Topological Kondo Insulator - SmB_6

Min-Feng

OUTLINE

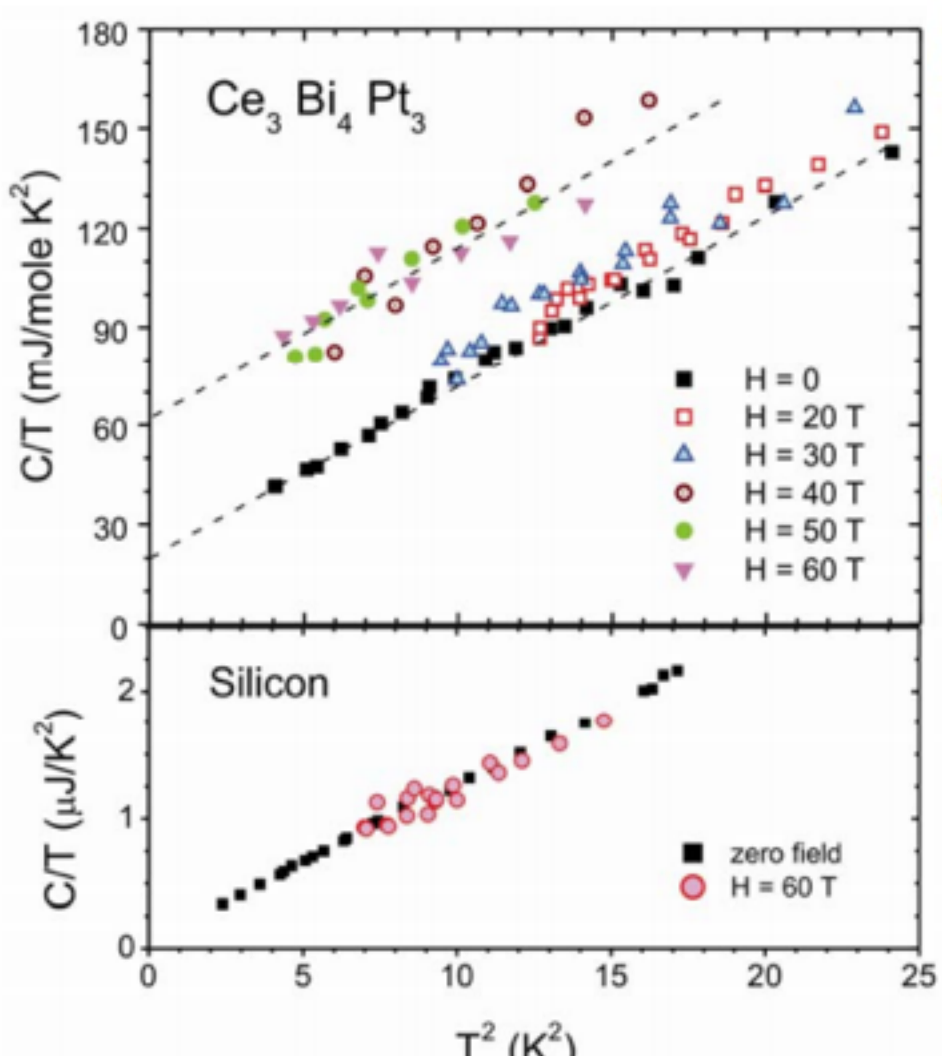
- MOTIVATION
- SmB_6 ANALYSIS
- IS IT REALLY TOPOLOGICAL?

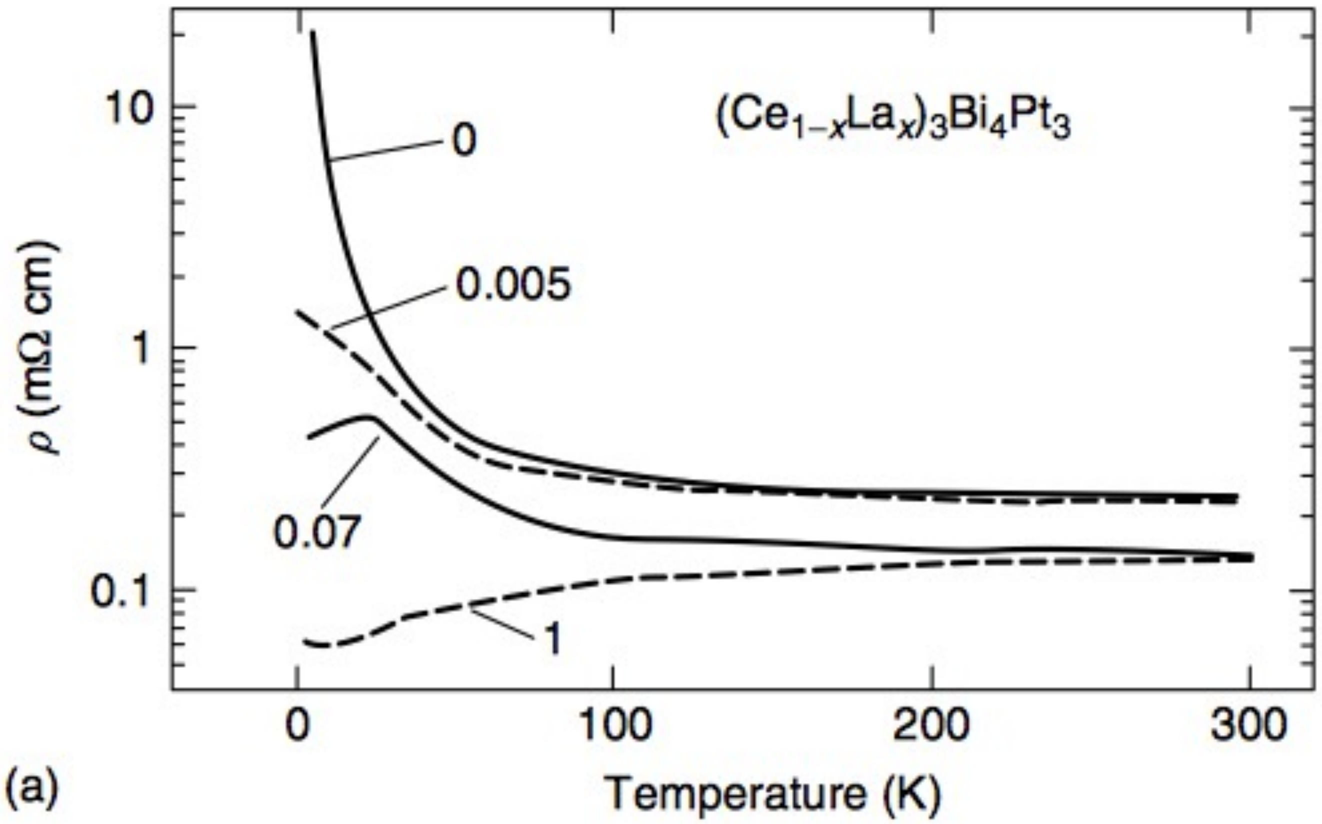
MOTIVATION

REMEMBER KONDO INSULATOR BEHAVIOR?

Kondo Insulator

$Ce_3Pt_4Bi_3$

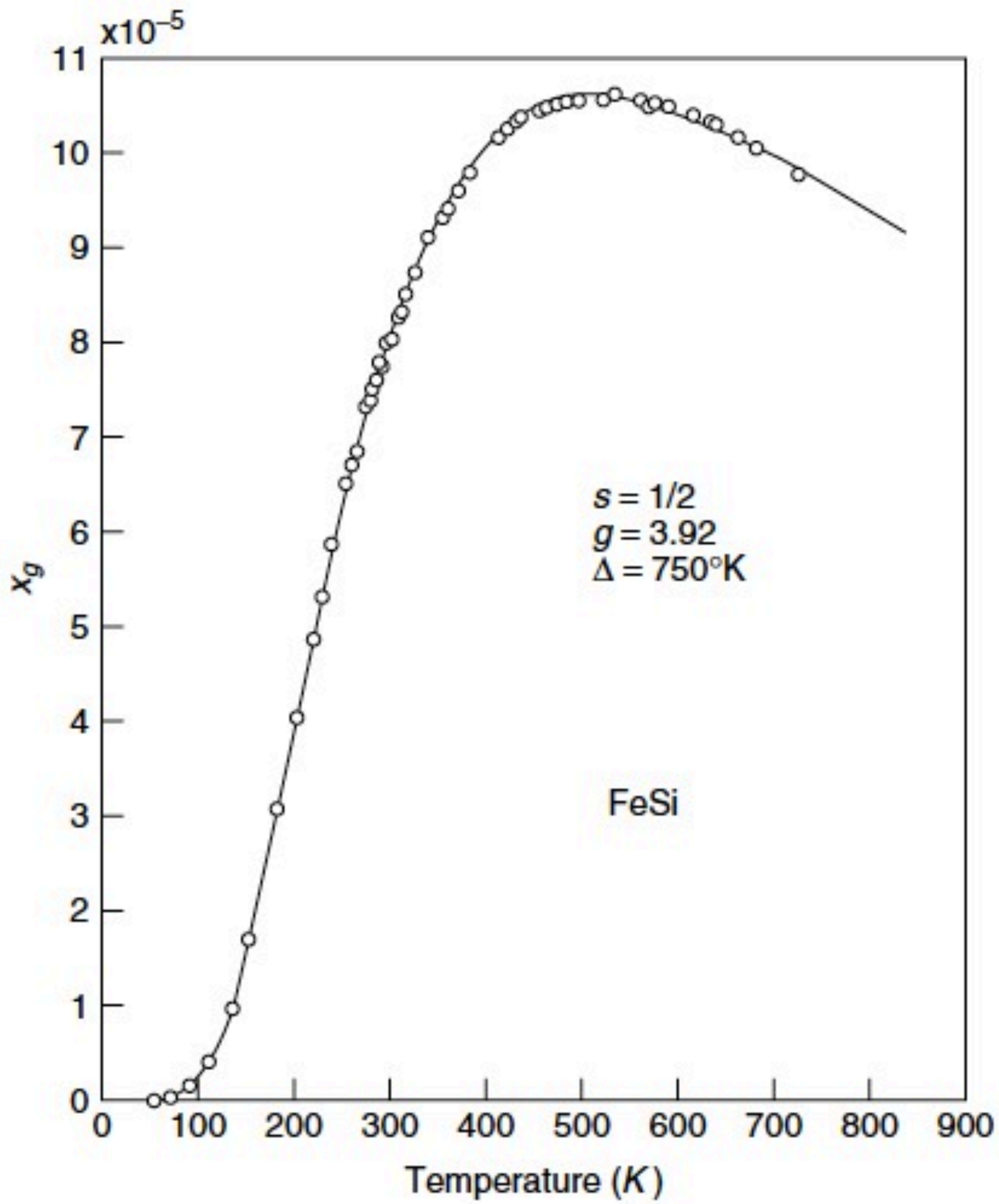




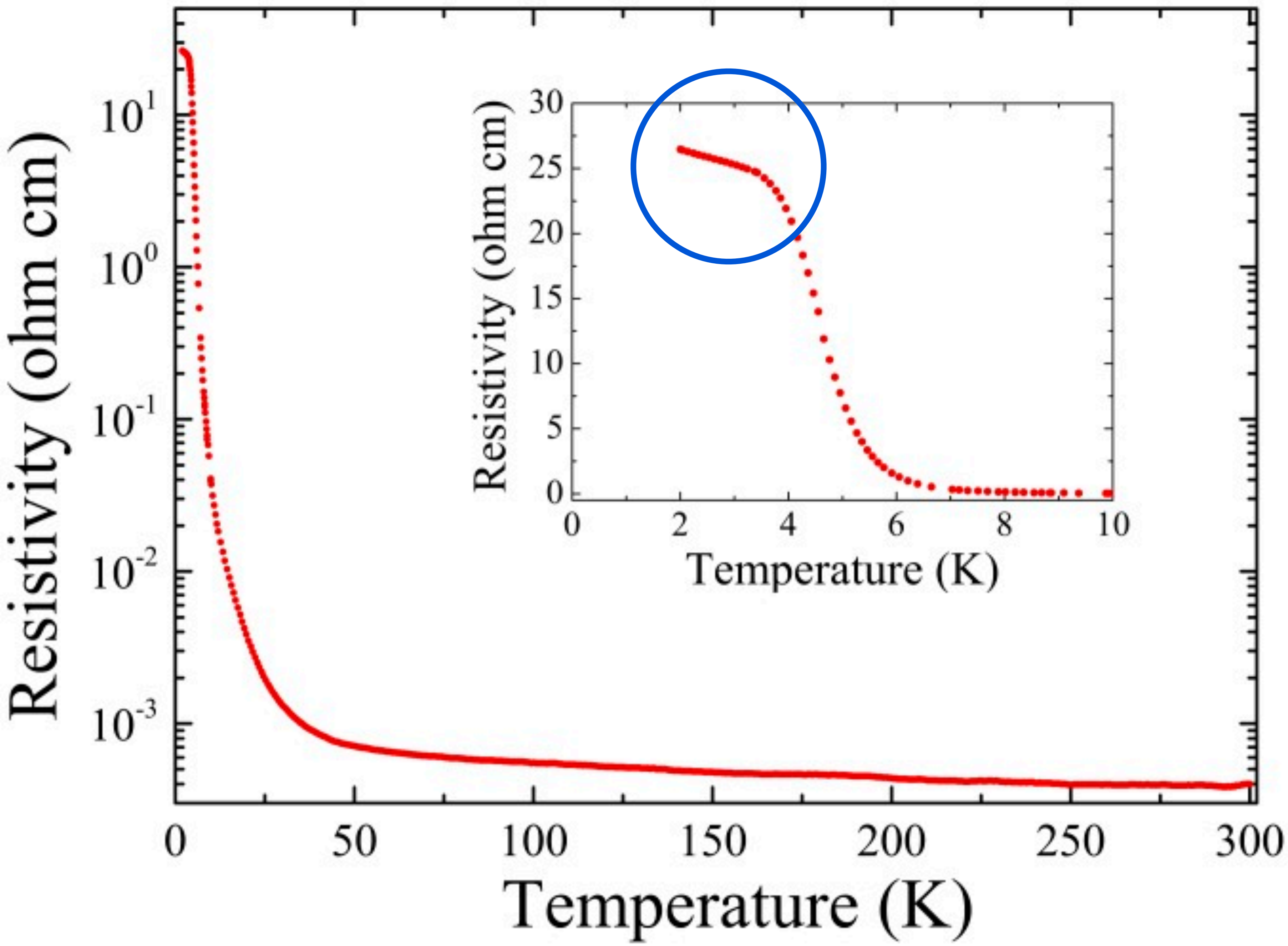
$$T_K = 80K$$

$$\gamma \rightarrow low$$

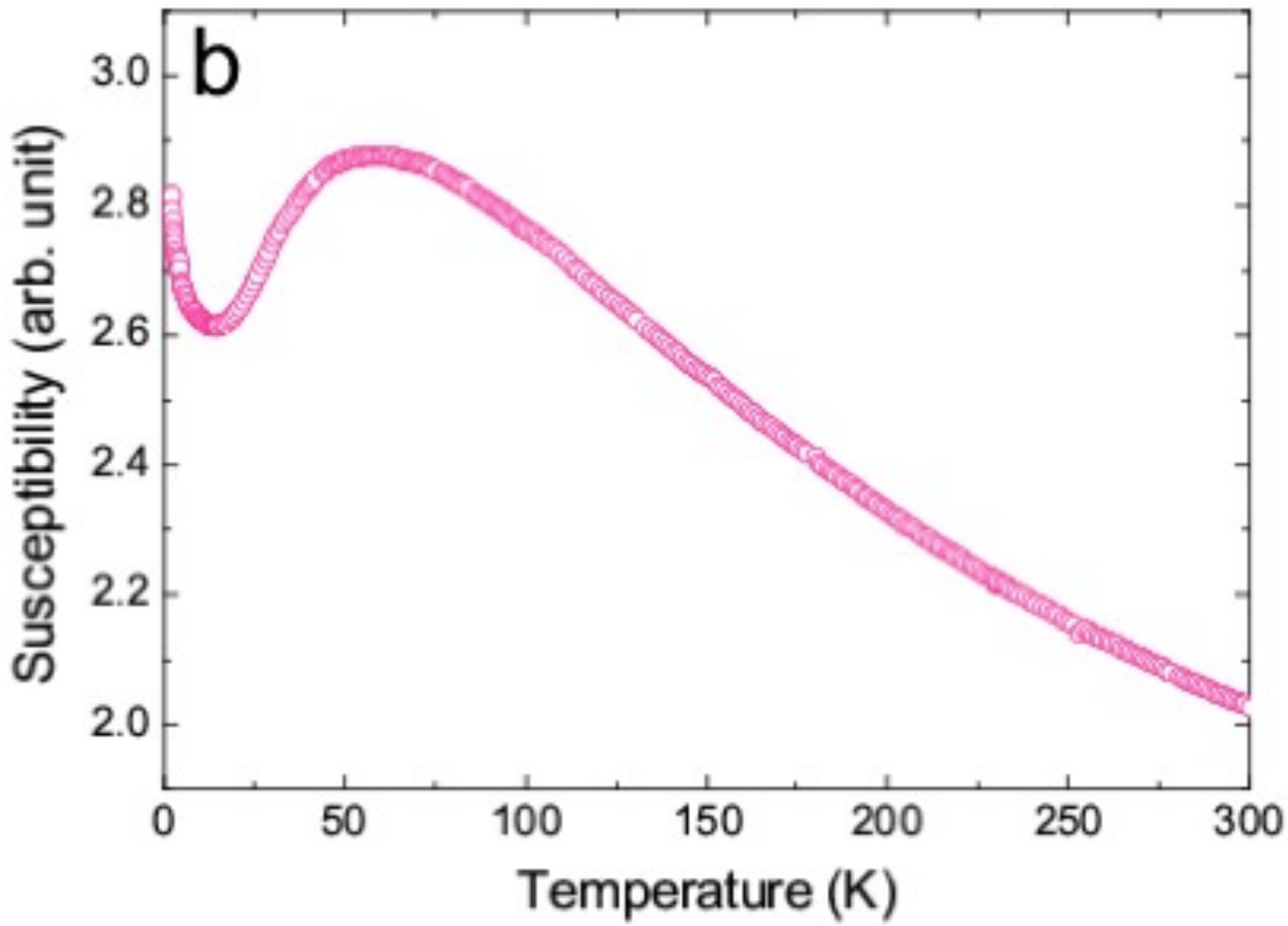
REMEMBER KONDO INSULATOR BEHAVIOR?



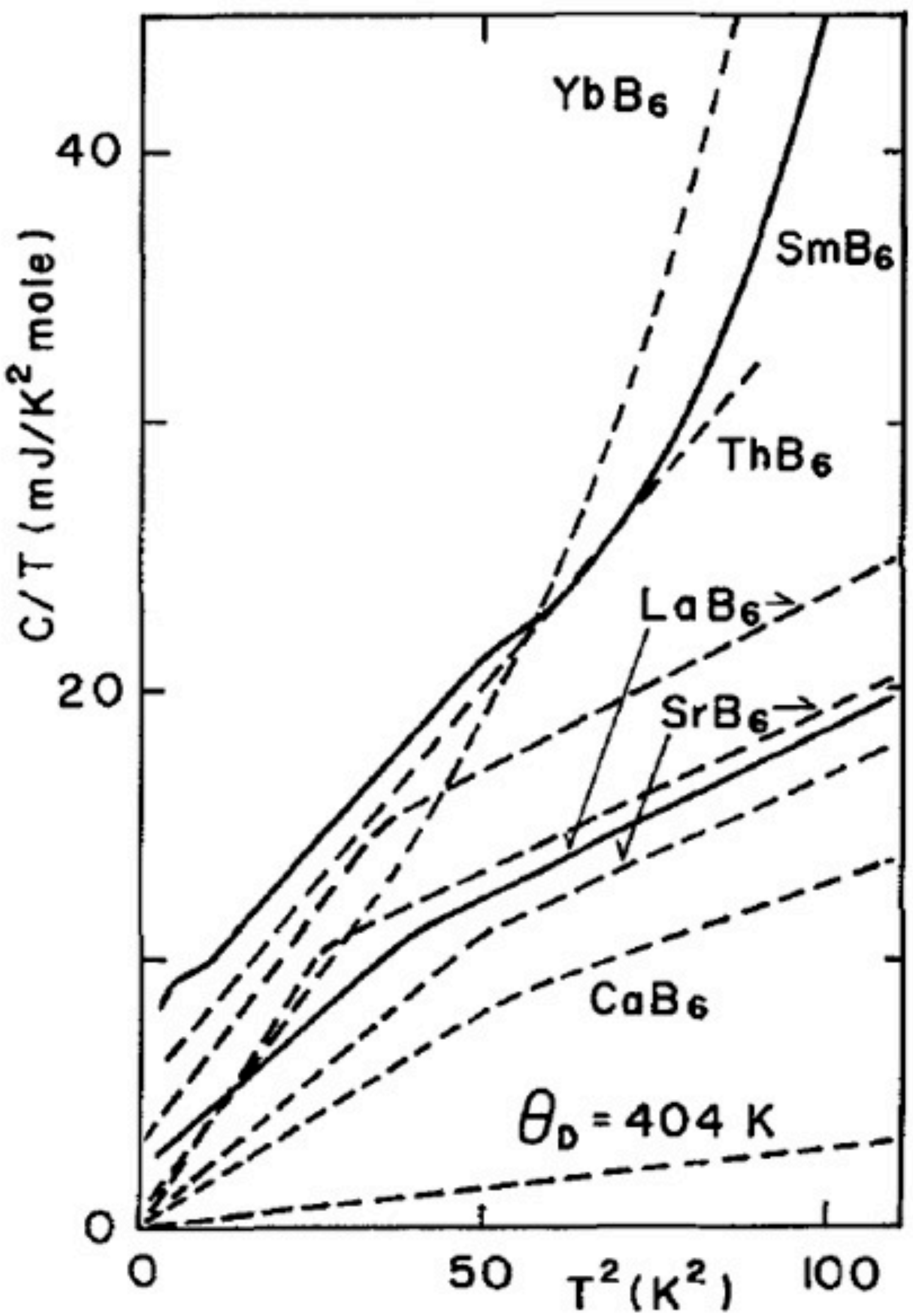
How about SmB6



How about SmB6



How about SmB6



So Why Are We Interested in SmB6

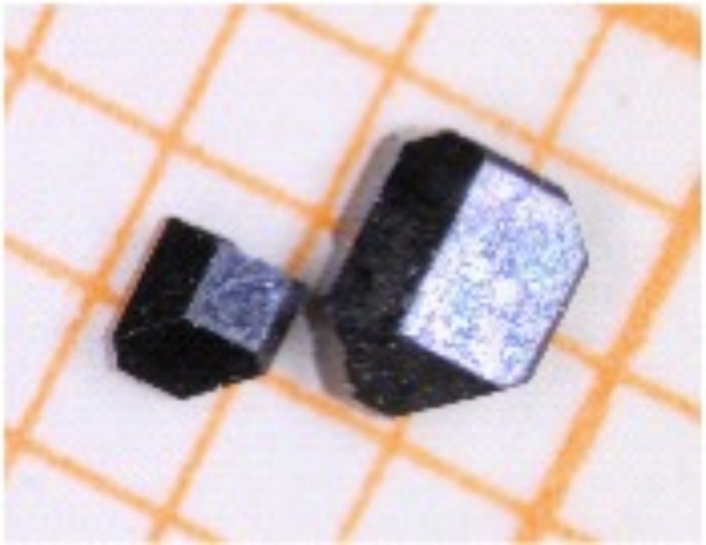
- Mystery at low temperature (T<3K)
  => resistivity plateau and anomalous susceptibility behavior

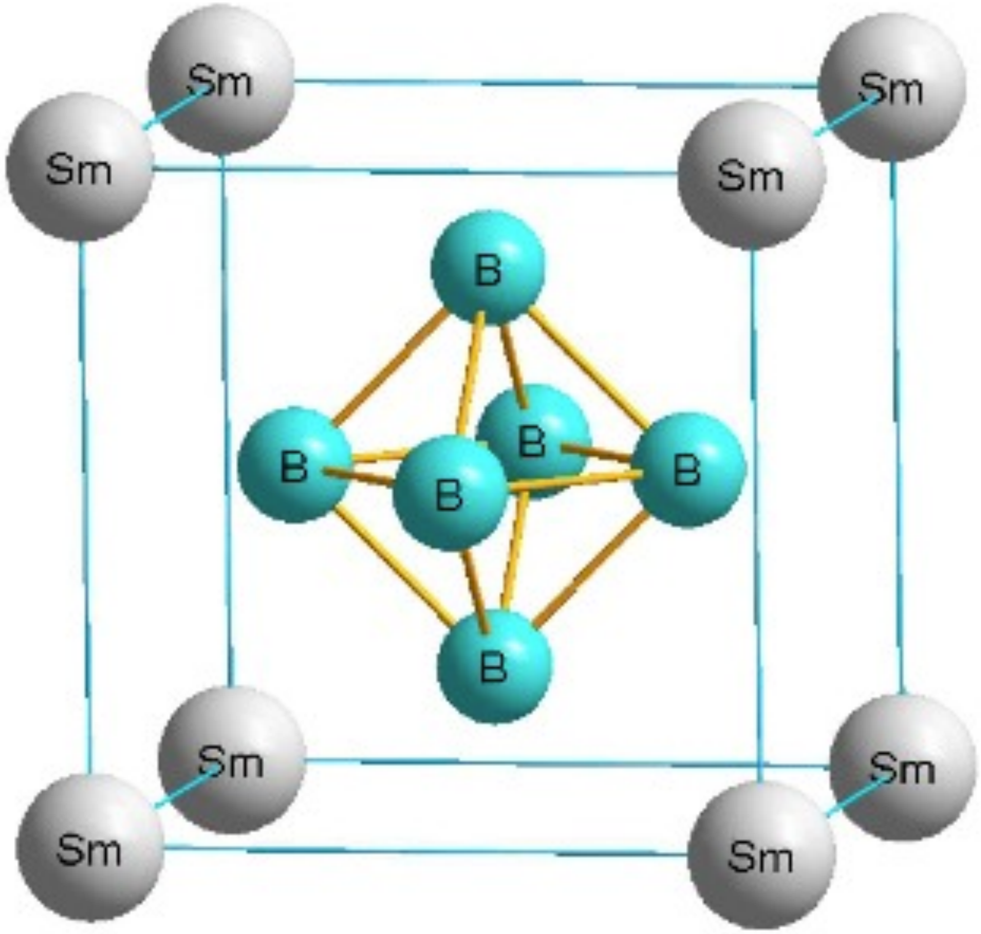
- The strong correlation + strong SO coupling +
  inversion of the bands with opposite parity
  => interacting TI candidate

- It is a true bulk insulator, unlike the other known TI

SmB6 Analysis - band theory and symmetry

What is SmB6





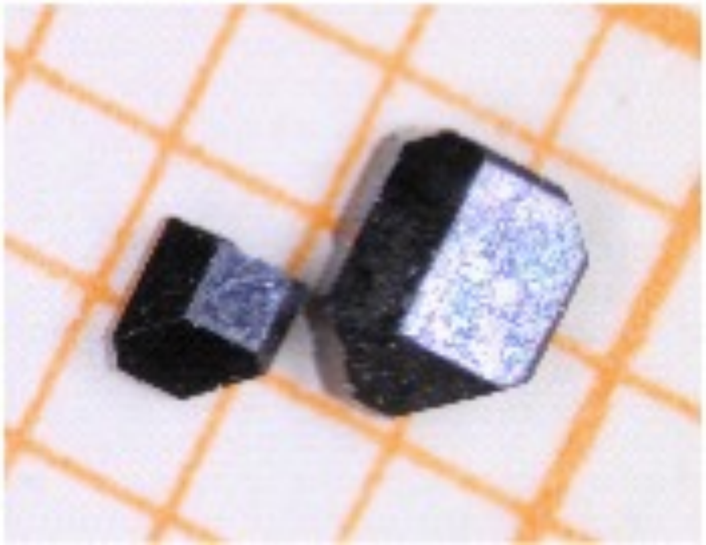
Ground state config of Sm

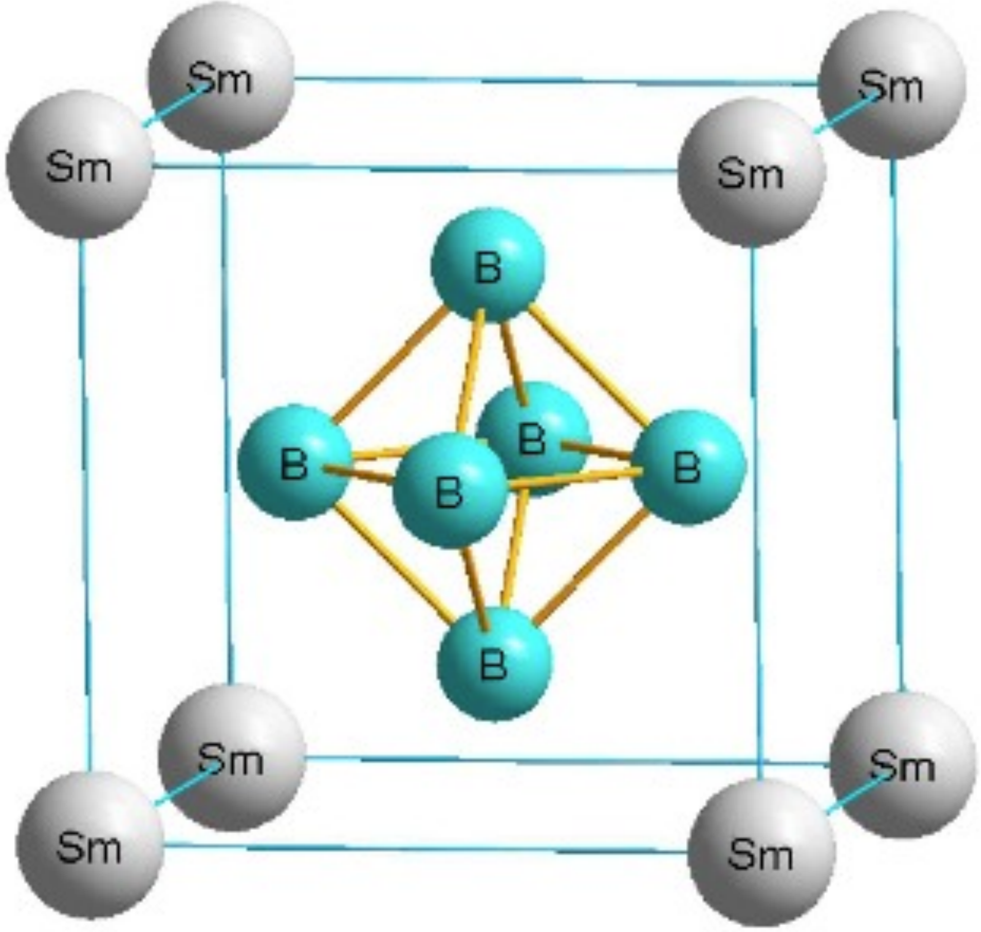
$$[Xe]4f^6 6s^2$$

Main role - Sm
Supporting role - B

draw the chemical picture

What is SmB6





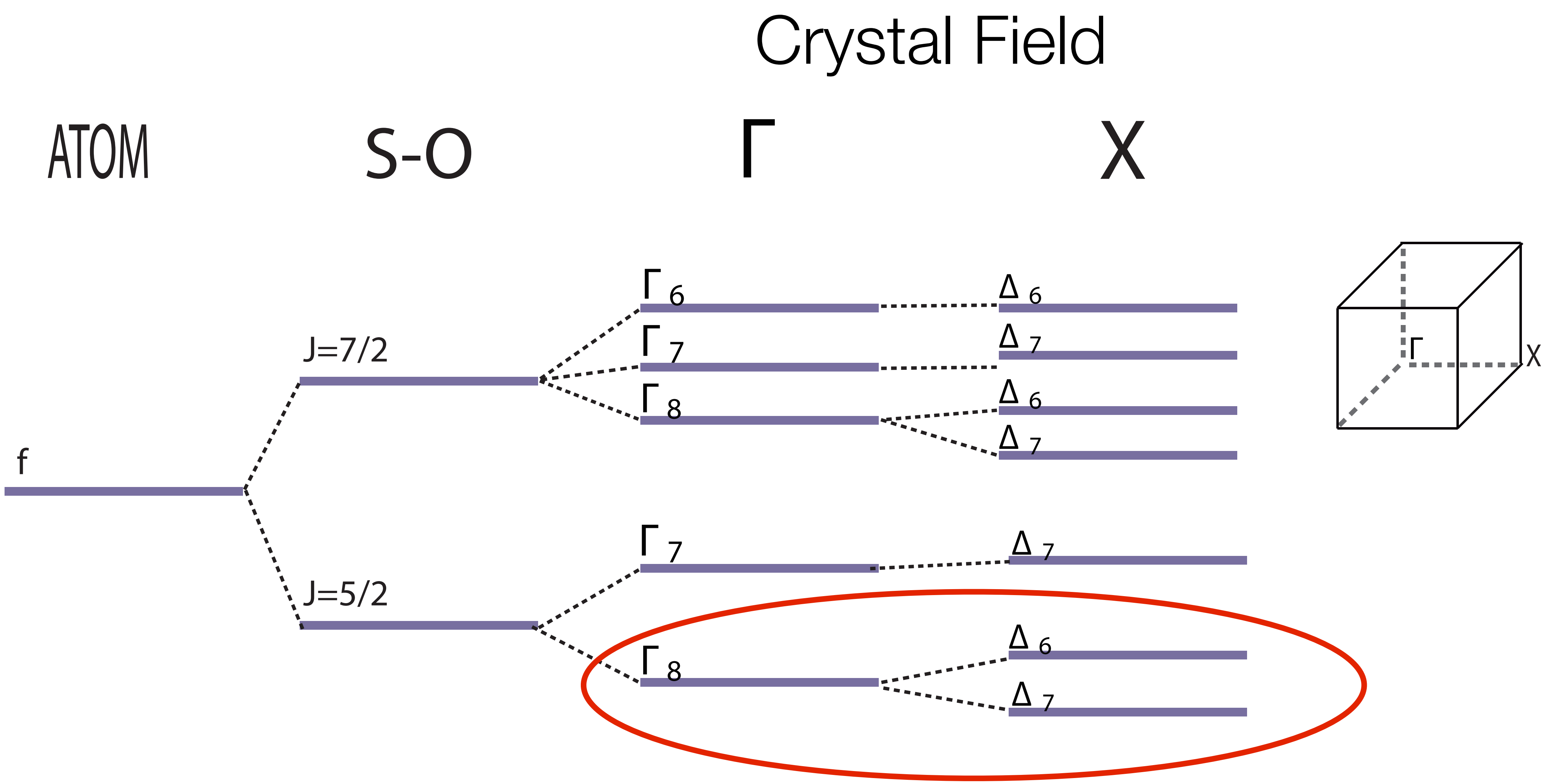
Conduction electron

Sm - 5d + B- 2p

Localized electron

Sm - 4f

SmB6 Band Configuration - Group Theory



Assuming atomic force > S-O > crystal field

mention the degeneracy and predict the band diagram from here

SmB6 Band Configuration - Group Theory

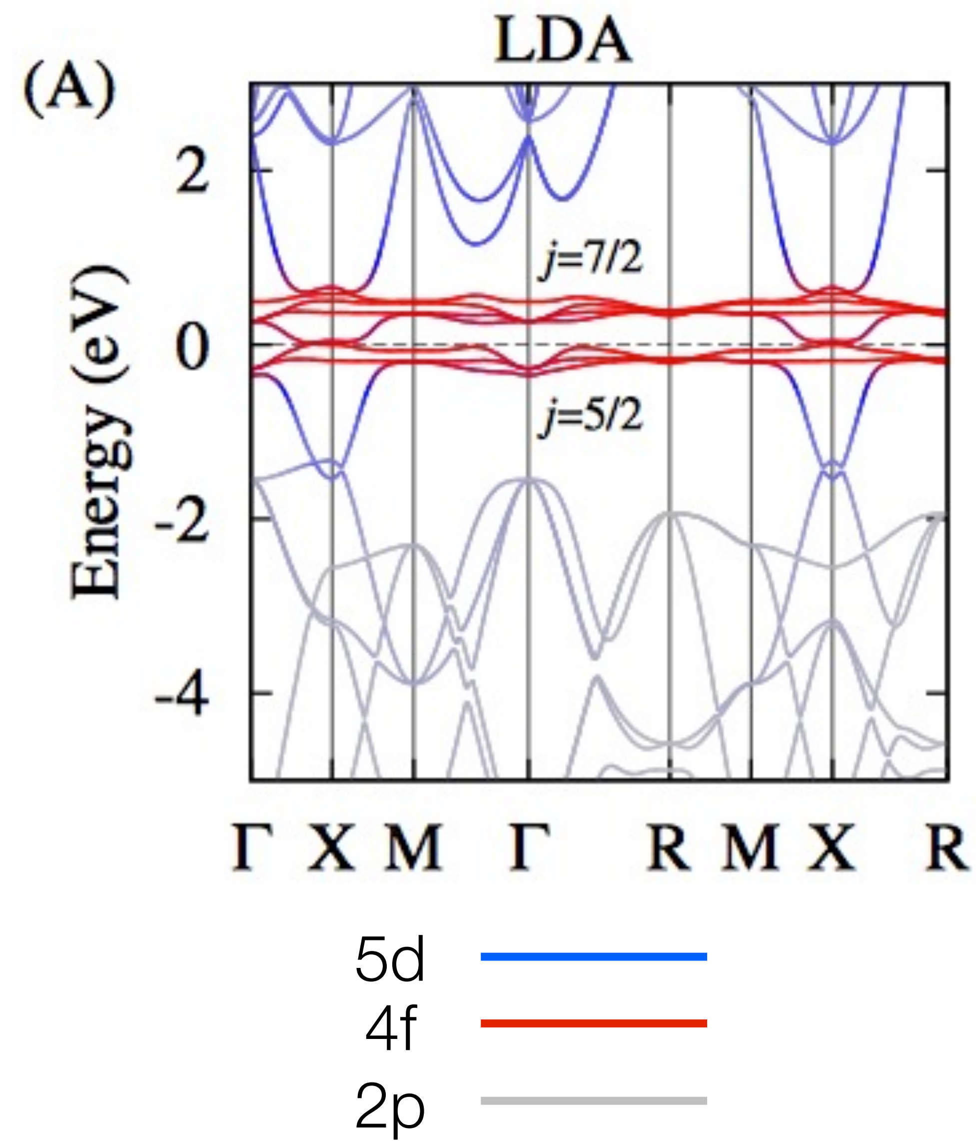
- Consider the bands near Fermi level.

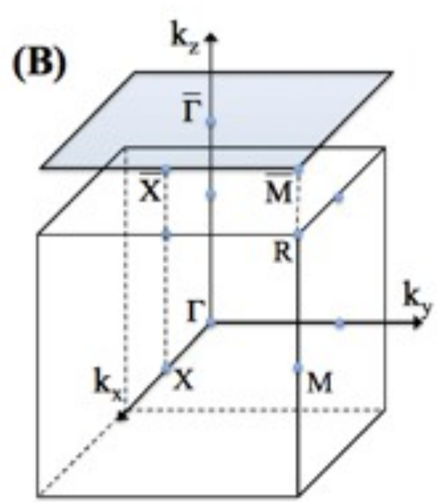
  Choose conduction e : $5d_{J=5/2}\Gamma_8$

  localized e : $4f_{J=5/2}\Gamma_8$

- These states are in the Double group $\tilde{O}$

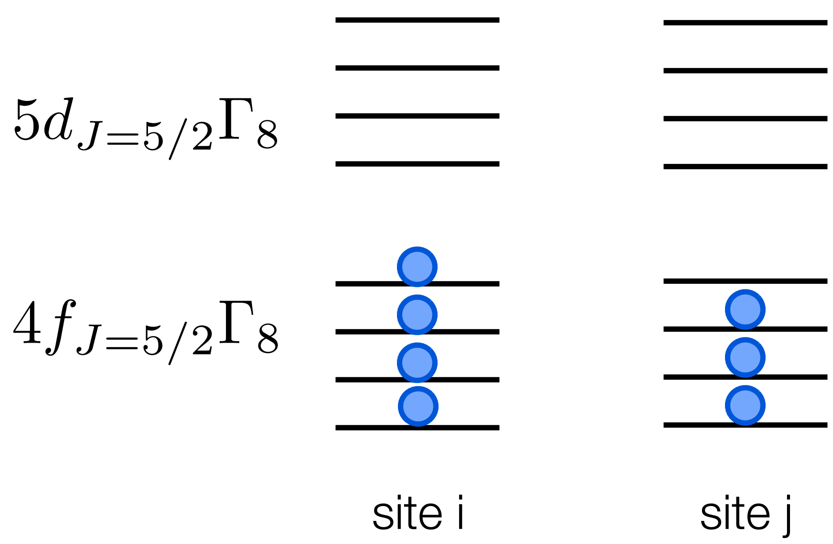
  Γ_8 is four fold degeneracy





Model Setup - PAM

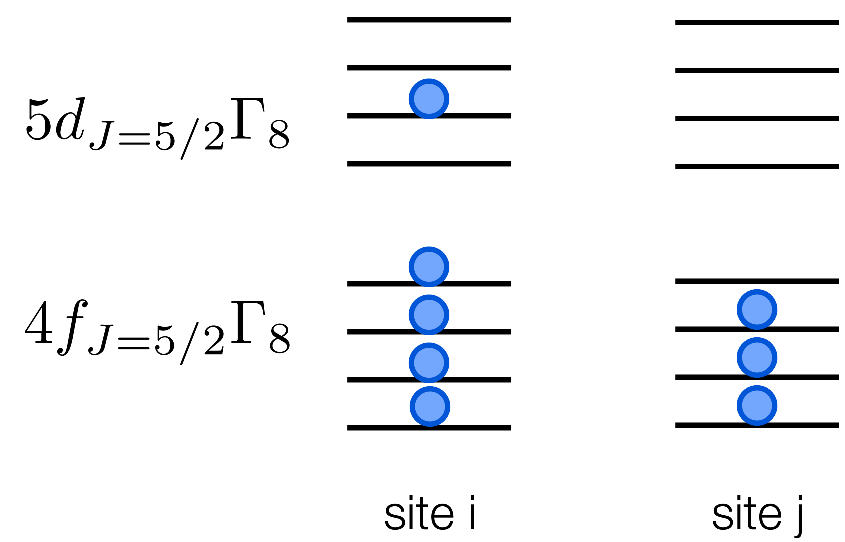
$$\hat{H} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mu} \varepsilon^{(f)}_{\mathbf{k}} \hat{f}^{\dagger}_{\mathbf{k}\mu} \hat{f}_{\mathbf{k}\mu} + \sum_{\mathbf{k}\mu\sigma} \left(V^{*}_{\mathbf{k}\sigma\mu} \hat{f}^{\dagger}_{\mathbf{k}\mu} \hat{c}_{\mathbf{k}\sigma} + \mathrm{h.c.} \right) + \frac{1}{2} U_{ff} \sum_{i;\mu\neq\mu'} \hat{f}^{\dagger}_{i\mu} \hat{f}_{i\mu} \hat{f}^{\dagger}_{i\mu'} \hat{f}_{i\mu'},$$



$$4f^6 : 4f^5 \approx 3 : 7$$

Model Setup

$$\hat{H} = \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mu} \varepsilon^{(f)}_{\mathbf{k}} \hat{f}^{\dagger}_{\mathbf{k}\mu} \hat{f}_{\mathbf{k}\mu} + \sum_{\mathbf{k}\mu\sigma} \left(V^{*}_{\mathbf{k}\sigma\mu} \hat{f}^{\dagger}_{\mathbf{k}\mu} \hat{c}_{\mathbf{k}\sigma} + \mathrm{h.c.} \right) + \frac{1}{2} U_{ff} \sum_{i;\mu\neq\mu'} \hat{f}^{\dagger}_{i\mu} \hat{f}_{i\mu} \hat{f}^{\dagger}_{i\mu'} \hat{f}_{i\mu'},$$



$$4f^6 : 4f^5 \approx 3 : 7$$

ξ_k onsite + n.n. hopping

ϵ_k onsite + n.n. hopping

V n.n. hopping anisotropy hybridization gap

U_{ff} onsite

Hamiltonian for SmB6

- STRATEGY

1. Find the possible Hamiltonian allowed by the symmetry.
   Ex: rotation or time reversal...

$$H_{sym} + U f^\dagger f^\dagger f f$$

2. Do the slave boson procedure to absorb the repulsion term into effective Hamiltonian

$$H_{eff}$$

3. Diagonalize the H and study the band diagram

$$E_k$$

Hamiltonian for SmB6

- STEP ONE

Symmetry in SmB6

$\frac{\pi}{2}$ rotation along x, y, z direction, π reflection to x, y, z plane, TR

Operator transformation

$$\begin{aligned}
R^z(\pi/2)a^\dagger_{lms}R^z(\pi/2)^\dagger &= e^{-im\pi/2}e^{-is_z\pi/4}a^\dagger_{lms_z} \\
R^y(\pi/2)a^\dagger_{lms}R^y(\pi/2)^\dagger &= \Sigma\Lambda_{m'm}e^{-is_y\pi/4}a^\dagger_{lm's_z} \\
R^x(\pi/2)a^\dagger_{lms}R^x(\pi/2)^\dagger &= \Sigma e^{im'\pi/2}\Lambda_{m'm}e^{-im\pi/2}e^{-is_x\pi/4}a^\dagger_{lm's_z} \\
R_x a^\dagger_{lms}R^\dagger_x &= \sigma_x a^\dagger_{l,-ms} \\
R_y a^\dagger_{lms}R^\dagger_y &= \sigma_y(-1)^m a^\dagger_{l,-ms} \\
R_z a^\dagger_{lms}R^\dagger_z &= \sigma_z(-1)^{l+m} a^\dagger_{lms} \\
T a^\dagger_{lms}T^\dagger &= e^{-i\pi\sigma_y/2}(-1)^m a^\dagger_{l-ms}
\end{aligned}$$

Hamiltonian for SmB6

- STEP ONE

Hamiltonian respect to Symmetry

$$OHO^\dagger = H$$

$$h(\mathbf{R}) = \begin{pmatrix} h^d(\mathbf{R}) & V(\mathbf{R}) \\ V^\dagger(\mathbf{R}) & h^f(\mathbf{R}) \end{pmatrix},$$

$$\begin{aligned}
H_d &= \mu_d \sum_r d_r^\dagger d_r + t^d \sum_r d_r^\dagger \begin{pmatrix} \mathbf{I} & 0 \\ 0 & \eta_d \mathbf{I} \end{pmatrix} d_{r\pm\hat{z}} \\
&+ t^d \sum_r d_r^\dagger \begin{pmatrix} (\frac{1}{4} + \frac{3}{4}\eta_d)\mathbf{I} & (\frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4}\eta_d)\mathbf{I} \\ (\frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4}\eta_d)\mathbf{I} & (\frac{3}{4} + \frac{1}{4}\eta_d)\mathbf{I} \end{pmatrix} d_{r\pm\hat{x}} \\
&+ t^d \sum_r d_r^\dagger \begin{pmatrix} (\frac{1}{4} + \frac{3}{4}\eta_d)\mathbf{I} & -(\frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4}\eta_d)\mathbf{I} \\ -(\frac{\sqrt{3}}{4} - \frac{\sqrt{3}}{4}\eta_d)\mathbf{I} & (\frac{3}{4} + \frac{1}{4}\eta_d)\mathbf{I} \end{pmatrix} d_{r\pm\hat{y}}
\end{aligned}$$

$$H_f = H_d(d \rightarrow f)$$
$$+U f^\dagger f^\dagger f f$$

$$\begin{aligned}
H_{df} &= \sum_r d_r^\dagger \begin{pmatrix} V_1\sigma_z & 0 \\ 0 & V_2\sigma_z \end{pmatrix} f_{r+\hat{z}} - d_r^\dagger h_{df}(\hat{z}) f_{r-\hat{z}} \\
&+ \sum_r d_r^\dagger \begin{pmatrix} -(\frac{1}{4}V_1 + \frac{3}{4}V_2)\sigma_x & -\frac{\sqrt{3}}{4}(V_1 - V_2)\sigma_x \\ -\frac{\sqrt{3}}{4}(V_1 - V_2)\sigma_x & -(\frac{3}{4}V_1 + \frac{1}{4}V_2)\sigma_x \end{pmatrix} f_{r+\hat{x}} - d_r^\dagger h_{df}(\hat{x}) f_{r-\hat{x}} \\
&+ \sum_r d_r^\dagger \begin{pmatrix} -(\frac{1}{4}V_1 + \frac{3}{4}V_2)\sigma_y & \frac{\sqrt{3}}{4}(V_1 - V_2)\sigma_y \\ \frac{\sqrt{3}}{4}(V_1 - V_2)\sigma_y & -(\frac{3}{4}V_1 + \frac{1}{4}V_2)\sigma_y \end{pmatrix} f_{r+\hat{y}} - d_r^\dagger h_{df}(\hat{y}) f_{r-\hat{y}}
\end{aligned}$$

Hamiltonian for SmB6

- STEP ONE

Hamiltonian in Momentum Space

$$H_d = \mu_d \sum_k d_k^\dagger d_k + \frac{t^d}{2} \sum_k d_k^\dagger \begin{pmatrix} (\phi_1 + \eta_d \phi_2)\mathbf{I} & (1-\eta_d)\phi_3 \mathbf{I} \\ (1-\eta_d)\phi_3 \mathbf{I} & (\phi_2 + \eta_d \phi_1)\mathbf{I} \end{pmatrix} d_k$$

where $\phi_1 = \cos k_x + \cos k_y + 4\cos k_z$, $\phi_2 = 3(\cos k_x + \cos k_y)$, $\phi_3 = \sqrt{3}(\cos k_x - \cos k_y)$,

$H_f = H_d(d \to f)$ $+U f^\dagger f^\dagger f f$

$$H_{df} = -\frac{i}{2} \sum_k d_k^\dagger \begin{pmatrix} 4V_1\tilde{\sigma}_z - (V_1 + 3V_2)(\tilde{\sigma}_x + \tilde{\sigma}_y) & \sqrt{3}(V_2 - V_1)(\tilde{\sigma}_x - \tilde{\sigma}_y) \\ \sqrt{3}(V_2 - V_1)(\tilde{\sigma}_x - \tilde{\sigma}_y) & 4V_2\tilde{\sigma}_z - (3V_1 + V_2)(\tilde{\sigma}_x + \tilde{\sigma}_y) \end{pmatrix} f_k$$

where $\tilde{\sigma}_i = \sigma_i \sin k_i$.

Hamiltonian for SmB6

- STEP TWO

Absorb the Correlation Term by Slave Boson

$$H_f = U \sum_i \sum_{\alpha=1}^{4} \sum_{\beta \neq \alpha} f_{i\alpha}^\dagger f_{i\alpha} f_{i\beta}^\dagger f_{i\beta}$$

consider infinite U, where we can project out all the states with $n_f > 1$, by replacing the bare f field by Hubbard operators X.

$$f_{i\alpha}^\dagger \to X_{\alpha 0}(i) = f_{i\alpha}^\dagger b_i, \quad f_{i\alpha} \to X_{0\alpha}(i) = b_i^\dagger f_{i\alpha},$$

$$\sum_{\alpha=1} f_{i\alpha}^\dagger f_{i\alpha} + b_i^\dagger b_i = 1.$$

Partition function

$$L = \sum_i b_i^\dagger \frac{d}{d\tau} b_i + \sum_{ij} \sum_{\alpha,\beta=1}^{4} f_{i\alpha}^\dagger \left[\delta_{ij}\delta_{\alpha\beta} \left(\frac{d}{d\tau} + \varepsilon_f \right) + b_i t_{ij,\alpha\beta}^{(f)} b_j^\dagger \right] f_{j\beta} + \sum_{\mathbf{k}\sigma} \sum_{a,b=1}^{2} c_{a\mathbf{k}\sigma}^\dagger \left(\frac{d}{d\tau} + \varepsilon_{ab}^{(d)}(\mathbf{k}) \right) c_{b\mathbf{k}\sigma}$$
$$+ \frac{1}{2} \sum_{\langle ij \rangle} \sum_{\mathbf{k}\sigma} \sum_{a=1}^{2} \sum_{\beta=1}^{4} \left(V_{ia\sigma,j\beta} c_{ai\sigma}^\dagger b_i^\dagger f_{j\beta} + \text{h.c.} \right) + \sum_j i\lambda_j \left(\sum_{\alpha=1}^{4} f_{j\alpha}^\dagger f_{j\alpha} + b_j^\dagger b_j - 1 \right)$$

Hamiltonian for SmB6

After the mean field approximation (saddle point), the min value is at

$$b_{\mathbf{q}}(\tau) = b\delta_{\mathbf{q},0}, \quad i\lambda_{\mathbf{q}}(\tau) = (E_f - \varepsilon_f)\delta_{\mathbf{q},0},$$

Put this back to Lagrangian, and it reduced to $L = L_0 + H_v$

$$L_0(\tau) = (b^2-1)(E_f-\varepsilon_f) + \sum_{\mathbf{k}\alpha}\sum_{n=1}^{2} \tilde{f}^{\dagger}_{n\mathbf{k}\alpha}\left(\frac{d}{d\tau} + E^{(f)}_{n\mathbf{k}}\right)\tilde{f}_{n\mathbf{k}\alpha} + \sum_{\mathbf{k}\sigma}\sum_{a=1}^{2} d^{\dagger}_{a\mathbf{k}\sigma}\left(\frac{d}{d\tau} + E^{(d)}_{a\mathbf{k}}\right)d_{a\mathbf{k}\sigma}$$

$$\widetilde{H}_V = iV_{df}\frac{b}{2}\sum_{\mathbf{k}} \hat{d}^{\dagger}_{\mathbf{k}\alpha}[\hat{\Phi}_{\mathbf{k}}]_{\alpha\beta}\tilde{f}_{\mathbf{k}\beta} + \text{h.c.},$$

In short, we will have a 2X2 effective H with renormalized $E_f \quad V$

$$\boxed{\begin{aligned} t_f &\to b^2 t_f \\ V_{df} &\to bV_{df}. \end{aligned}}$$

$$b^2 + \langle n_f \rangle = 1$$

Hamiltonian for SmB6

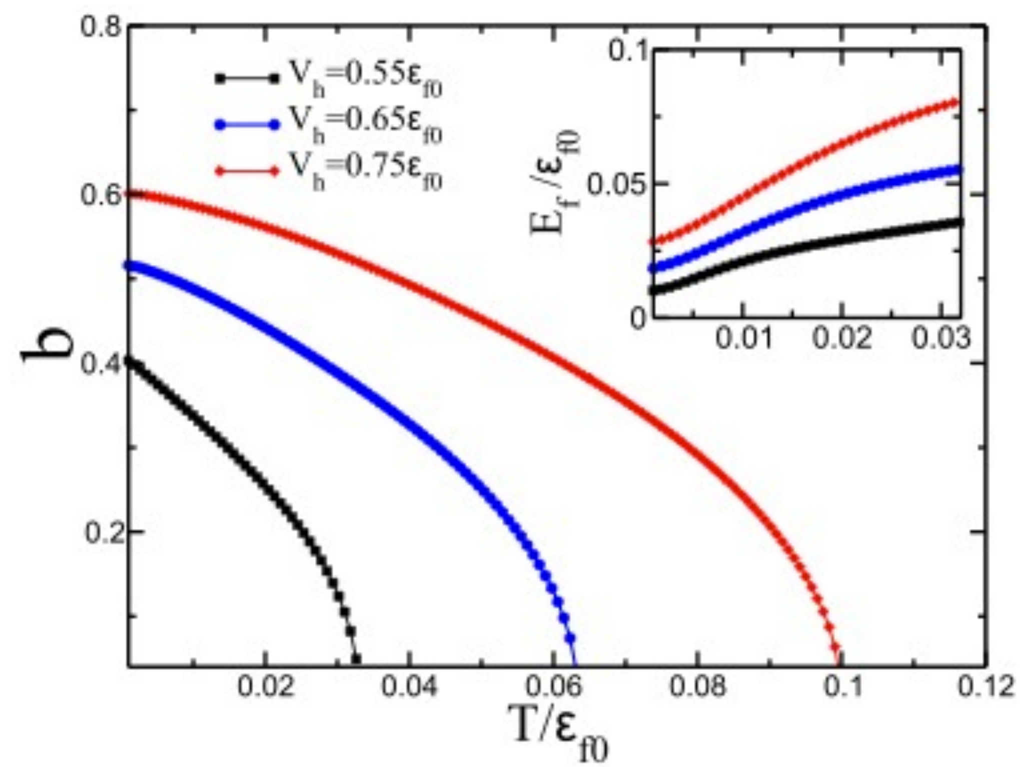
We can further integrate out the conduction field, and run the saddle point again. Then we can study the Lagrangian with finite temperature.

$$\frac{\partial S_{eff}}{\partial E_f} = 0, \quad \frac{\partial S_{eff}}{\partial b} = 0.$$

$$b^2 - 1 + 2\sum_{i=1}^{4}\sum_{\mathbf{k}} \frac{f(\varepsilon_{i\mathbf{k}}) n_F(\varepsilon_{i\mathbf{k}})}{\prod_{l\neq i}(\varepsilon_{i\mathbf{k}} - \varepsilon_{l\mathbf{k}})} = 0, \quad n_F(x) = \frac{1}{e^{\beta x}+1},$$

Mean Field Equation

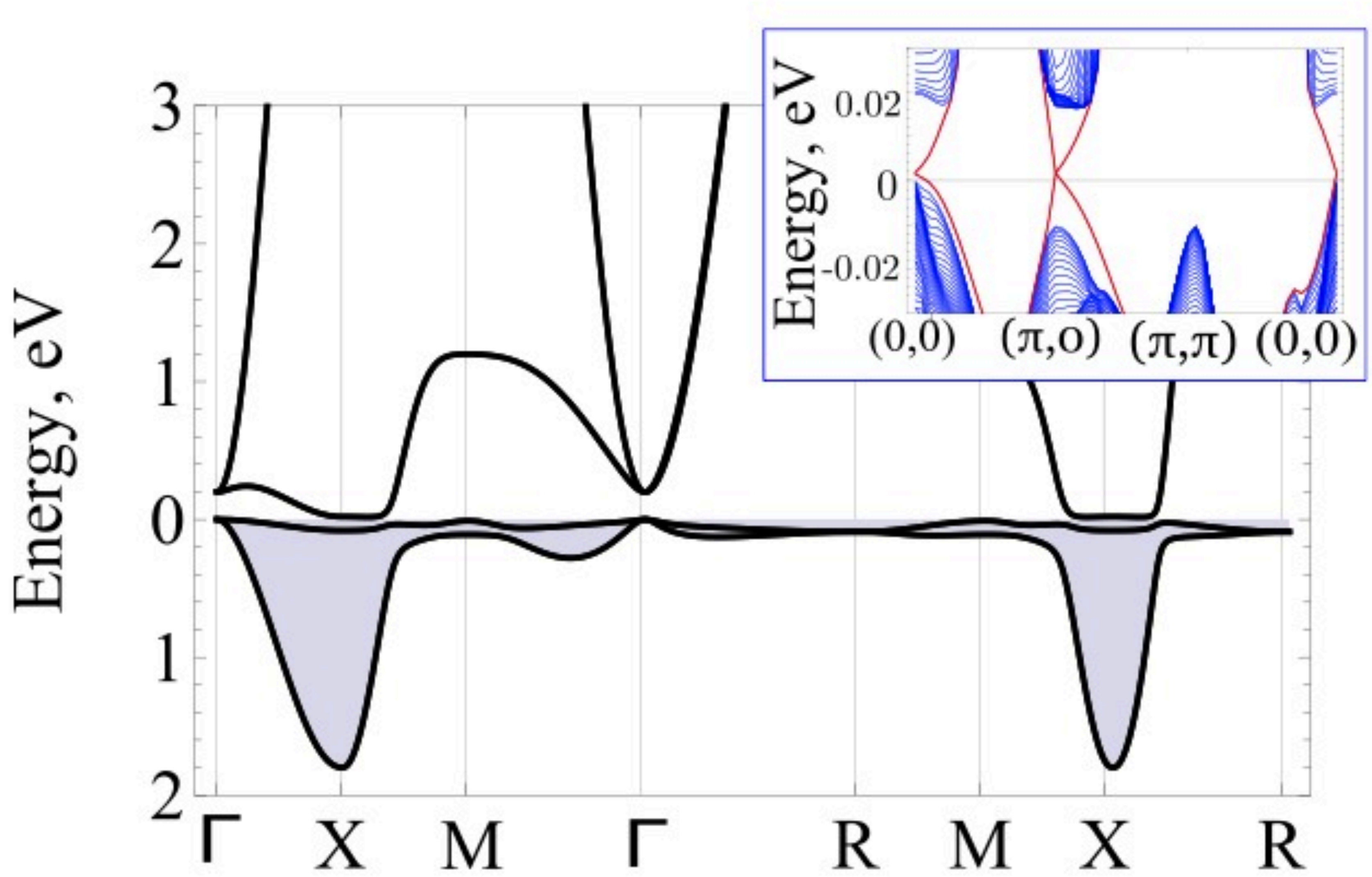
$$8(E_f - \varepsilon_f) + 2\sum_{i=1}^{4}\sum_{\mathbf{k}} \frac{\partial \varepsilon_{i\mathbf{k}}}{\partial E_f} n_F(\varepsilon_{i\mathbf{k}}) = 0.$$

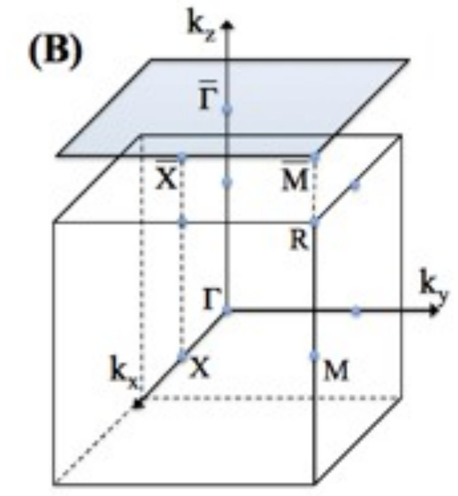


Hamiltonian for SmB6

- STEP THREE

ENERGY DIAGRAM AND PFT DIAGRAM





$\Delta = 15meV$

The gap is opened by the hybridization of d, f bands

SmB6 - Is it topological? Really?

Z2 number

- Based on Hasan and Kane's work, a 3D TI insulator is characterize by four $\mathbb{Z}_2$ topological invariants $(\nu_0;\nu_1\nu_2\nu_3)$

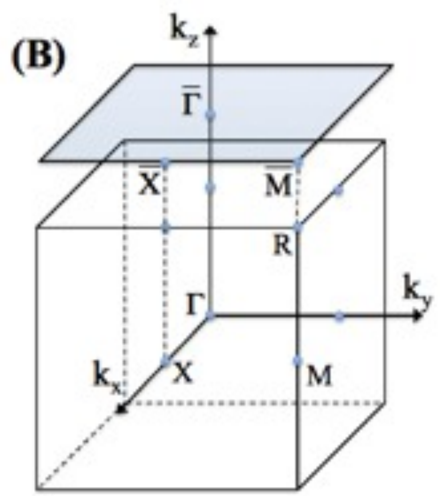
strong TI index

$$I_{STI} = (-1)^{\nu_0} = \prod_{m=1}^{8} \delta_m = \pm 1$$

weak TI index

$$I^a_{WTI} = (-1)^{\nu_a} = \prod_{k_m \in P_j} \delta_m = \pm 1$$

$$\delta_m = \mathrm{sgn}(\xi_{\mathbf{k}^*_m} - \tilde{\varepsilon}^{(f)}_{\mathbf{k}^*_m})$$



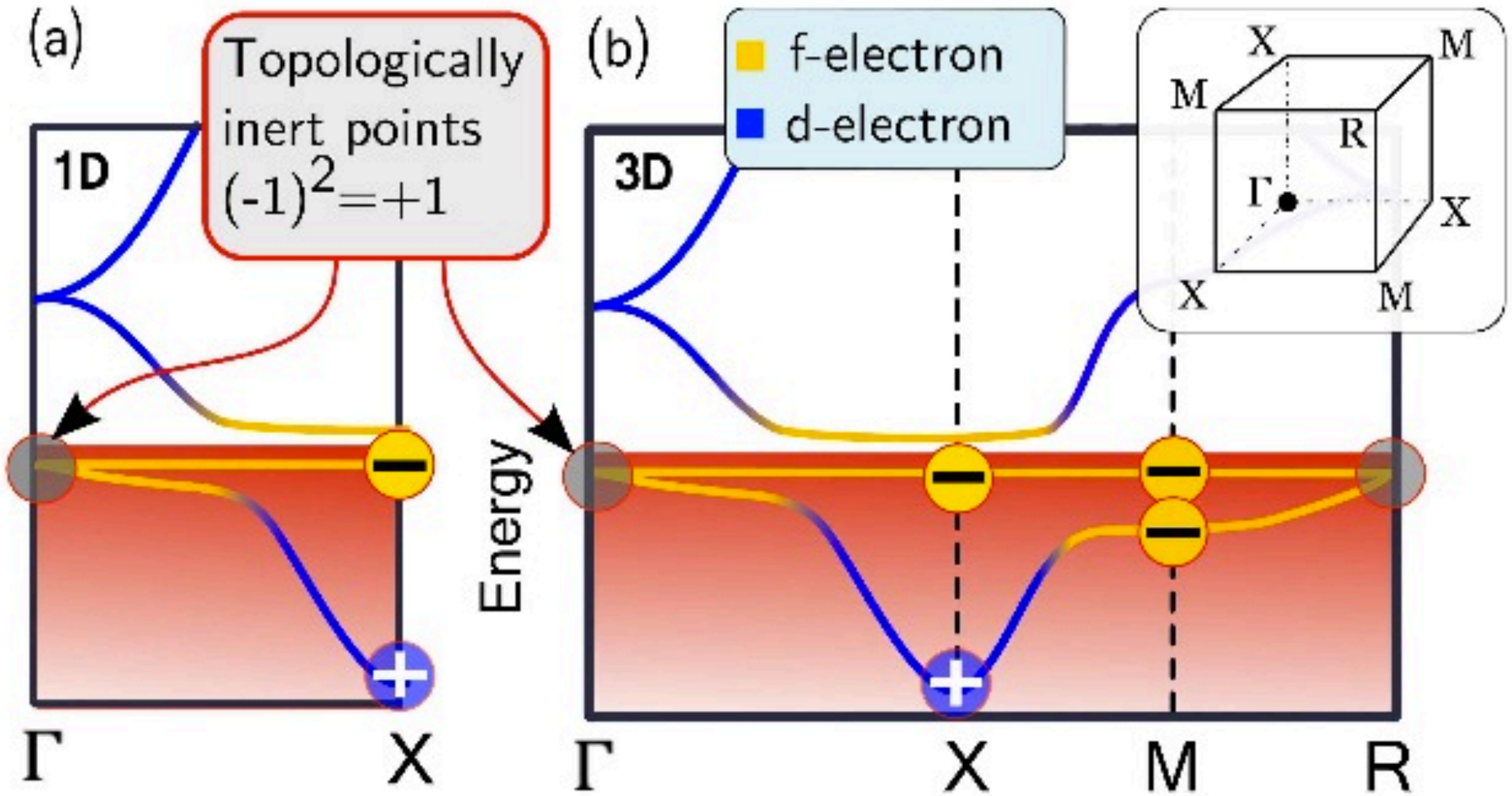
Example

conventional insulator $(0;0,0,0)$

STI $(1;0,0,0)$

WTI $(0;1,1,1)$

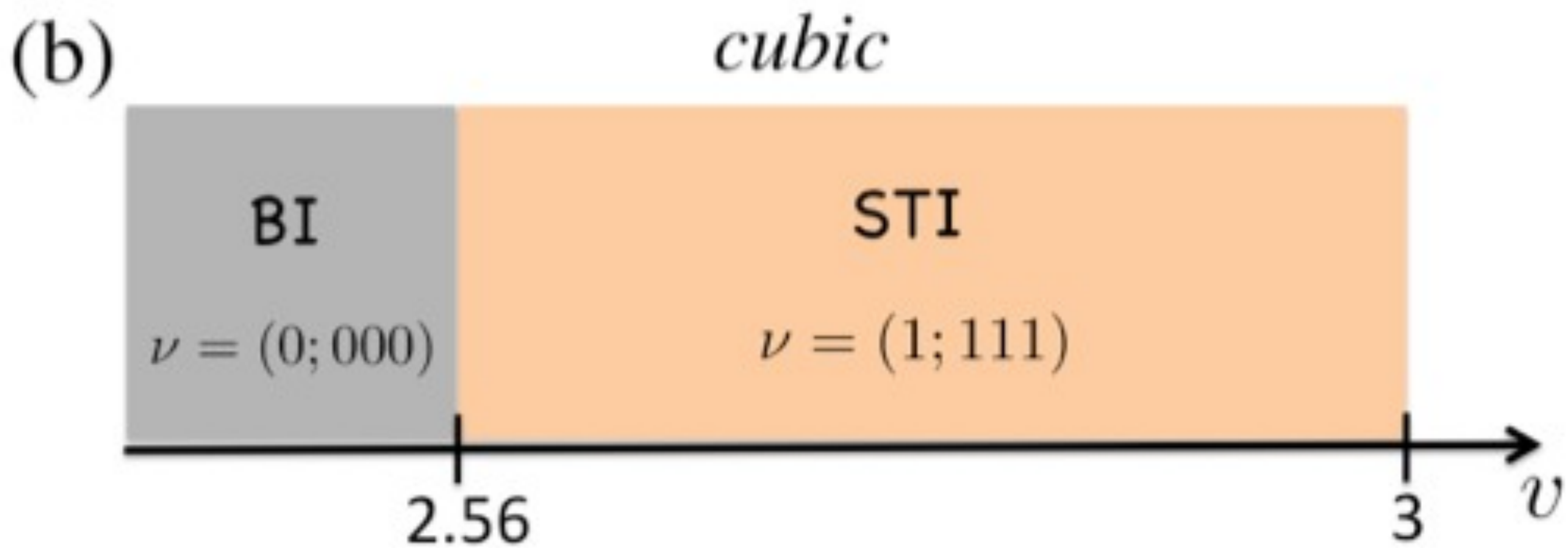
Z2 number for SmB6



$\delta =$ 1 -1 1 1

Z2 number = (1; 1, 1, 1)

Z2 number for SmB6



$$v = 3 - n_f$$

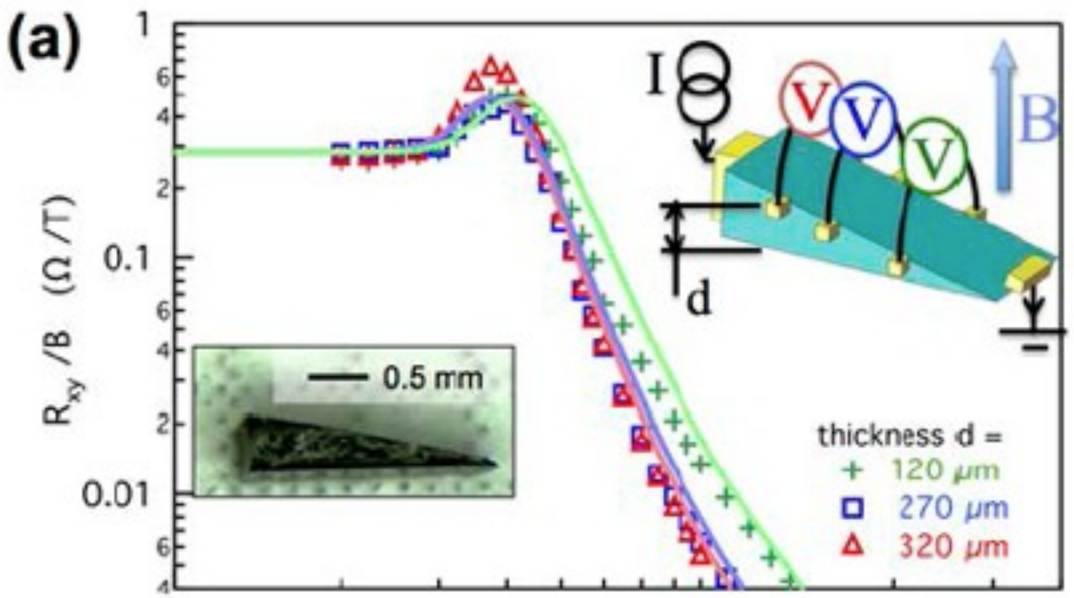
- v gives the valence of the Sm ion, while n_f measures the number of f-holes in the filled $4f^6$ state, so that $n_f = 1$ corresponds to the $4f^5$ configuration.

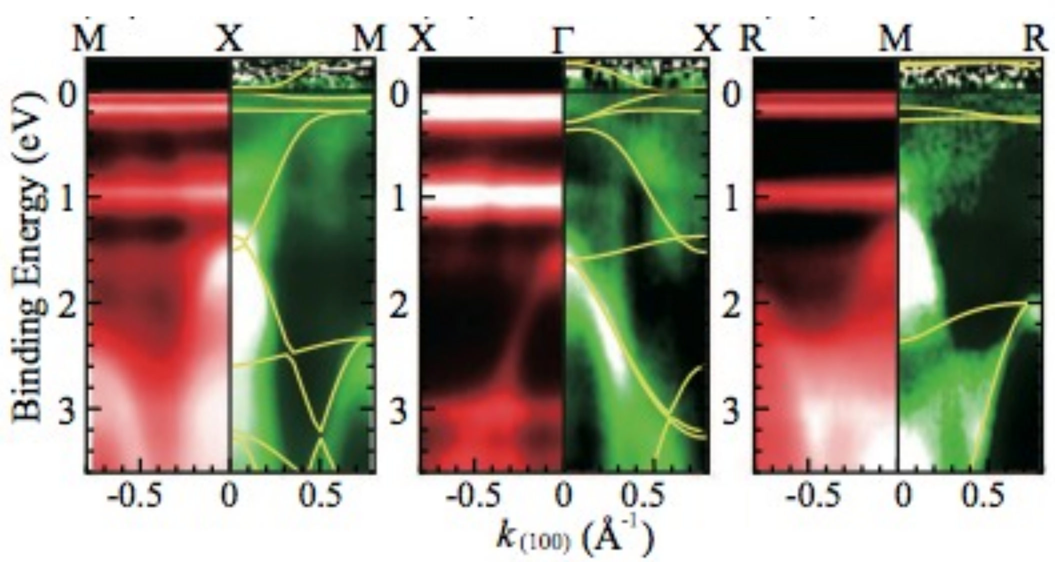
- SmB6 is mixed valence materials. $4f^{5.7}$

$$v = 3 - 0.3 = 2.7$$

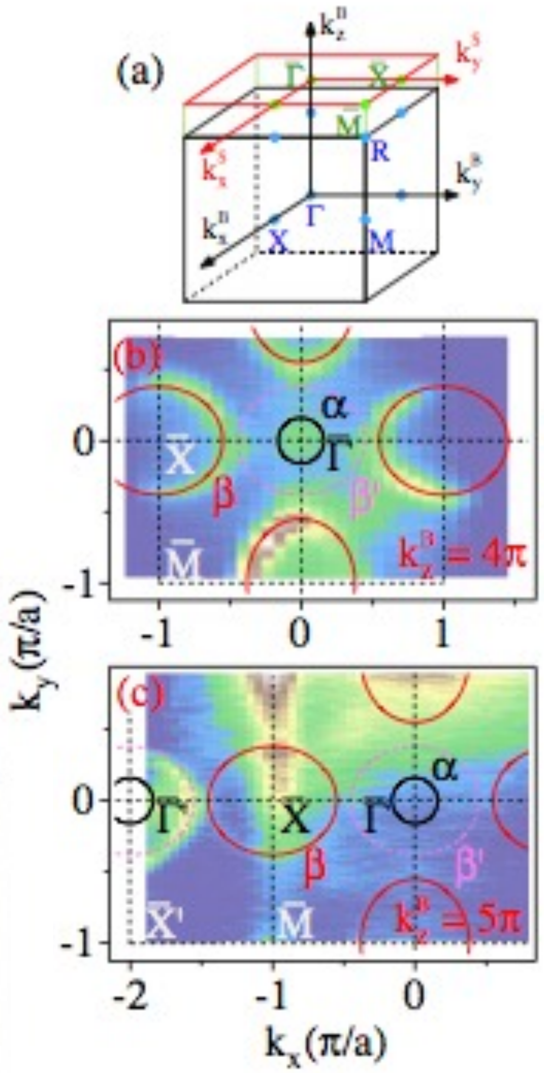
How does the experiment say?

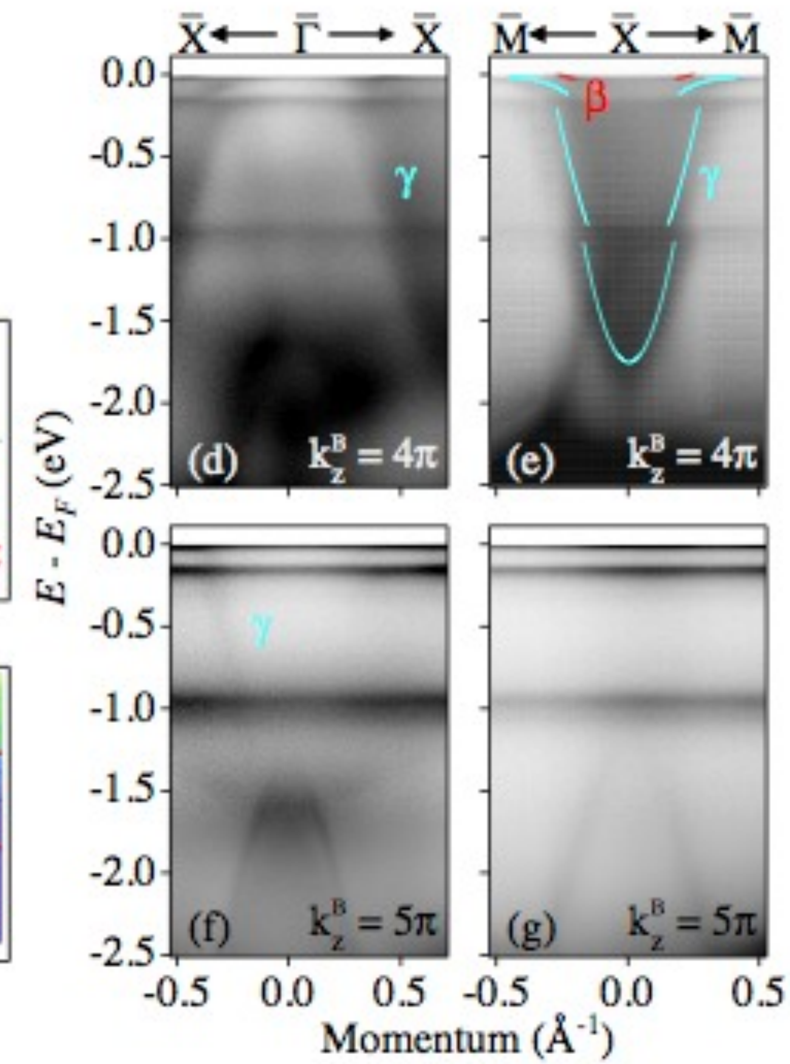
Transport





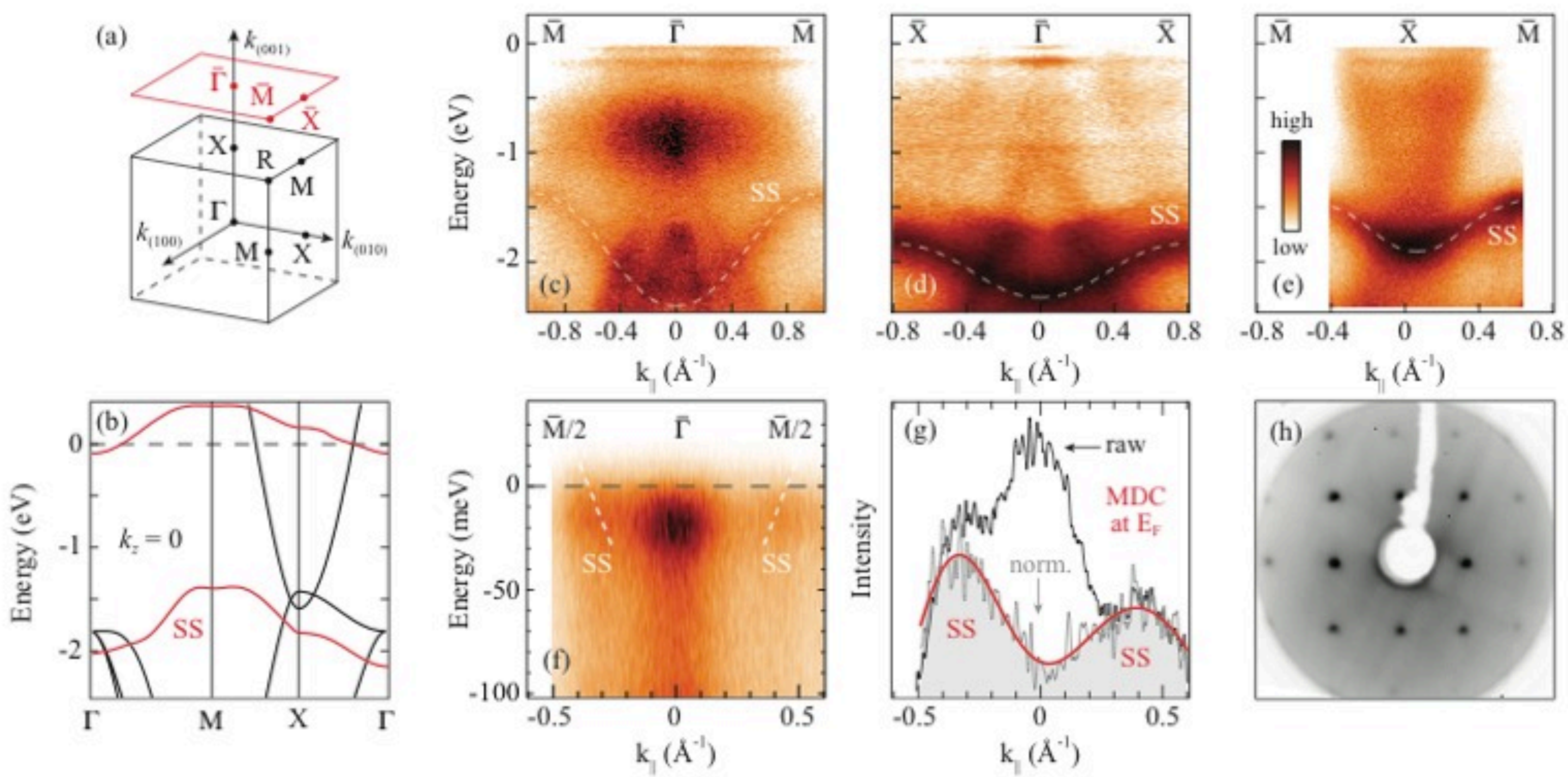
ARPES





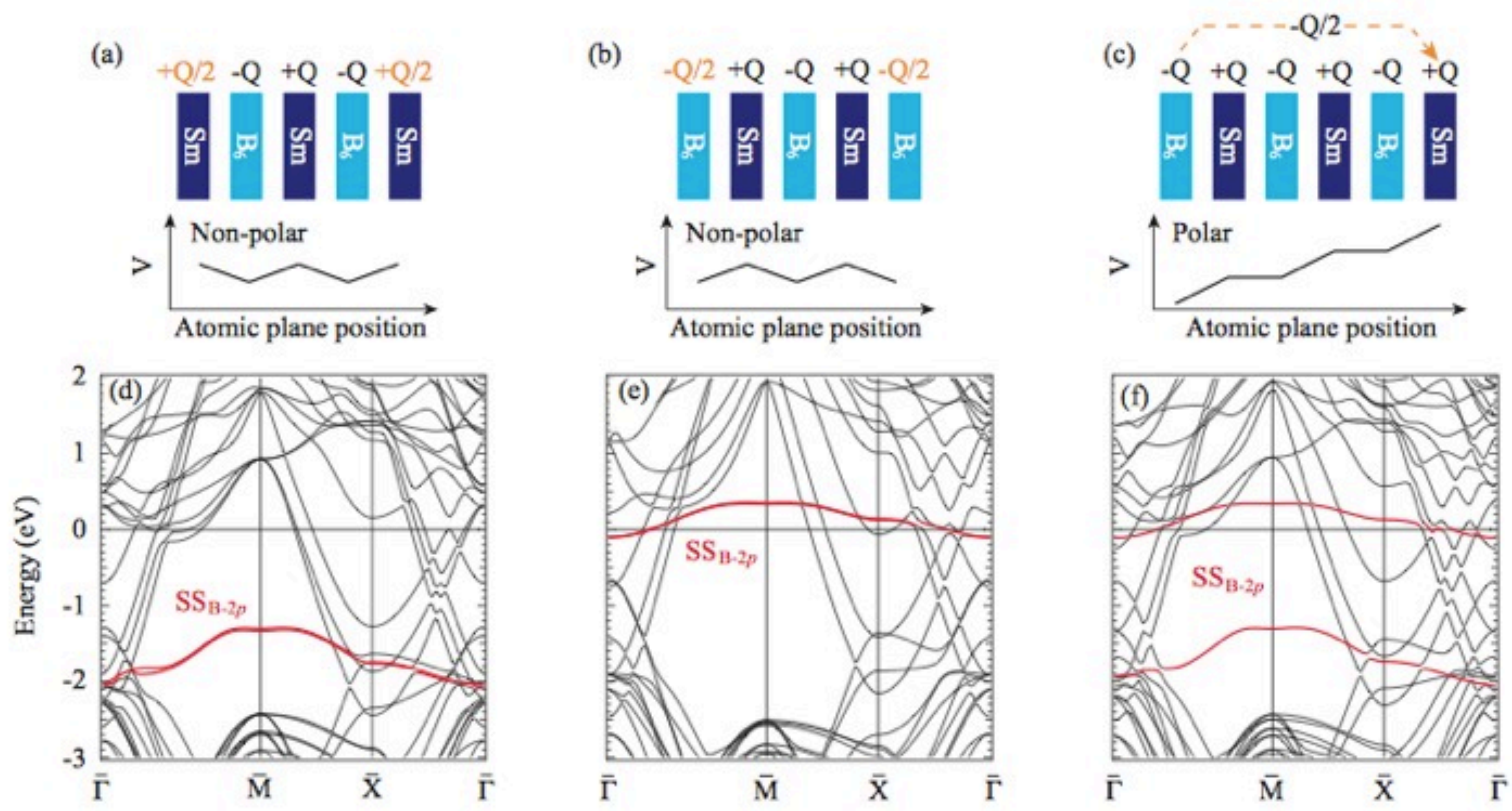
How does the experiment say?

- Other SS?



How does the experiment say?

- Some other possible SS... polarity.. band bending Fermi gas.. more



- More experiments like MR, QO, and magnetic doping .... Some support topo. SS, and some against it...

Review and Question

Review

- The Kondo insulator which is a true insulator has strong electron correlation and spin-orbital coupling => An ideal TI candidate
- The PAM + symmetry constraint + slave boson => effective H
- The energy diagram and the PFT result show the existence of gap and edge state
- The Z2 number = -1. Theoretical prediction of TKI. However, experiments are needed to verify it.

Question

- Can Kondo insulator adiabatically connect to normal insulator?
- Does U help to increase the TI phase?
- How does SmB6 behave under different T, P, B ? And the phase diagram?
- The Kondo screening, spin configuration in SmB6?
- Is the edge state really topological? What is the origin of the S.S
- ......