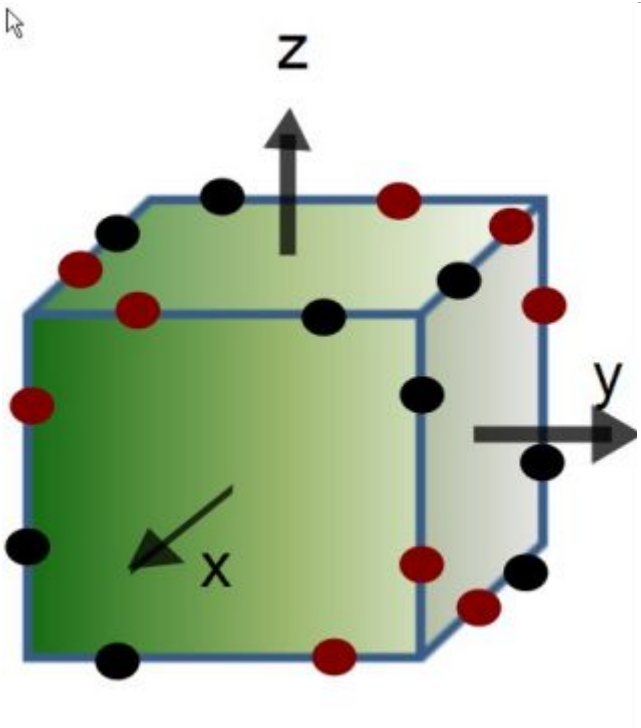




Three positive Weyl points around L **Positive and negative Weyl points in BZ**

Annihilation of Weyl Points and Change in Band Topology

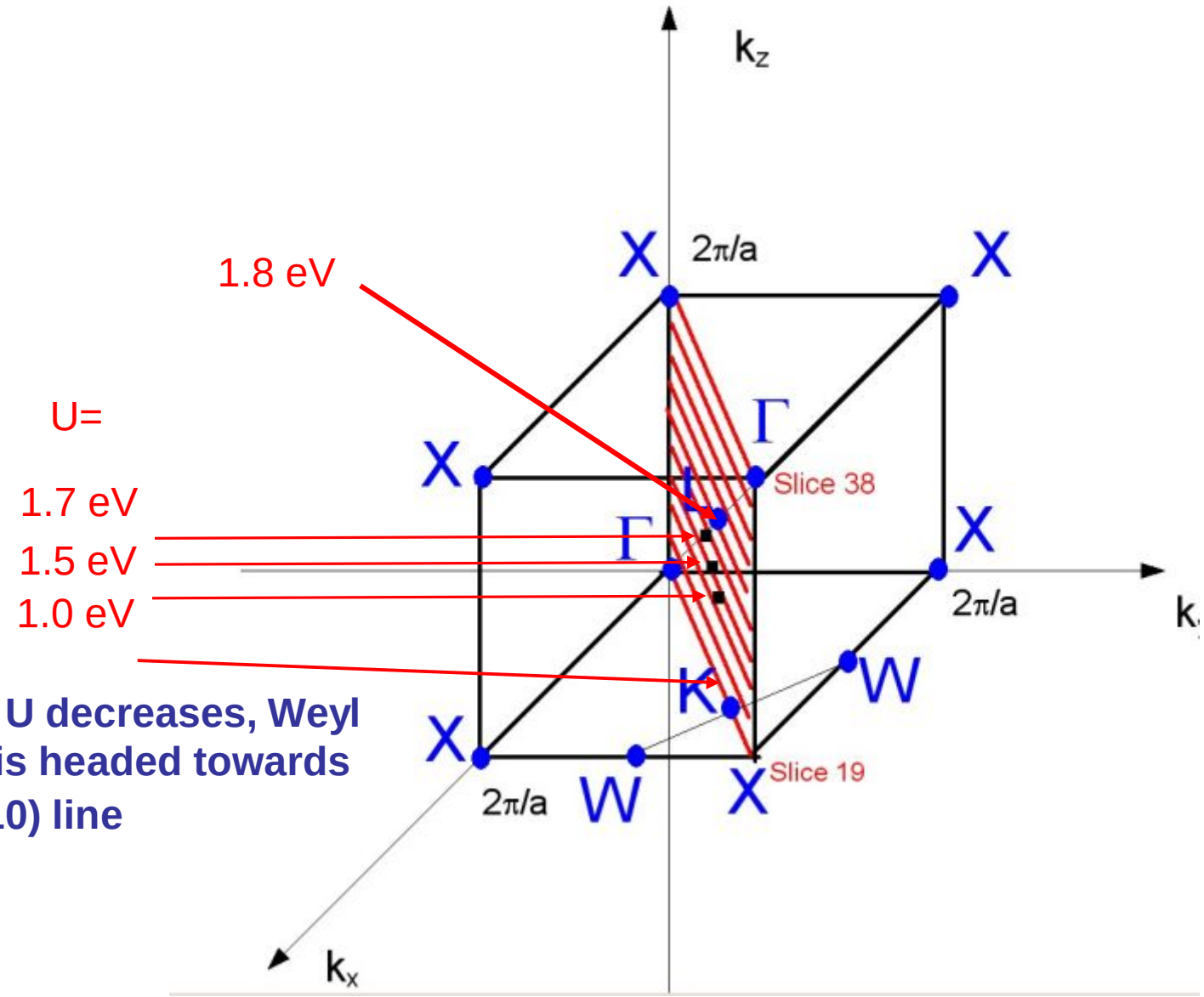
When Weyl Points annihilate, their chiral charges get added together and the resulting charge is zero: the system becomes insulator!



For example, when U goes above 1.8 eV,
every 6 Weyl points collapse at L points, three with positive chiral charge and three with negative chiral charge at equivalent "–L" points, and Weyl metal phase goes to Mott insulator phase.

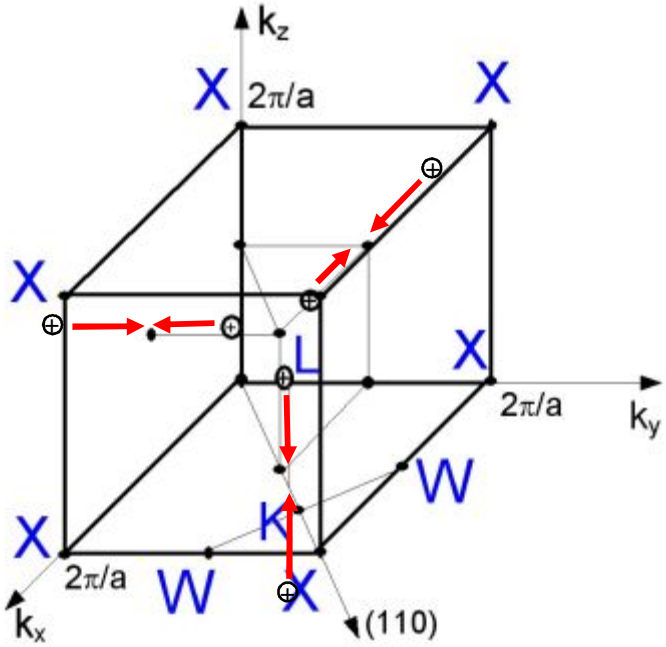
Q: How exactly Weyl Phase disappears when U decreases?

Collapse of Weyl Points at small Us



When U decreases, Weyl point is headed towards ΓX (110) line

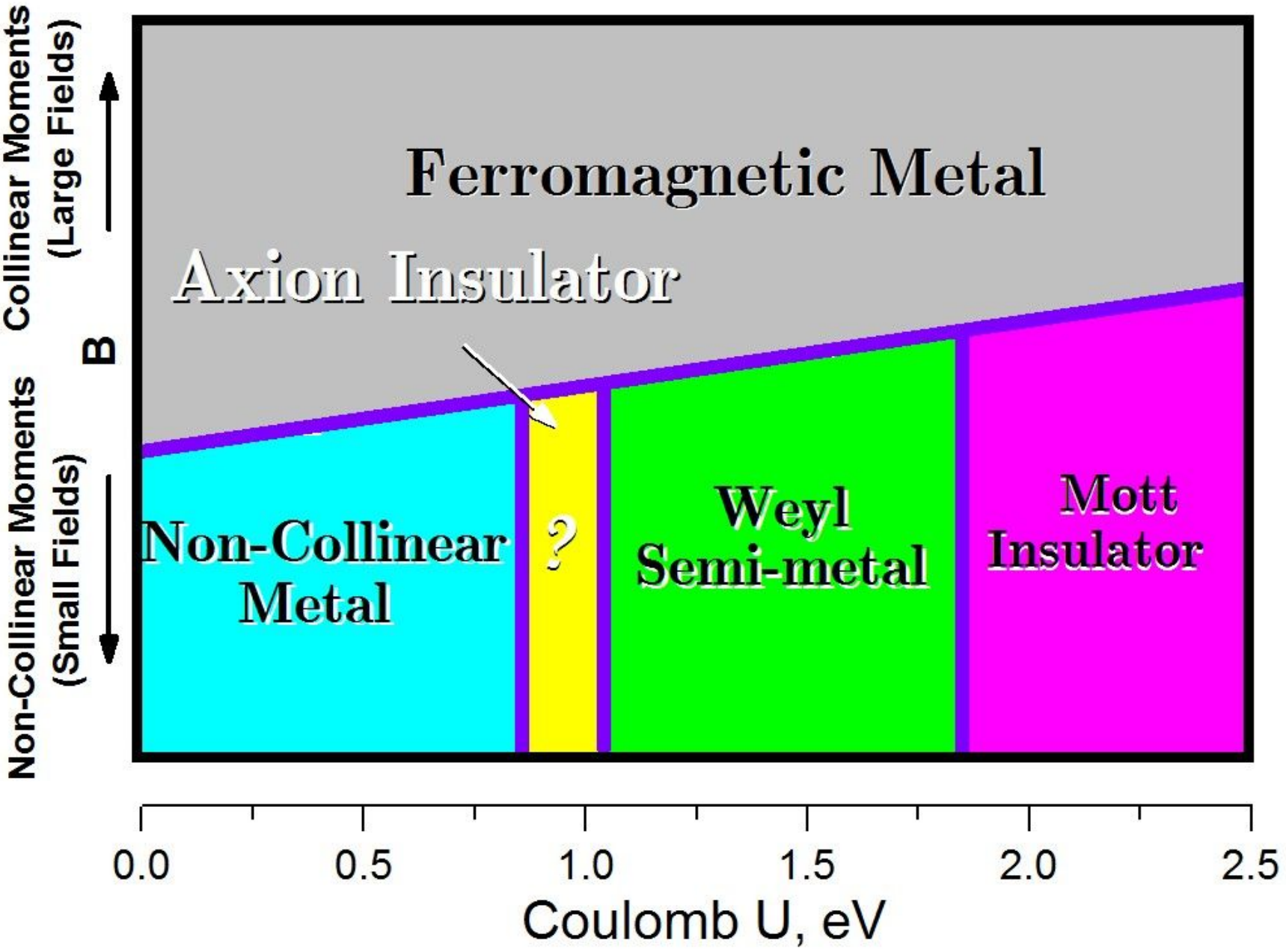
If Weyl points would collapse somewhere along ΓX line (not exactly at X point), they would annihilate pairwise by meeting with the Weyl points of the opposite chirality. Thus band properties will change again. If this would be true a **Magnetic Topological (Axion) Insulator** will be born!



This unfortunately does not happen in LDA+U calculation since the gap closes at other portions of the Brillouin Zone which prevents the collapse of the Weyl points. However, due to well-known underestimation of gaps and metallization threshold by LDA this opportunity still remains!

Our recent work on hypothetical Os spinels (MOs_2O_4, M=Ca,Sr) shows realization of this scenario (Wan, Vishwanath, SS, PRL 2012, in press)

Suggested Electronic Phase Diagram of Iridates



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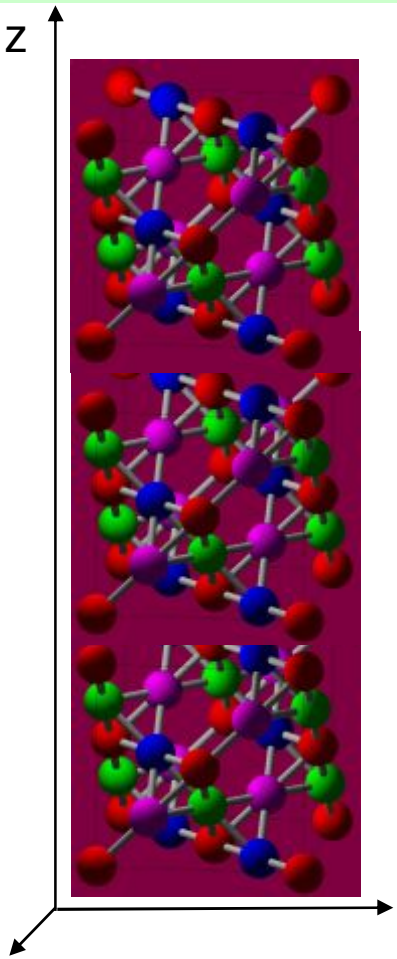
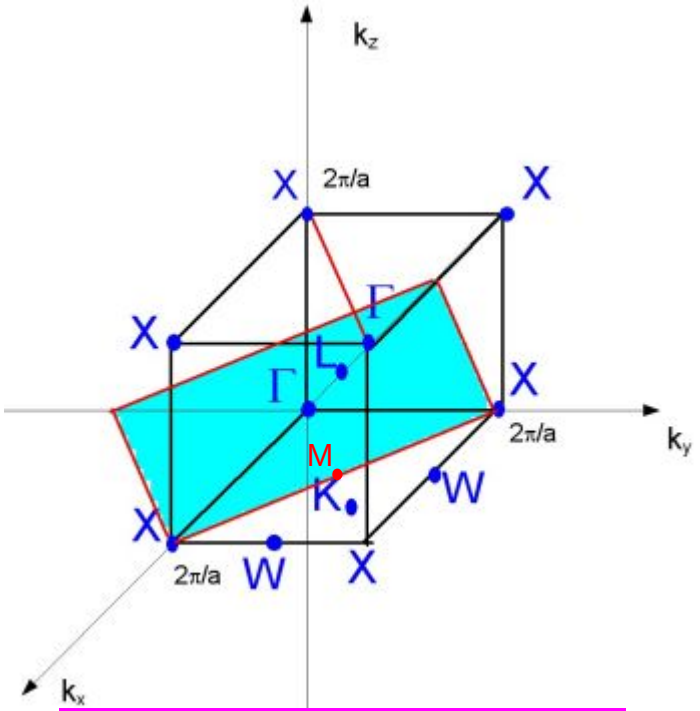
Surface Band Structures – Projected Bulk Spectrum

Increasing the size of cell along z axis

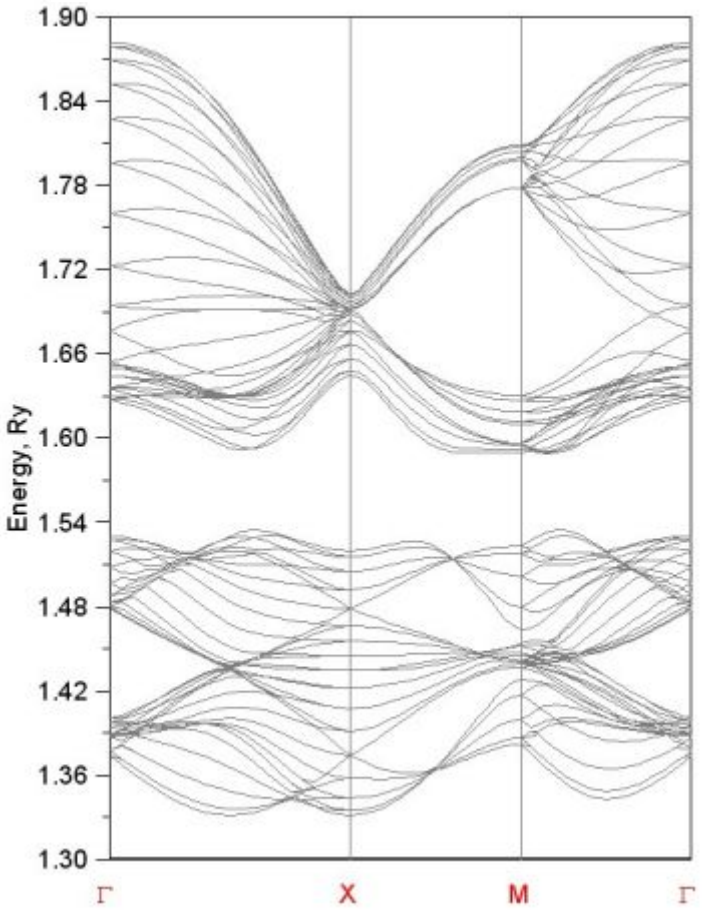
shrinks the size of the BZ along kz axis





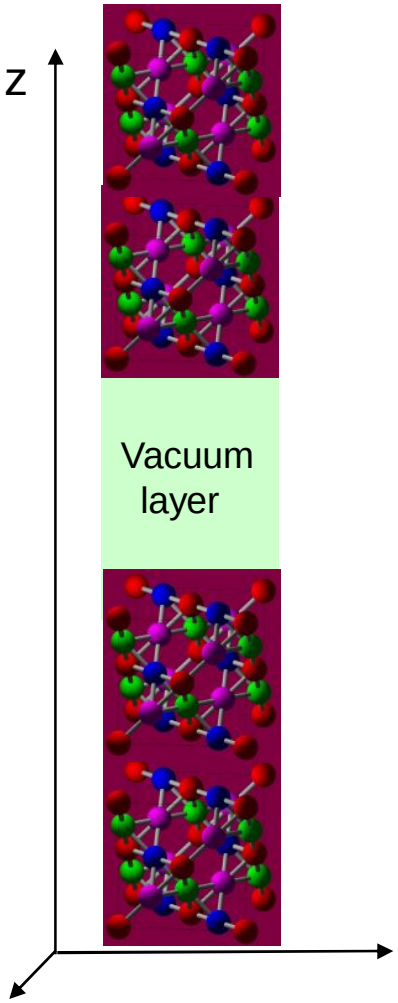
(001) Surface BZ
ΓXM are surface TRIMs

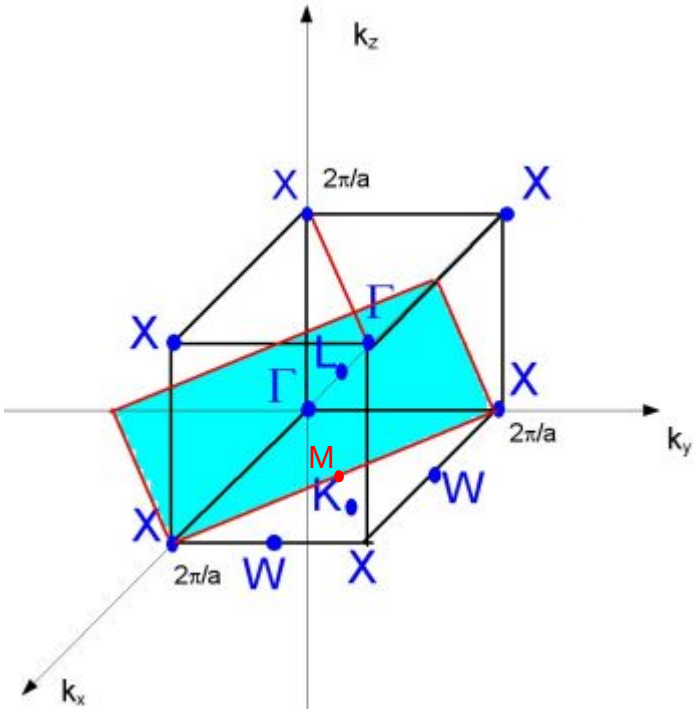
Eight Cells - Periodic



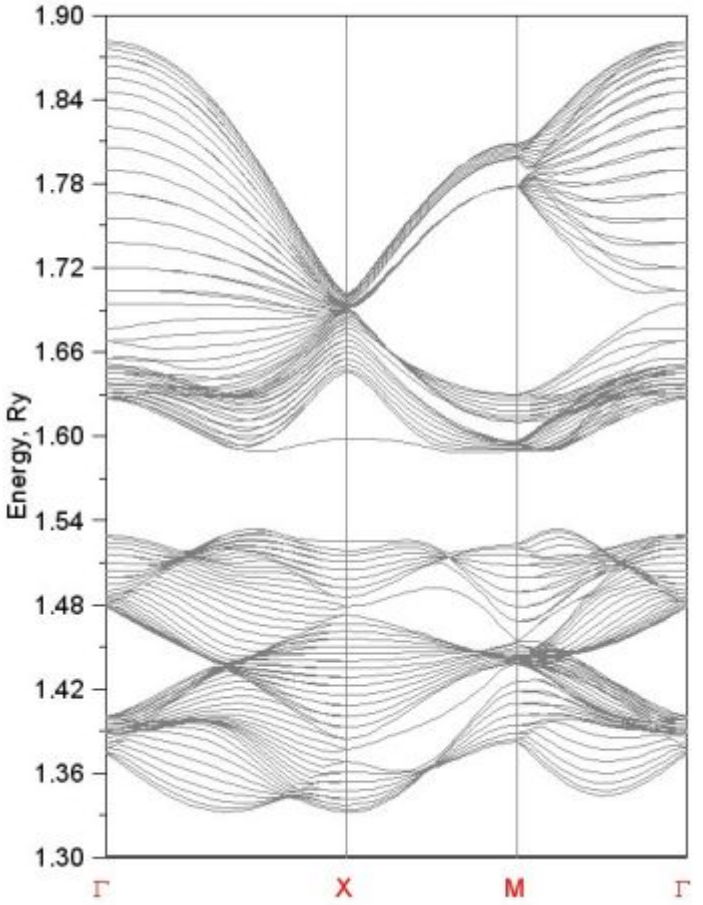
Band Structures for all k_z=const planes are projected to k_z=0 plane

Surface States - Slab Calculations





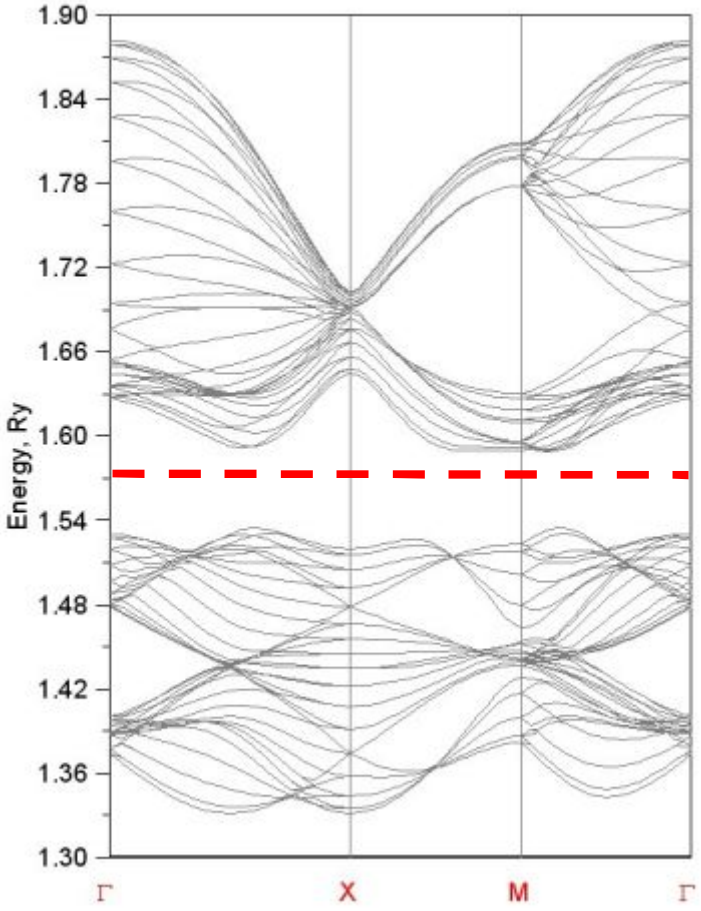
Eight Cells Slab



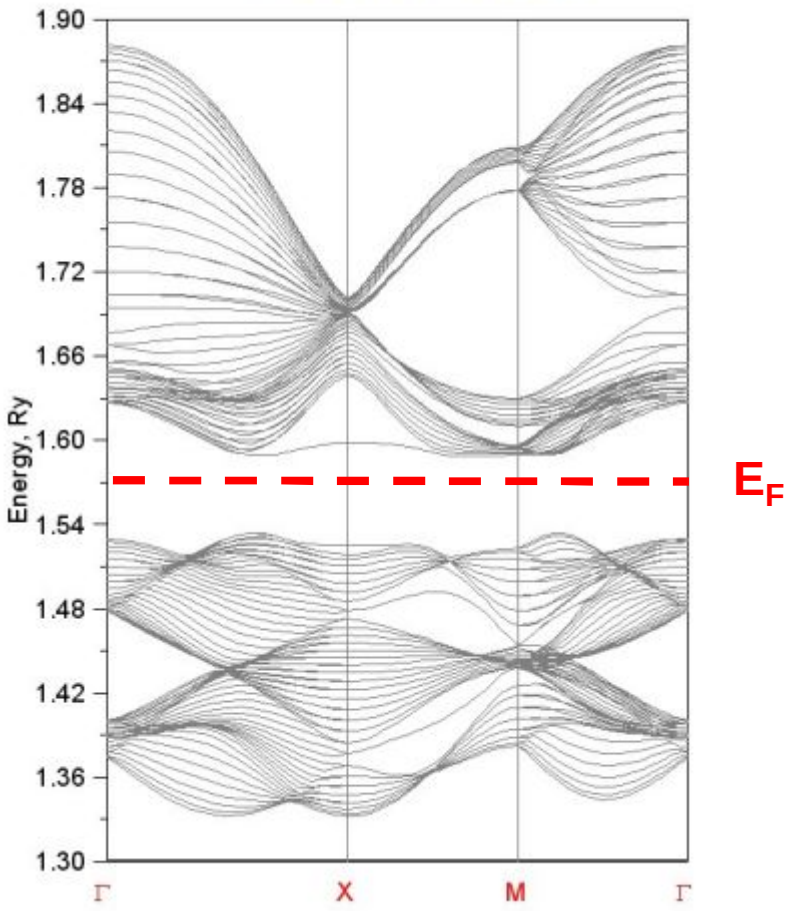
(001) Surface BZ
ΓXM are surface TRIMs

In Slab Calculation Surface(s) Spectrum appears on top of projected bulk E(k)

Trivial insulators: Surface state show energy gap as in projected bulk spectrum



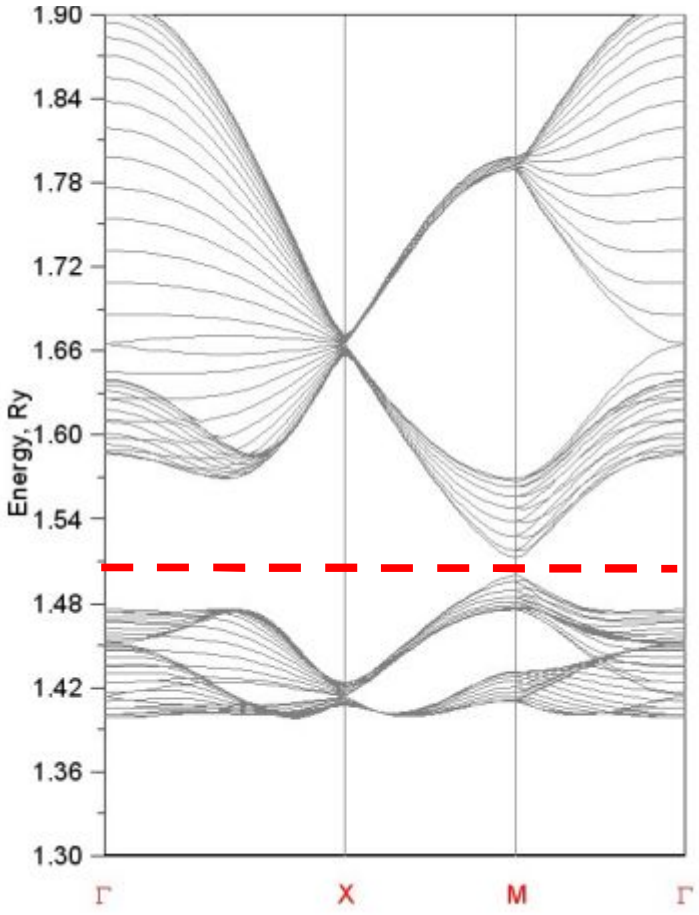
Projected Bulk Spectrum



Slab Spectrum

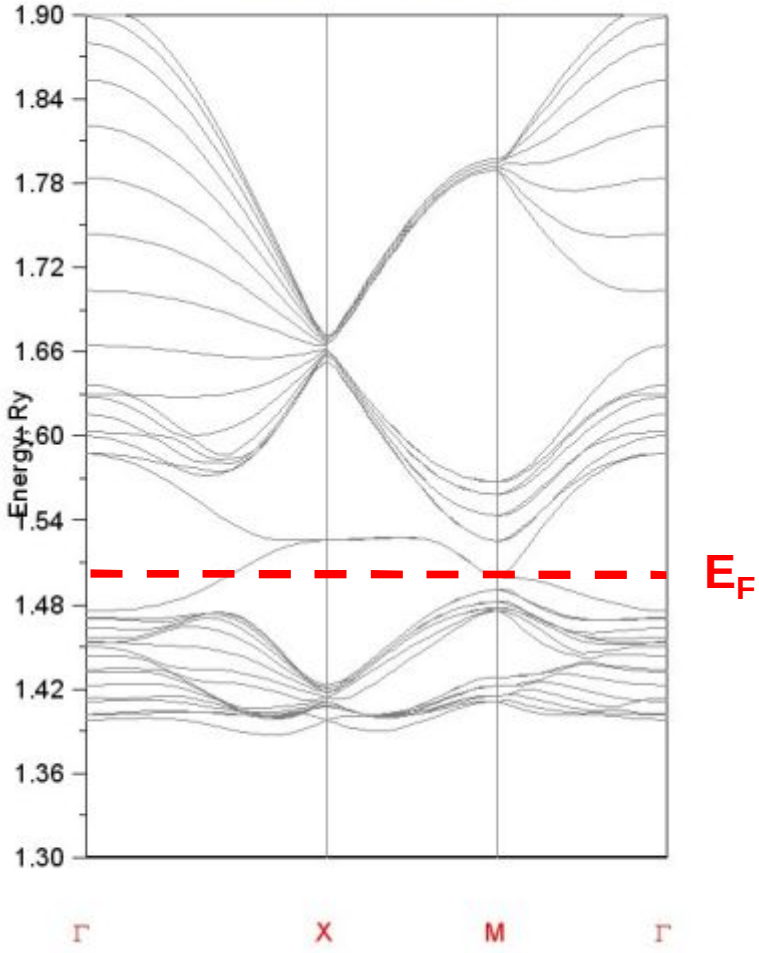
Topological insulators: Surface states show protected metallic behavior

Pesin Balents Topological Insulator



Projected Bulk Spectrum

Pesin Balents Topological Insulator



Slab Spectrum

Our Story: Weyl Semi-Metal and its Berry Flux

In the vicinity of Weyl Point: $q=k\text{-}k_W$

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

The Berry curvature is evaluated to be

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

(only Weyl point contributes)

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

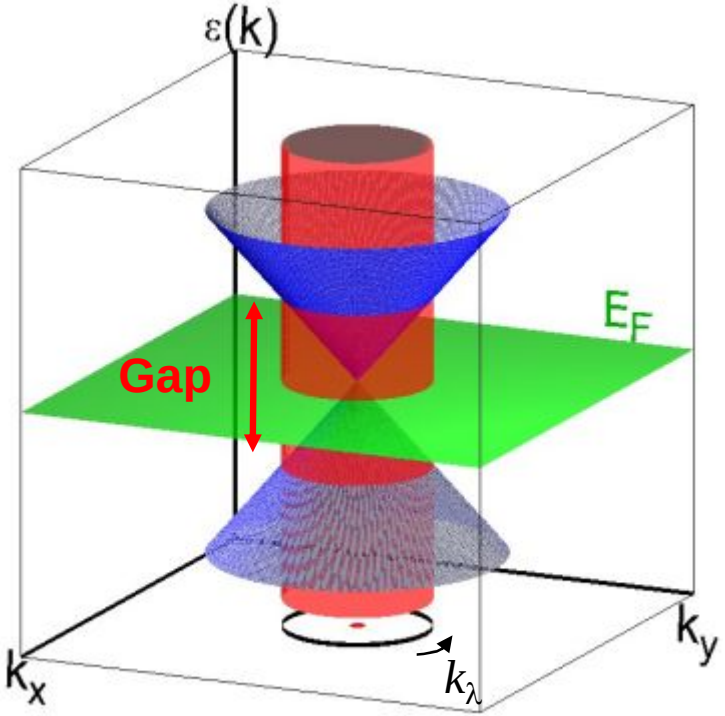
$$c=\frac{1}{2\pi}\oint_S dS\Omega(k)=\text{sign}(v_1\bullet v_2\times v_3)$$

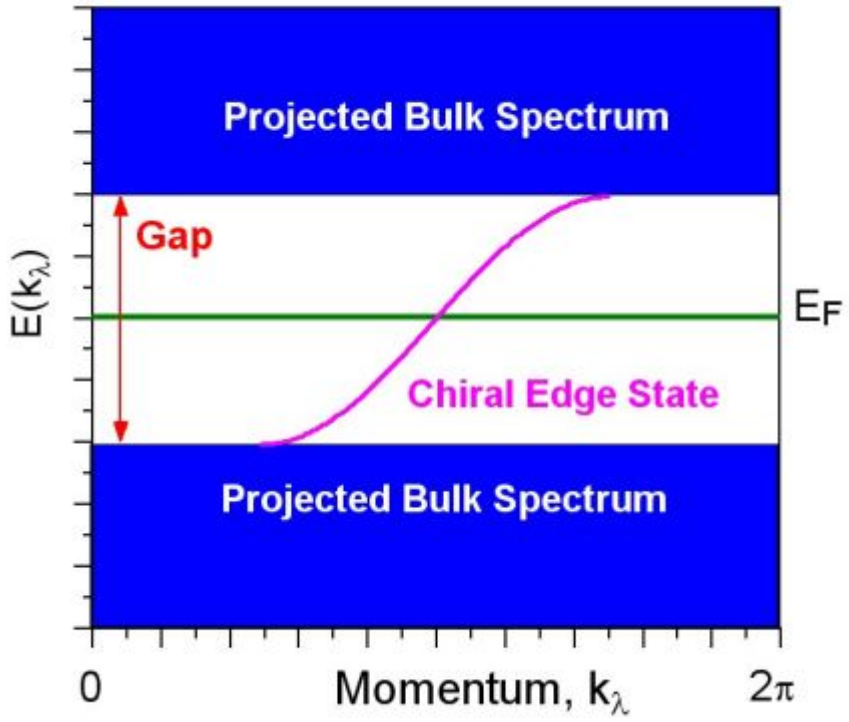
Weyl point acts as a **magnetic monopole** at the origin:

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

whose charge is given by chirality

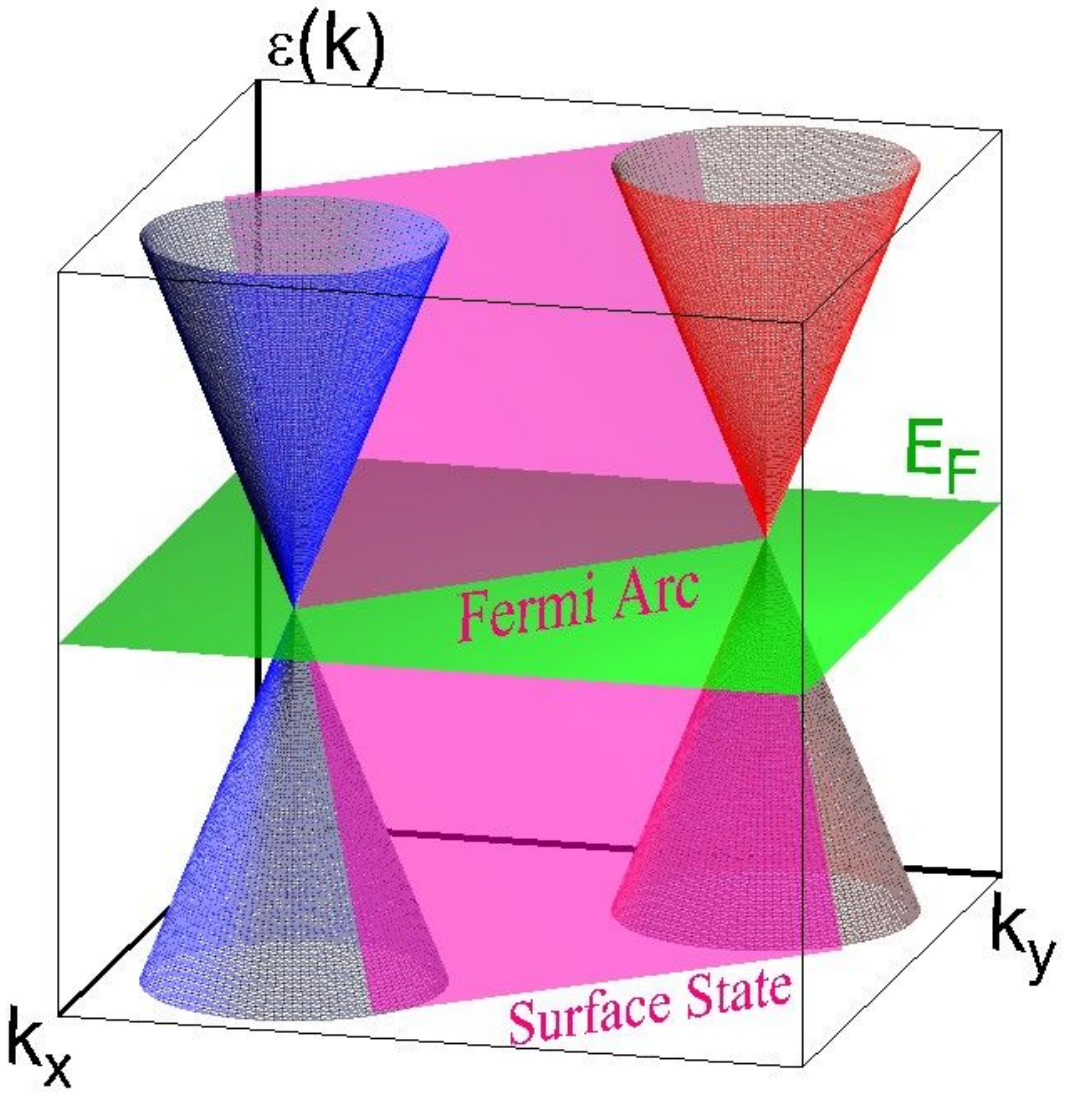
Weyl Semi-Metal: Formation of Surface States





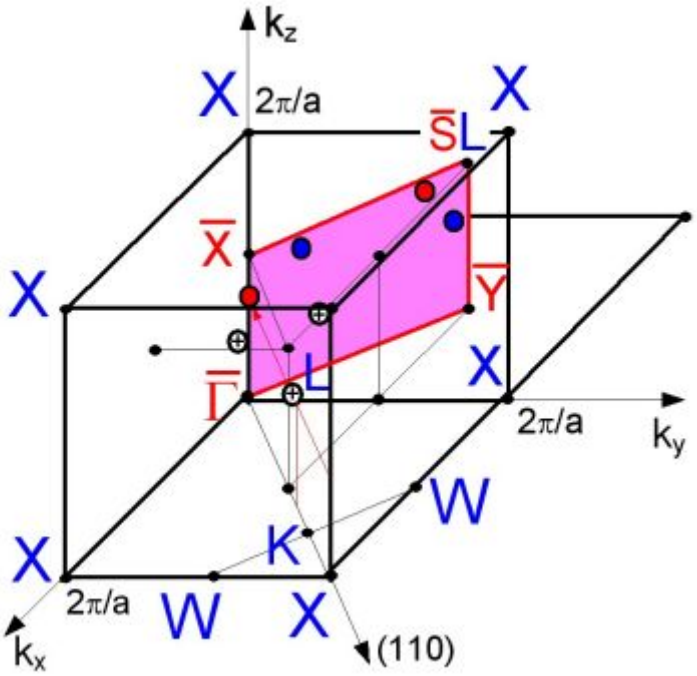
k_λ defines a 2D subsystem with non-zero C number: we expect a **Chiral Edge State**

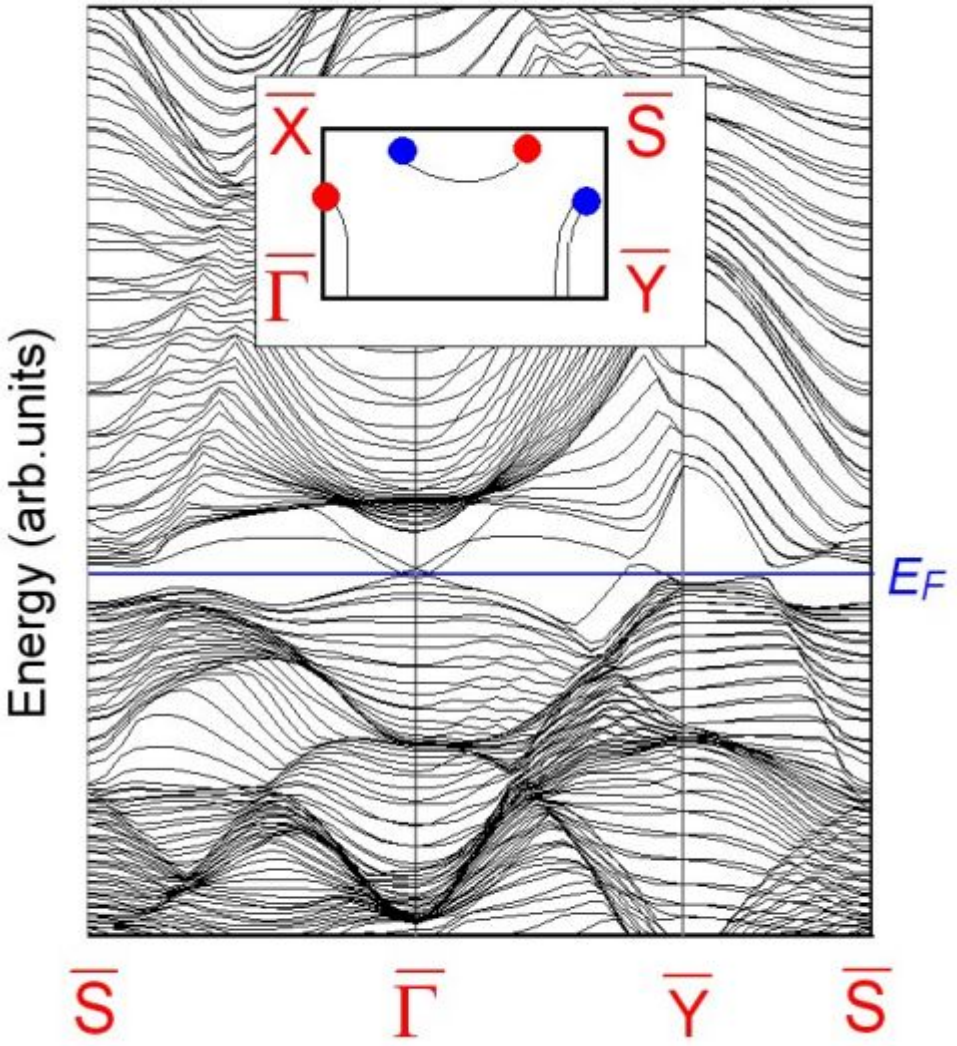
Weyl Semi-Metal: Formation of Fermi Arc



Fermi Arc connects Weyl points of opposite chirality

Tight-Binding Simulation of (110) Surface Band Structure for Iridates





Fermi Arcs connecting Weyl points of opposite chirality can be directly observed

How to detect Weyl semimetal experimentally?

Anomalous Hall conductivity is characterized by Chern vector ν_c (Haldane, 2004)

$$\sigma_{ab} = \sum_c \frac{e^2}{2\pi h} \varepsilon_{abc} \nu_c = \frac{-ie^2}{2\pi h} \sum_{bands} [\partial_{k_a} \langle u_k | \partial_{k_b} | u_k \rangle - \partial_{k_b} \langle u_k | \partial_{k_a} | u_k \rangle]$$

- **Yang, Lu, and Ran, PRB 2011:** In general Weyl semimetal

$$\vec{\nu}_{nodes} = \sum_i (-1)^{\xi_i} \vec{P}_i$$

where P_i is momentum of each node and ξ_i is its chirality.

For 24 Weyl nodes of $Y_2Ir_2O_7$ we get zero due to cubic symmetry but if it gets broken by uniaxial pressure along [111] direction one can induce large anomalous Hall effect.

- **Xu, Weng, Wang, Dai, Fang, PRL 2011:** $HgCr_2Se_4$ is existing Weyl semimetal.

- **Burkov Balents, PRL 2011:** Realization of Weyl semimetal via multilayer structure of magnetically doped TI separated by insulating spacers.

Conclusion

- **Novel electronic phases have been predicted for Pyrochlore Iridates: Weyl semi-metal and Mott insulators: they compete in the vicinity of Hubbard U~1.5-2 eV**

- **Non-collinear semi-metallic/insulating magnetism can be switched to normal metallic behavior by collinear alignment of moments (such as magnetic field)**

- **Weyl nodes are topological objects, they can be removed by annihilating with each other. They give rise to protected surface states similar to topological insulators. They produce Fermi arcs at surface BZ.**

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Metal-Nonmetal Changeover in Pyrochlore Iridates

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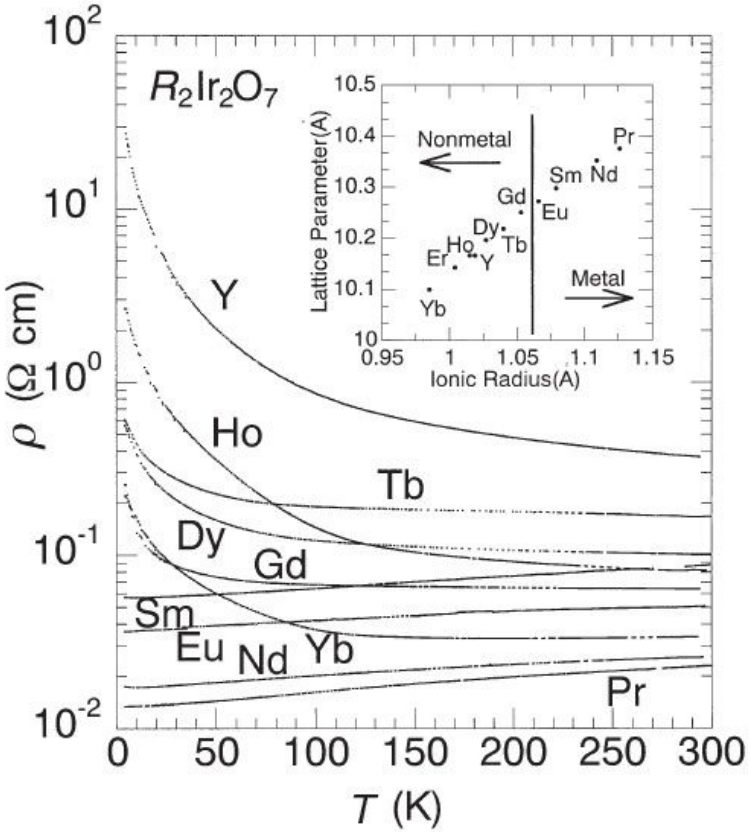

Fig. 1. Resistivity of polycrystalline $R_2Ir_2O_7$. Inset: Relationship between the ionic radius of R^{3+} and the observed cubic lattice parameter.

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Metal–Insulator Transition in Pyrochlore Iridates $Ln_2Ir_2O_7$ (Ln = Nd, Sm, and Eu)

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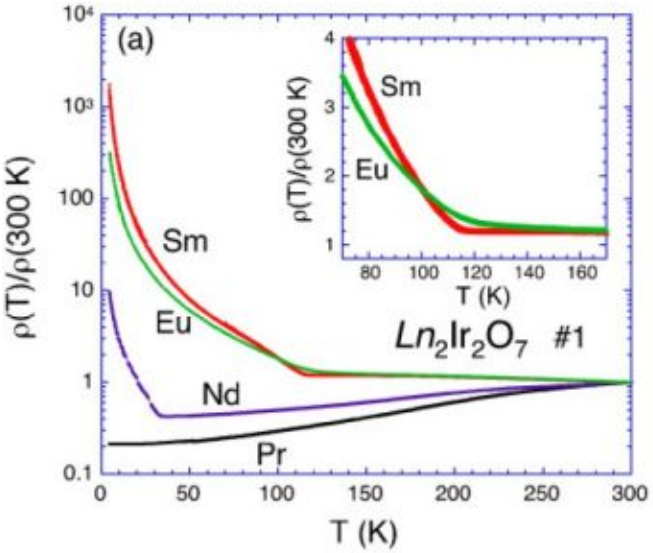
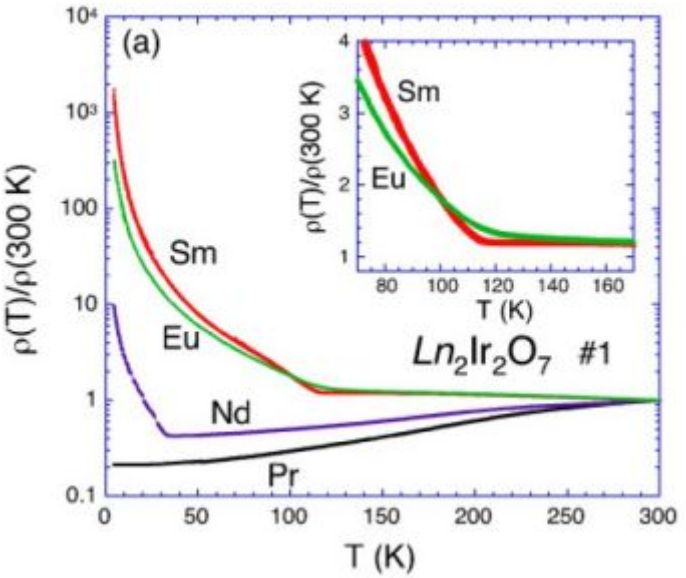
We report that $Ln_2Ir_2O_7$ for Ln = Nd, Sm, and Eu have metal–insulator transitions (MITs) at 36, 117, and 120 K, respectively. Their electrical resistivities and thermoelectric powers are not discontinuous and exhibit no thermal hysteresis at their transition temperatures T_{MI}, indicating second-order phase transitions. In this letter, we focus on the MIT of $Sm_2Ir_2O_7$. The specific heat and the magnetic susceptibility show a clear anomaly at T_{MI}. These results indicate that this MIT involves a magnetic ordering produced by 5*d* electrons in Ir.





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

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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 anomalously long Ir^{4+} spin correlation time, suggesting a singular density of low-lying spin excitations. Similar behavior is found in other pyrochlores and geometrically frustrated systems, but also in the unfrustrated iridates $BaIrO_3$ and $Sr_2Ir_2O_4$. $Eu_2Ir_2O_7$ may be only weakly frustrated; if so, the singularity might be associated with the small-gap insulating state rather than frustration.