The topological insulator with strong correlation effects

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Lu et al, PRL 110, 096401 (2013)

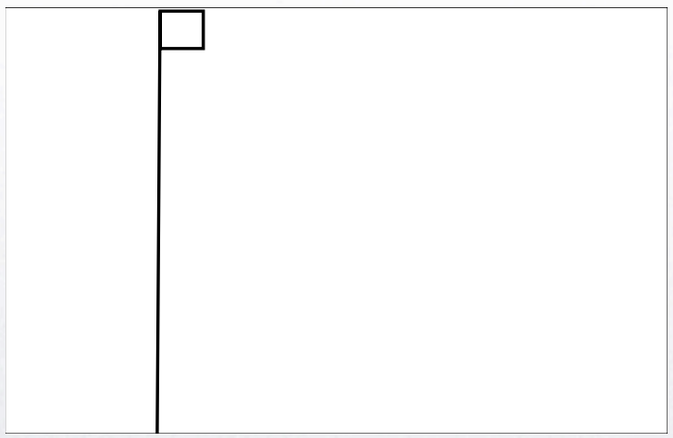
outline

- Band inversion and TI
- Mix valen e ompound: Band inversion between d and f bands; the important role of e-e intera tion
- SmB6 , YbB6, and YbB12
- Con lusion

Topologi al lassifi ation of band insulators

- normal insulator: the ele troni stru ture an be smoothly transformed to isolated atoms
- an not be smoothly transformed to isolated atoms without going through a phase transition, Z2 invarian e defined for non-intera ting TI
- TI with intera tion an be defined by the Theta angle of of topologi al magneto-ele tri effe t

Evolution of band stru ture from solid to isolated atoms

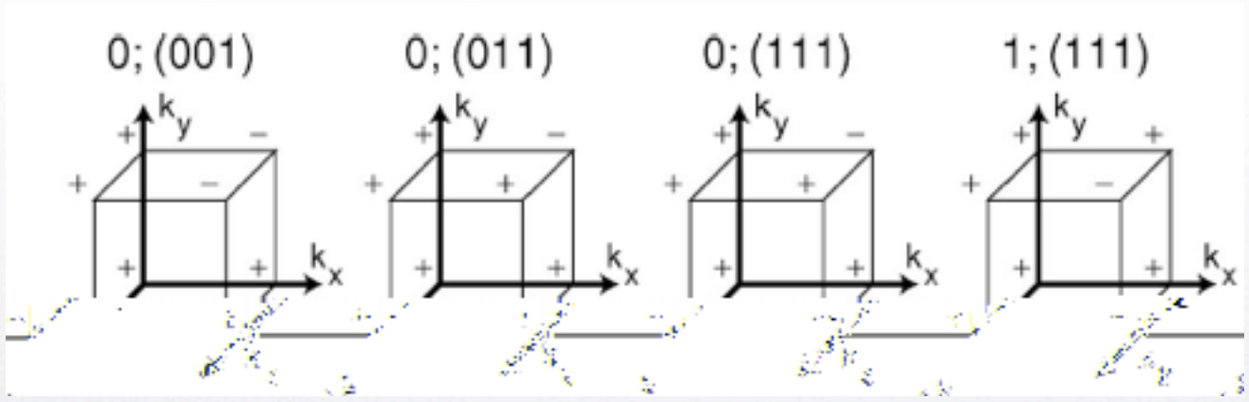


Z2 invarian e for non-intera ting TI with inversion symmetry

- **Simple rules for TI with inversion symmetry: strong index and weak indices; K=-K high symmetry points**

$$(-1)^{\nu_0} = \prod_{i=1}^{8} \delta_i .$$

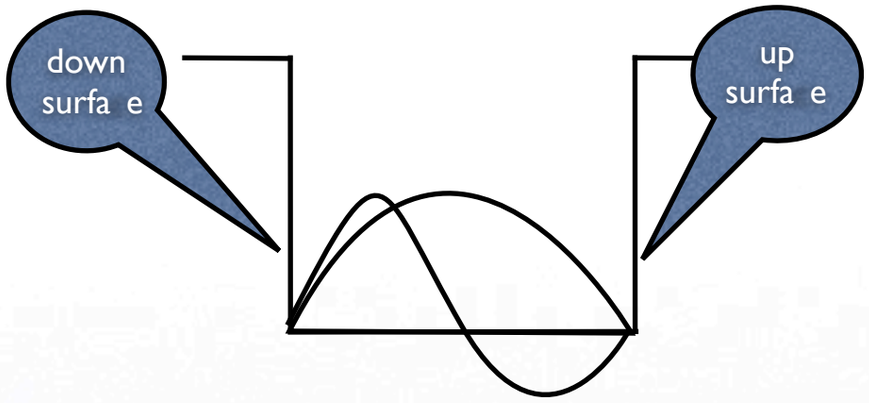
$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) .$$



L. Fu and C. Kane, PRB 76,045302

TI and surfa e states

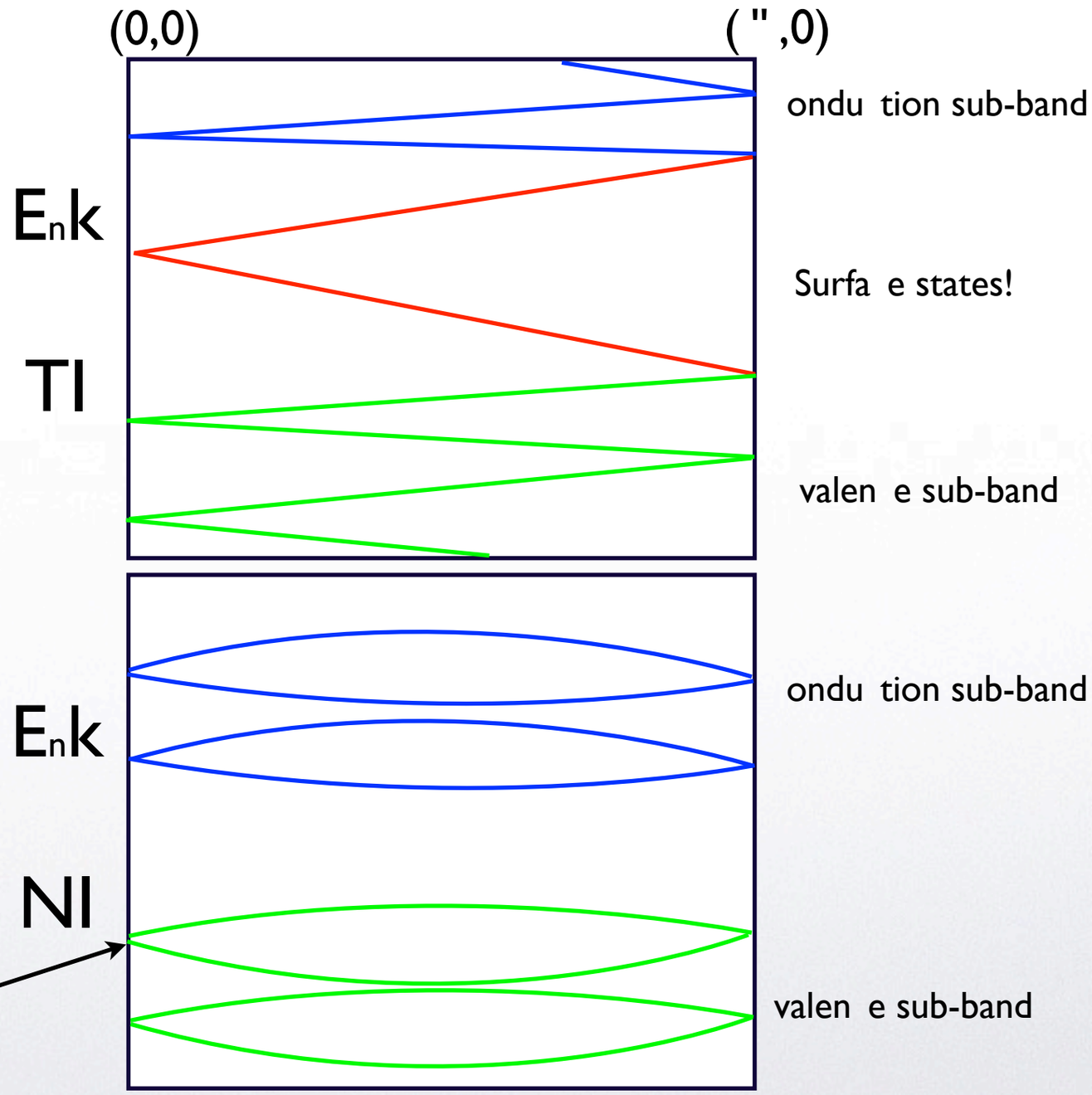
Consider a slab of TI



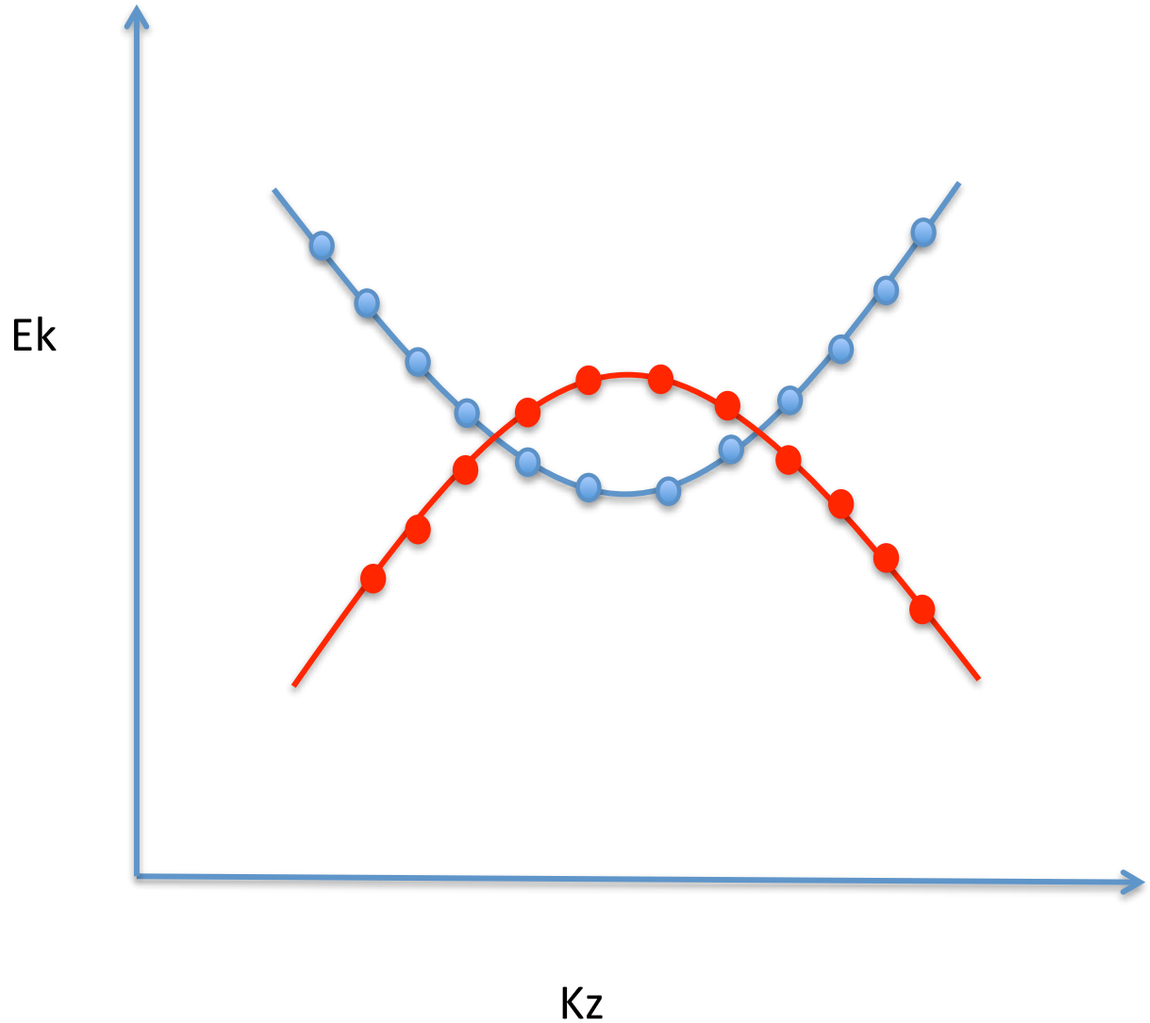
! n(kx,ky)

z

k= – k+G; Kramers degenera y



I d c :Ba d I e a d TI



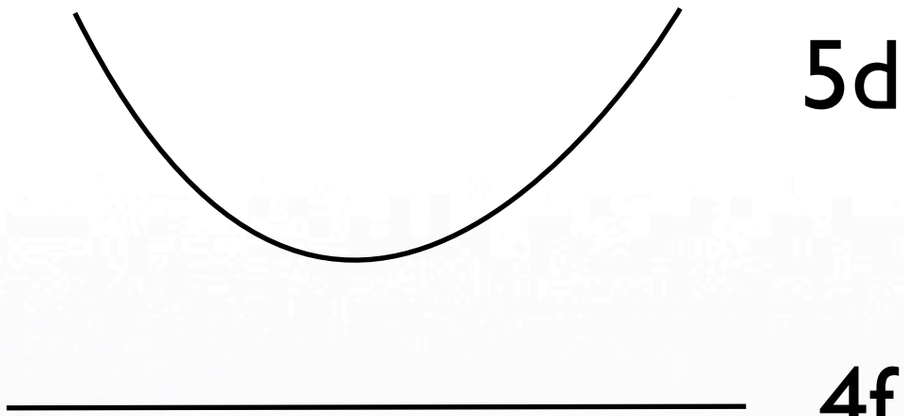
The different types of band inversion

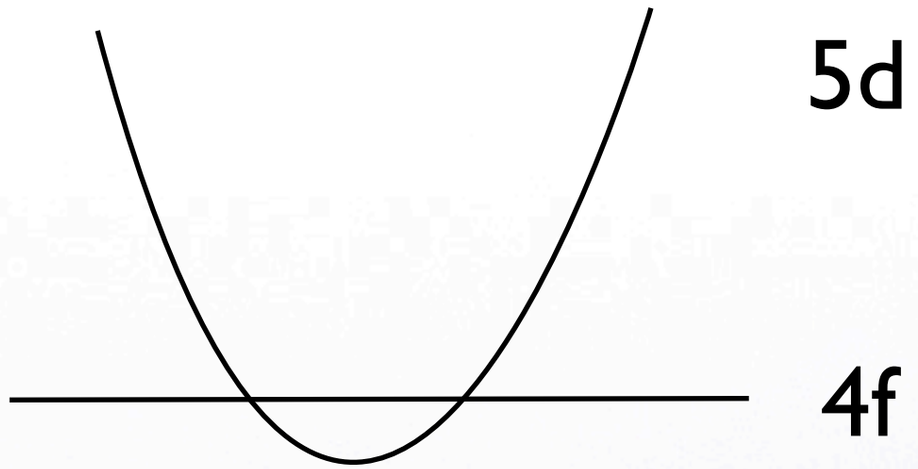
- Band inversion between s and p bands: HgTe
- Band inversion between bonding and anti-bonding p-bands: Bi2Se3, Sb
- Band inversion generated by valen e flu tuation of 4f/5f bands
- Very strong orrelation effe ts in f-ele tron materials:
- Does these materials topologi ally non-trivial?

4f/5f ompounds with intermediate valen e

- golden phase of SmS
- SmB6, YbB6, YbB12
- PuTe and PuSe
- Are these materials topologi al Kondo insulator? M. Dzero et al, Phys. Rev. Lett. **104, 119901,2010**

Intermediate Valen e and band inversion: from the band theory point of view





Rare earth ompounds with divalen e (not very stable), Sm, Eu, Yb.....

intermediate valen e state band theory point of view

Is the band des ription orre t for these ompounds?

- from non-intera ting band insulator to strong oupling "Kondo insulator"
- how to apture the orre t ele troni stru ture?
- how to des ribe its topologi al nature?

How to ompute the Z2 invarian e for intera ting system?

Formula derived from the topologi al field theory:
PRL.105,256803 (2010)

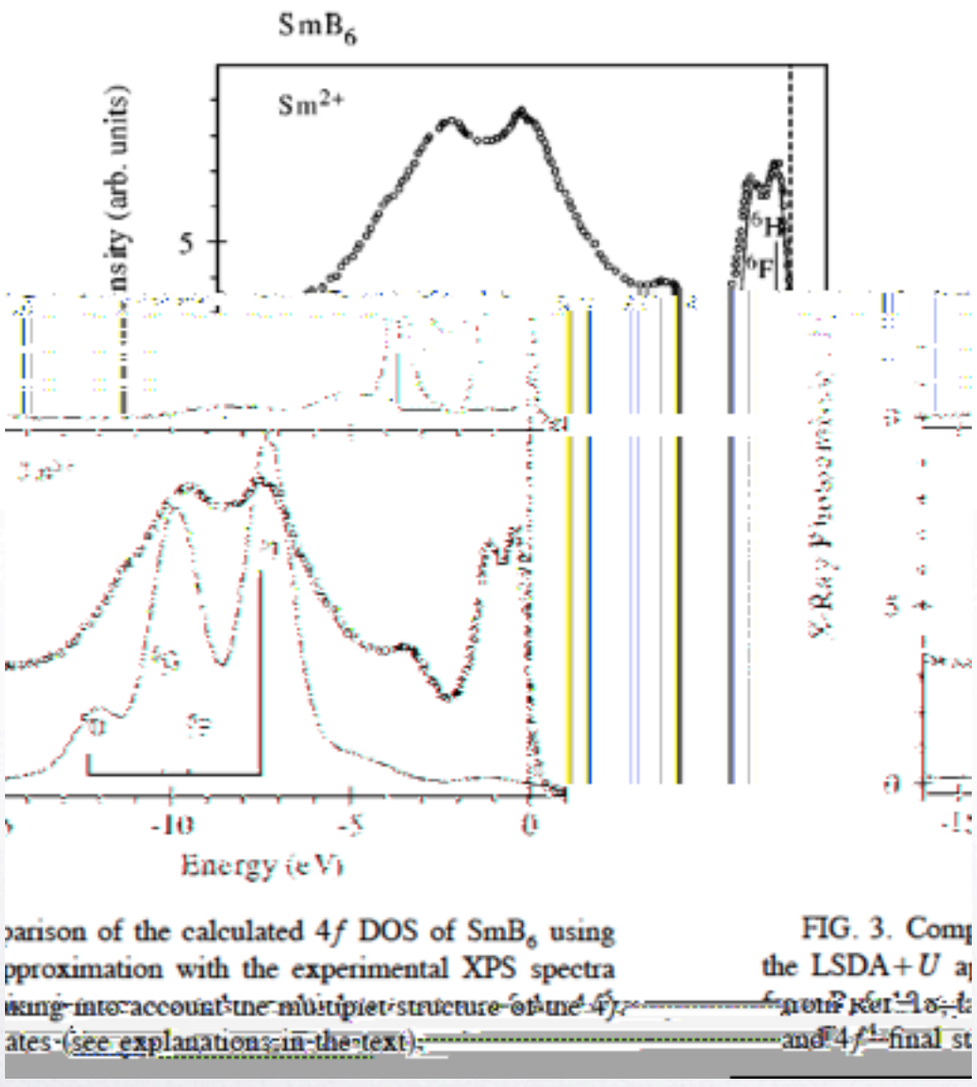
$$P_3 = \frac{\pi}{6}\int_0^1 du \int \frac{d^4k}{(2\pi)^4} \mathrm{Tr}\epsilon^{\mu\nu\rho\sigma}[G\partial_\mu G^{-1} G\partial_\nu G^{-1} \times G\partial_\rho G^{-1} G\partial_\sigma G^{-1} G\partial_u G^{-1}] \quad (1)$$

- Pole expansion of the self energy without k dependen e PRB , 235135 (2012); EPL98 (2012) 57001
- Using the eigenstate of H0+Σ(0), condition: there is no singularity along the imaginary axis of self energy, PRB 85, 165126 (2012)

Our method: LDA+Gutzwiller

- Gutzwiller type of ground state wave fun tion
- Combined with first prin iple ode
- Suitable for the study of f-ele trons
- Has been applied to many orrelated system: LaOFeAs; NaxCoO2; Ce; Pu....PHYSICAL REVIEW B , 075114 ,2009

from PHYSICAL REVIEW B **66**, 165209, 2002

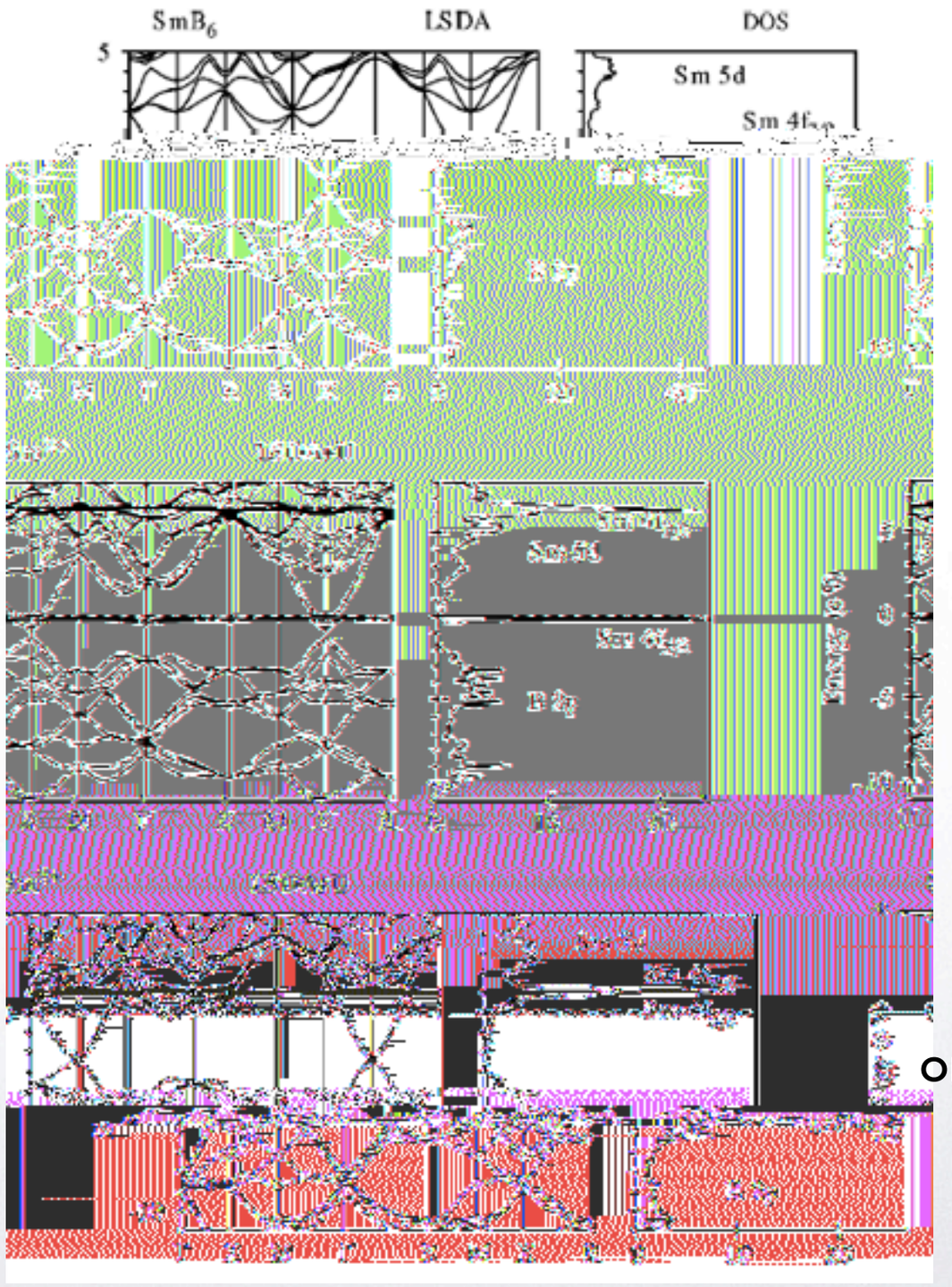


parison of the calculated 4*f* DOS of SmB_6 using
pproximation with the experimental XPS spectra
aking into account the multiplet structure of the 4*f*
ates (see explanation in the text).

FIG. 3. Comp
the LSDA+*U* a
and $4f^5$ final st

ompare to XPS

The valen e determined by XPS is 2.54



band stru ture obtained by LDA and LDA+U

Assuming some kind of orbital ordering from Sm3+ phase

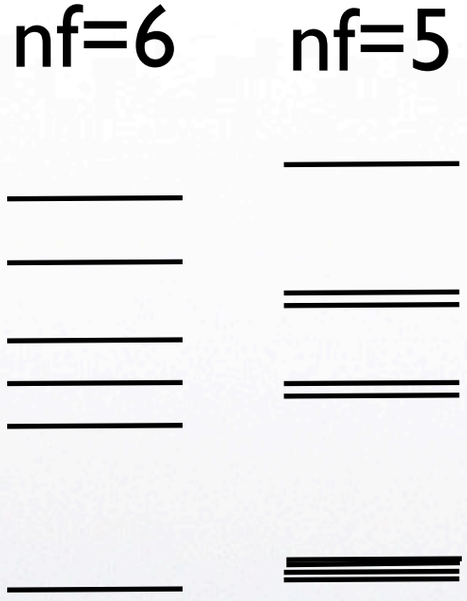
Atomi multiplets or Band states?

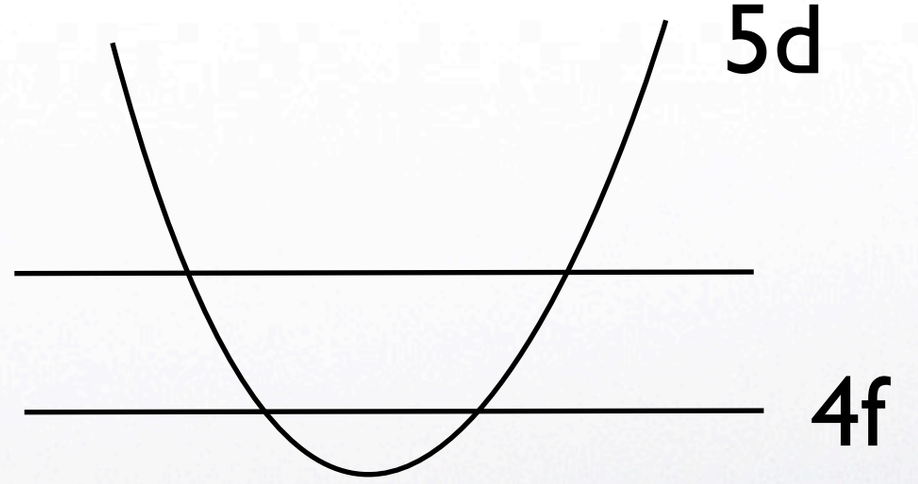
= +

$$= \ _0 \frac{\left(\quad -1\right)}{2} + \sum_{=1,\alpha\beta\gamma\delta}^{3} \ _2^{\alpha\beta\gamma\delta} \ _\alpha^+ \ _\beta^+ \ _\delta \ _\gamma + \sum_\alpha \varepsilon_\alpha \ _\alpha^+ \ _\alpha$$

$$H_{hopping} = \sum_{ij\alpha\beta} t_{ij}^{\alpha\beta} f_{i\alpha}^{+} f_{j\beta} + h.c.$$

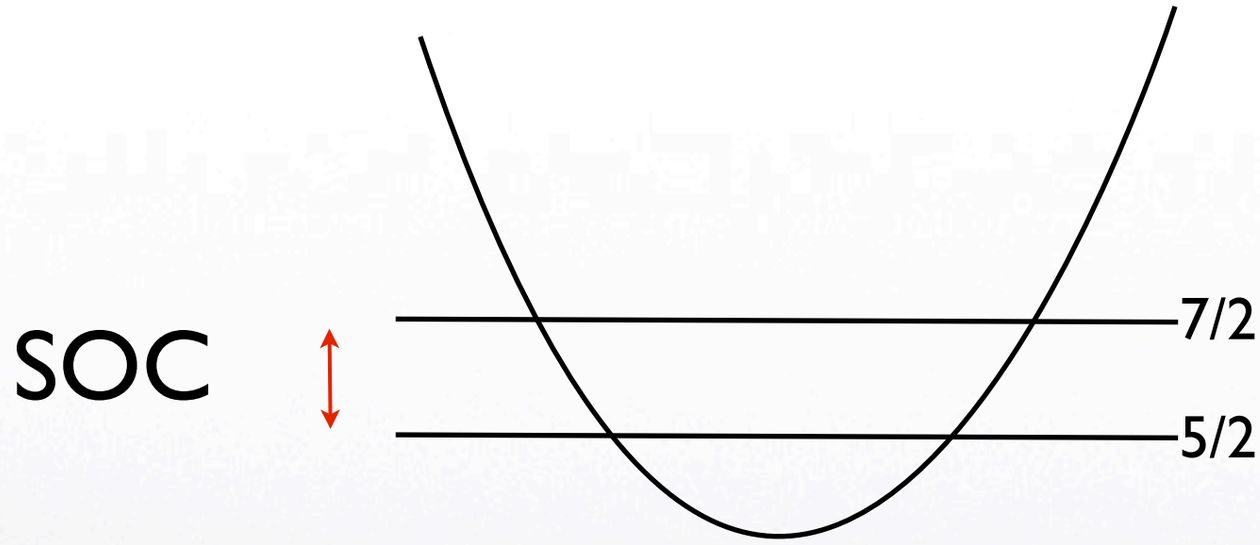
... nf=6 nf=5 ...



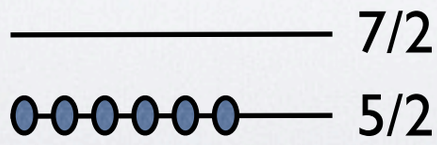


Both are non-fo k states!

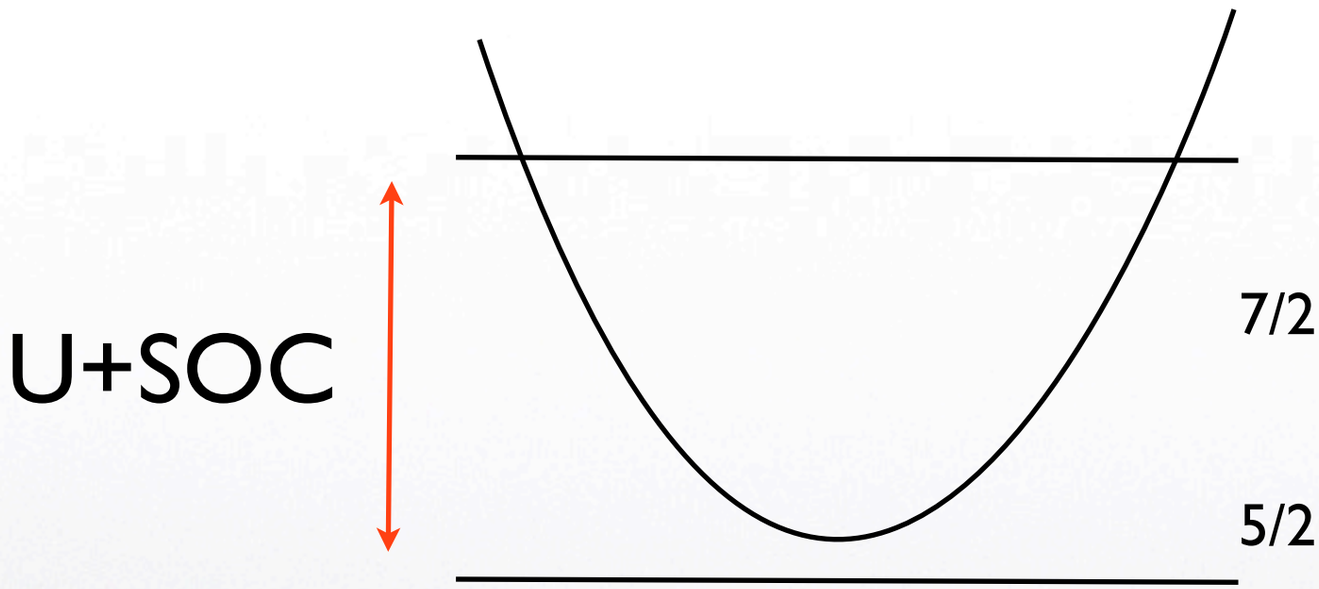
Problem of Hatree-Fo k treatment



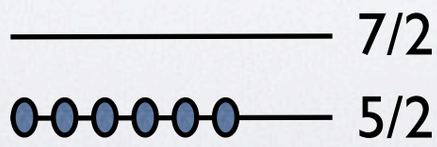
MF atomi state:



Problem of Hatree-Fo k treatment



MF atomi state:



The Gutzwiller Trial wave fun tion used in this study

Rotational Invariant Gutzwiller Approximation

Gutzwiller variational wavefunction:

$$|\Psi_G\rangle = \mathcal{P}|\Psi_0\rangle = \prod_{\mathbf{R}} \mathcal{P}_{\mathbf{R}} |\Psi_0\rangle$$

$$\mathcal{P}_{\mathbf{R}} = \sum_{\Gamma\Gamma'} \lambda(\mathbf{R})_{\Gamma\Gamma'} |\Gamma, \mathbf{R}\rangle\langle\Gamma', \mathbf{R}|$$

$|\Gamma\rangle$: eigenstates of atomic Hamiltonian H_{at}

$|\Psi_0\rangle$: uncorrelated wavefunction (Wick's Theorem holds)

$\mathcal{P}_{\mathbf{R}}$: projector operator modify weight of local configuration

Gutzwiller Constraints:

$$\langle\Psi_0|\mathcal{P}^\dagger\mathcal{P}|\Psi_0\rangle = 1$$

$$\langle\Psi_0|\mathcal{P}^\dagger\mathcal{P}n_{i\alpha}|\Psi_0\rangle = \langle\Psi_0|n_{i\alpha}|\Psi_0\rangle$$

We only apply trun ation respe t to the o upation number, for SmB6, we keep all the atomi states with nf=5,6,7, about 8000 variational parameters!

Effe tive Hamiltonian in Gutzwiller approximation

- Under Gutzwiller approximation, we an define

$$E_G = < 0|P H_{LDA} P|0 > + E_{int} \approx < 0|H_{eff}|0 > + \sum_{\Gamma} \lambda_{\Gamma,\Gamma} E_{\Gamma}$$

It an be easily proved that Heff is equivalent to $H0+\Sigma(0)$ by omparing the Green s fun tion in low frequen y limit

$$G(i\omega) = \frac{z}{i\omega - H_{eff}} = \frac{1}{i\omega/z - H_{eff}/z}$$

$$H_0 + \Sigma(0) = -G^{-1}(0) = H_{eff}/z$$

Main difficulties for the electronic structure calculation for f-electron systems

- Strong interactions among f-electrons, which can be expressed in terms of Slater integrals:F0,F2,F4,F6
- for SmB6 F0=5.8eV, F2=9.9eV, F4=7.09eV, F6=4.99eV
- Typical interaction strength is one order bigger than the f-band width
- Multiplet state VS the band state

The double ounting problem

- The total Hamiltonian treated in LDA+Gutzwiller

$$H_{total} = H_{LDA} + H_U + H_{DC}$$

$$H_{DC} = V_{DC} \sum_{k\sigma} f^{\dagger}_{k\sigma} f_{k\sigma}$$

- A ommonly used form for DC term:

$$V_{ab}^{\mathrm{DC}} = \delta_{ab}\left[\bar{U}\left(\bar{n}_c - \frac{1}{2}\right) - \bar{J}\left(\bar{n}_c^{\sigma} - \frac{1}{2}\right)\right].$$

- Kotliar et al, RMP78, 865,2006

Valence of Sm determined by exp

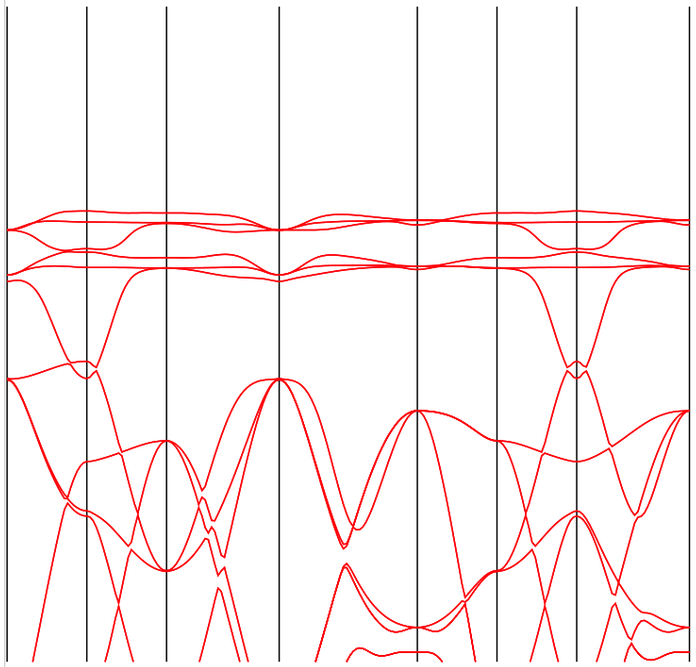
	paper	experiment	nf	Average valence
! " #$	%&#'(() *+$( ) ,(-(, . /$	0%!	.12	31+
! " #$	45%'(() *+6(,)(-(/ * /	7 899 : ;<=>(=?=@A	.1,	31$
! " #$	%BC9D@;(#'() ** .(3) .-(**	E=<A>8E(=FG=>D " =EA9	.1, ,	31.$
! " #$	4%H!'(366*( )+$-(6)362,	05!	.1,+	31.2

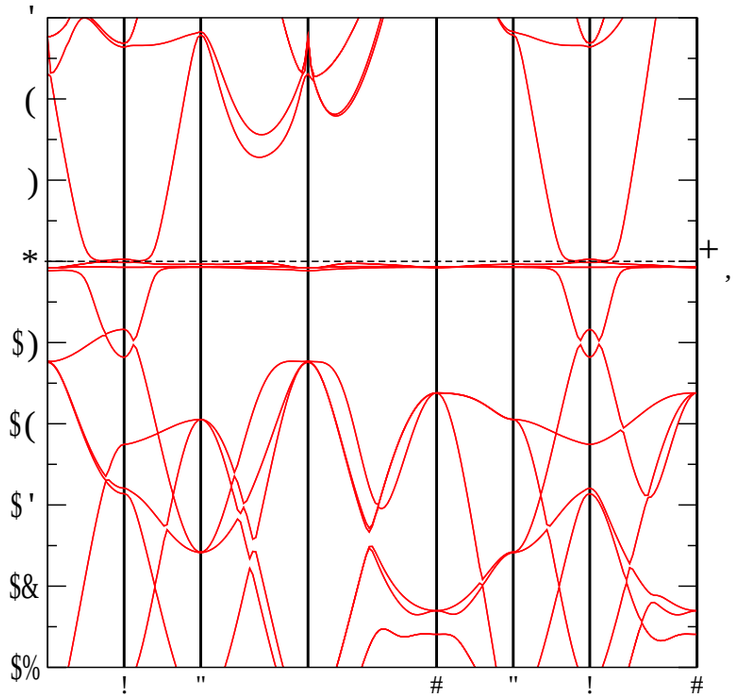
SmB6: Z, nf, Gap vs Parity

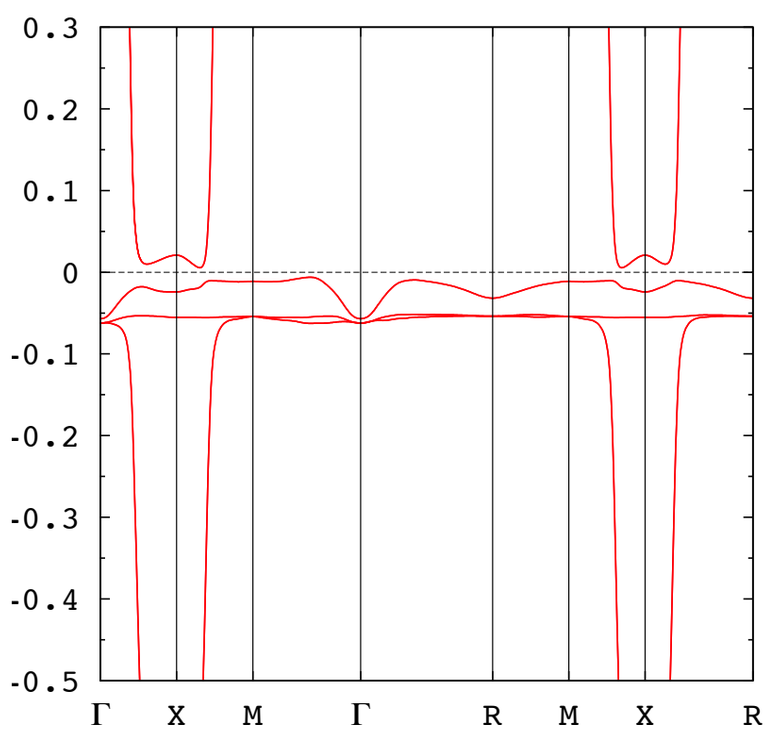
		3_4	5	26	(	27	89:
;*<=	>?@	).*AB	C	D	C	C	D
	+		C	D	C	C	

!"#	$%		&'()*+,-	
			./)	0/)
	.12.			

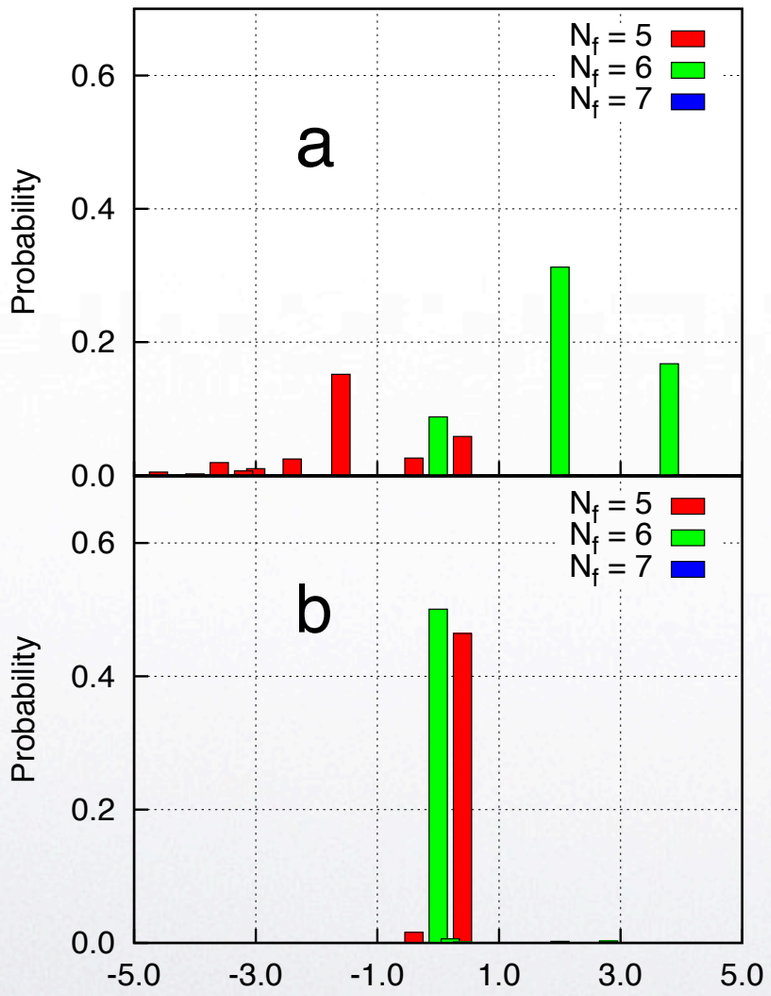
Band structure obtained by LDA and LDA+G







The probability of atomi eigenstates for SmB6

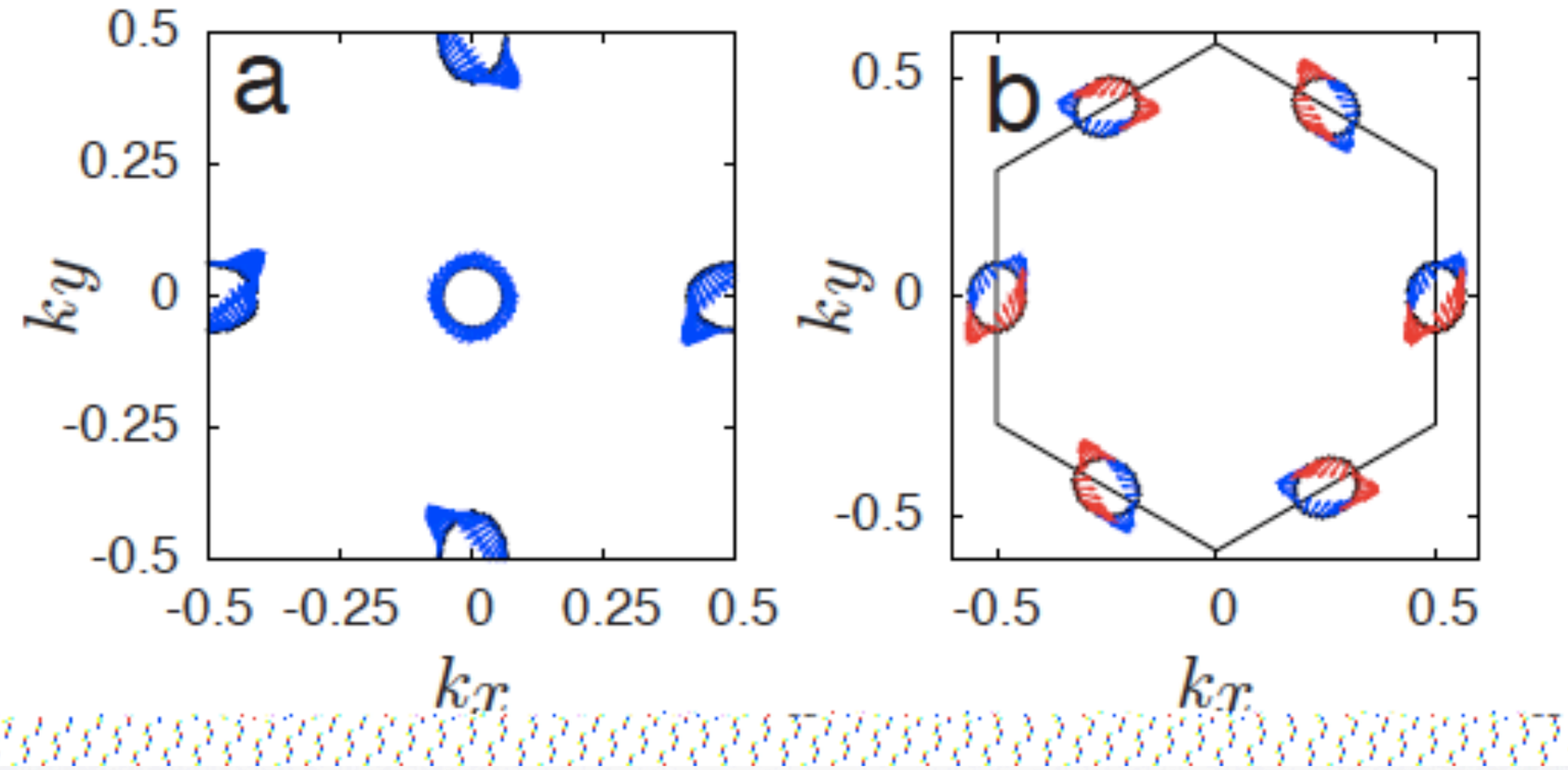


LDA

LDA+G

The unique surfa e states of SmB6 on (001) surfa e

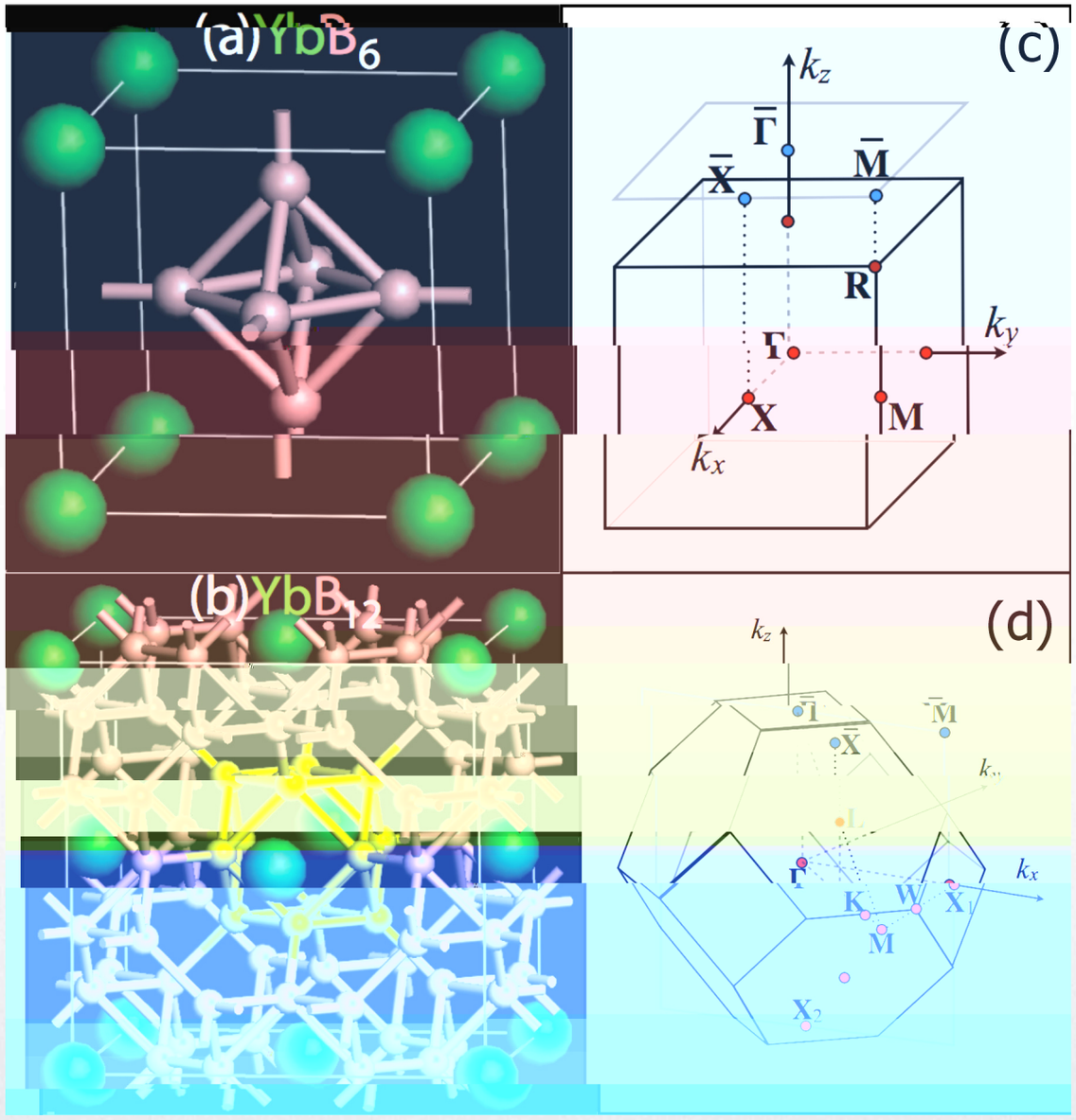
Spin texture for surfa e states



001 surfa e

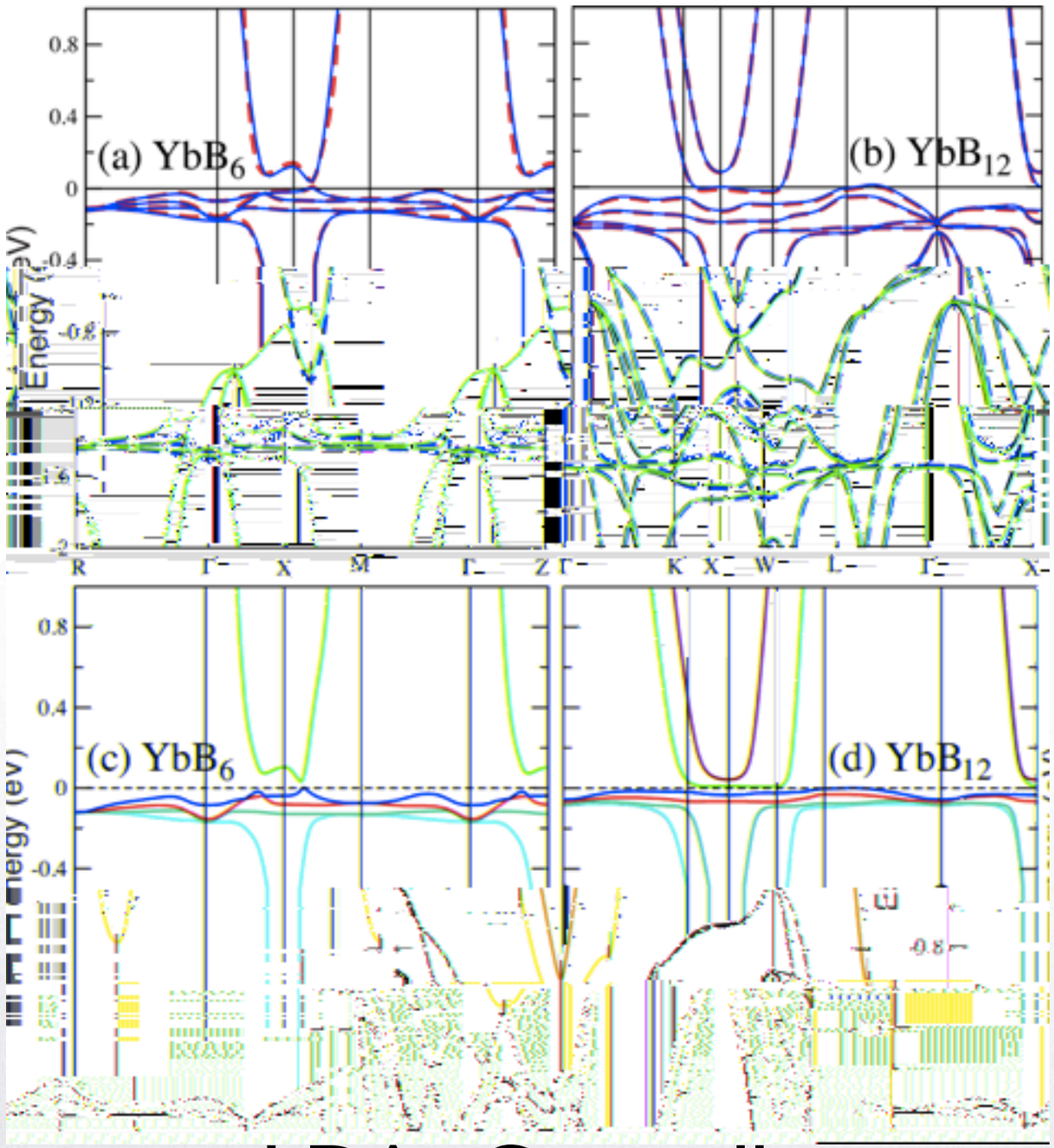
111 surfa e

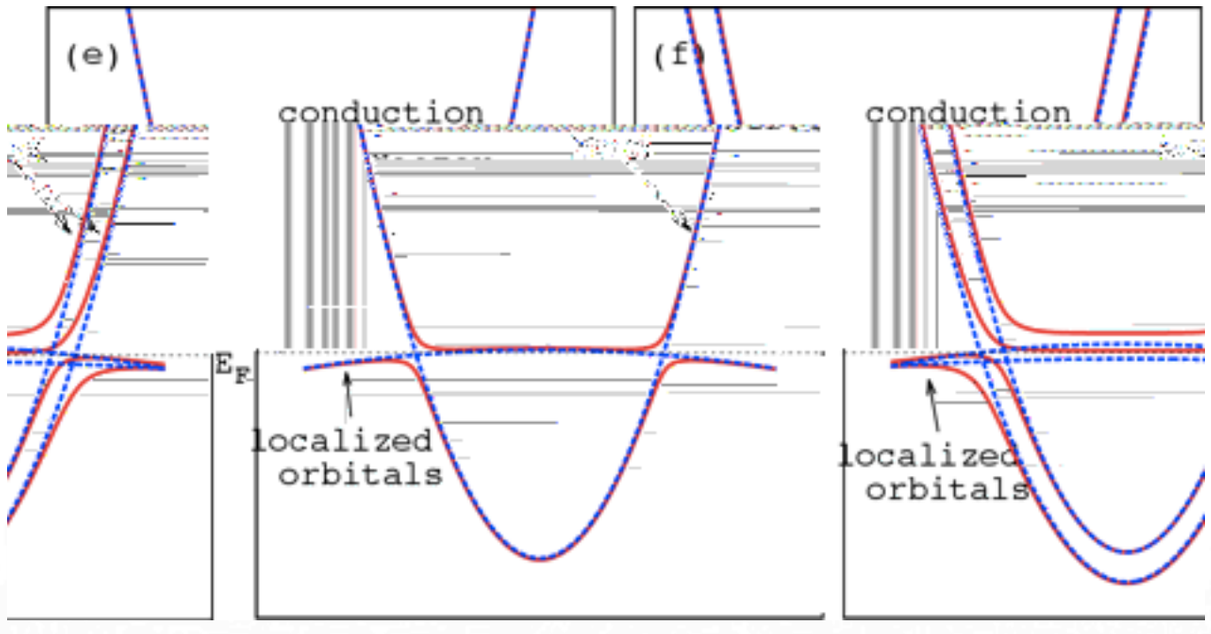
Structure of YbB6 and YbB12



Renormalized Band stru ture

LDA





	Γ	$3X$	$3M$	R	n_f	z
YbB_6					13.80(13.58)	0.87

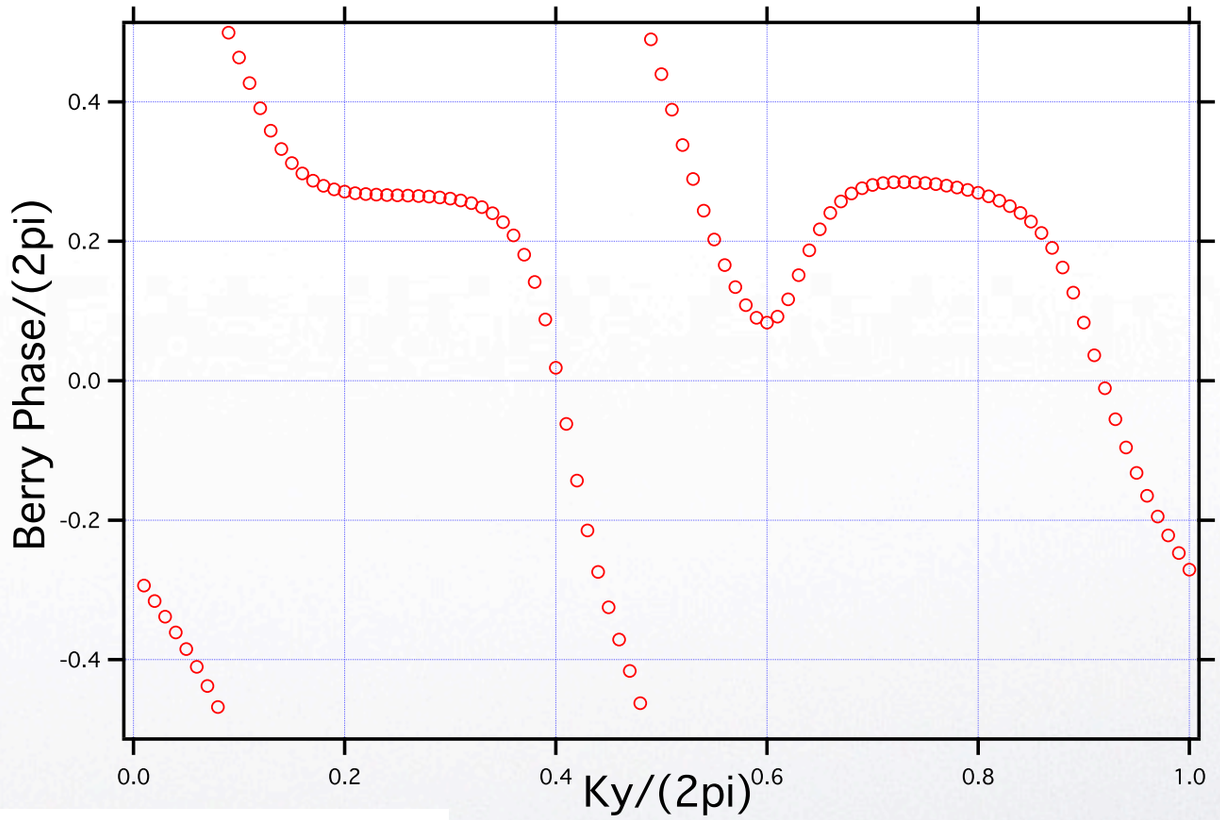
LDA+Gutzwiller

Determine the Mirror Chern number

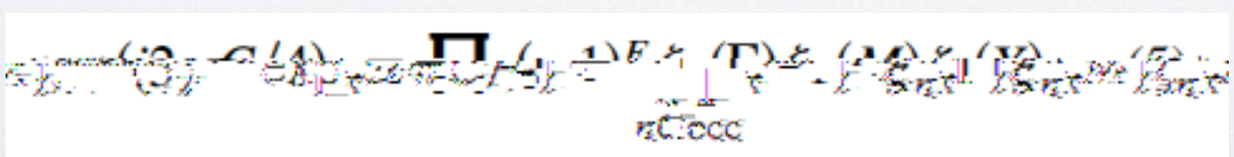
By the eigenvalue of the Cn rotational at high symmetry point

	C4	C2	M
4f7/2 jz=1/2	exp(i " /4)	exp(i " /2)	-i
5d5/2 jz=-1/2	exp(-i " /4)	exp(-i " /2)	-i
4f7/2 jz=-3/2	exp(-i3 " /4)	exp(-i3 " /2)	-i
5d5/2 jz=3/2	exp(i3 " /4)	exp(i3 " /2)	-i

By Wilson Loop method

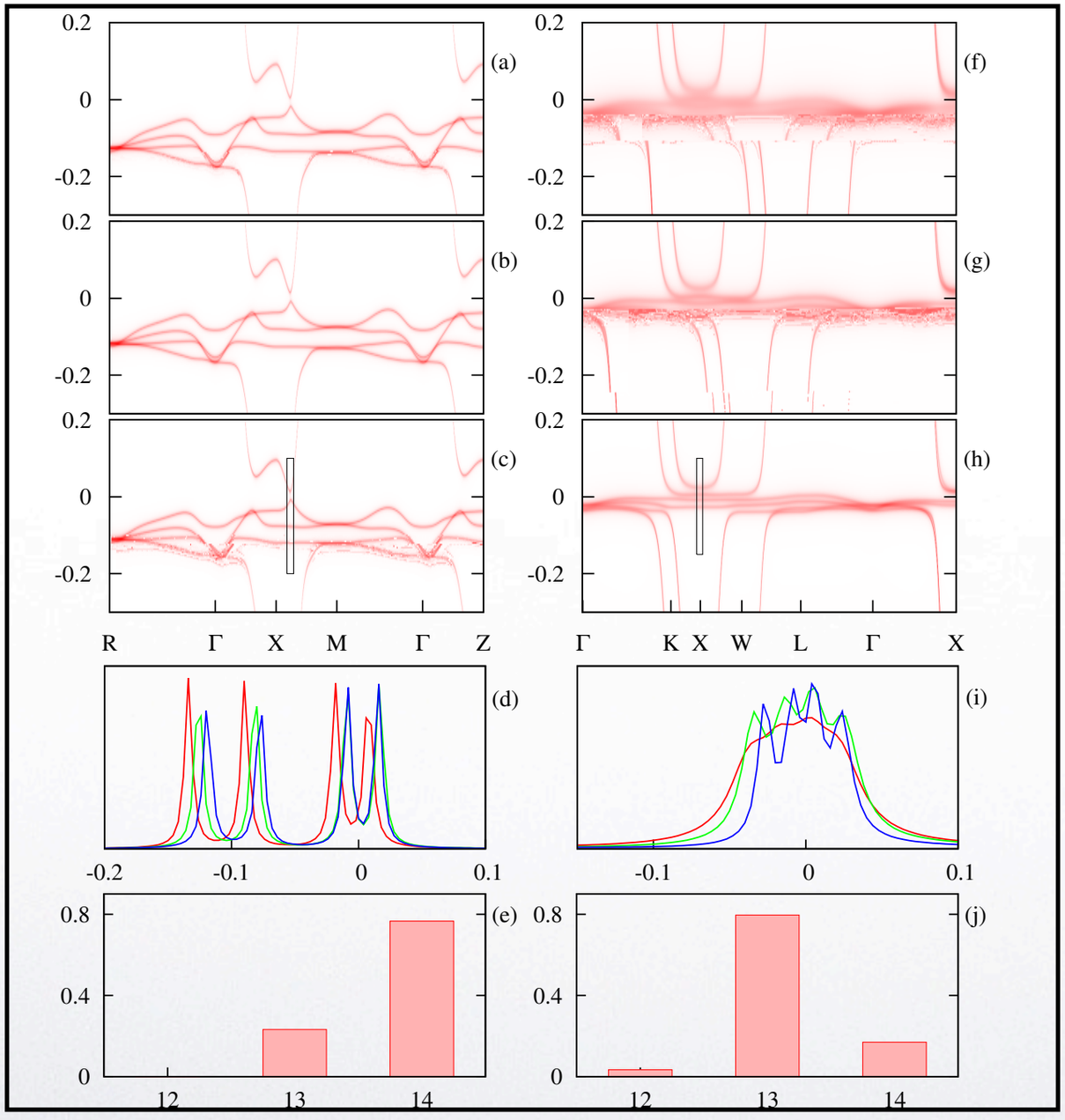


$$i^C = -1$$



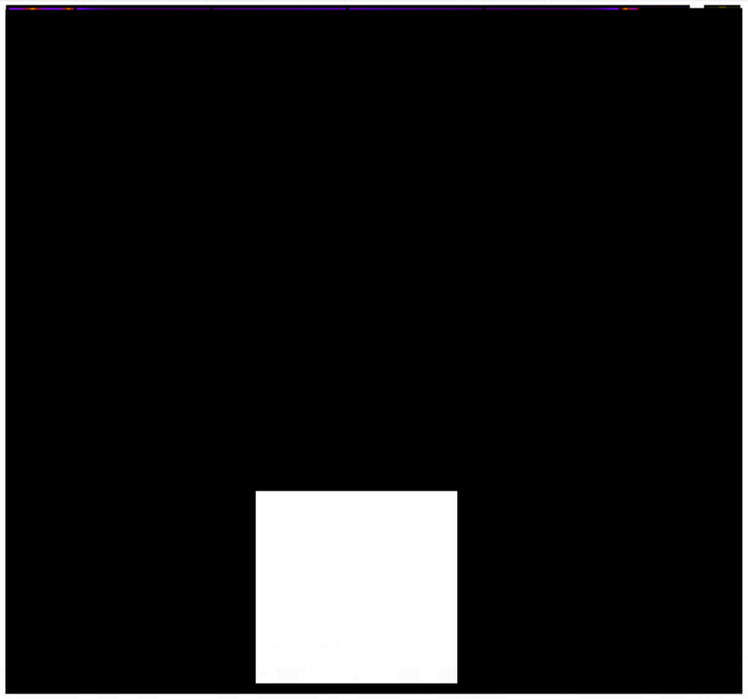
C. Fang et al, PRL 108, 266802 (2012); R. Yu, et al, Phys. Rev. B **84**, 075119 (2011)

Temperature dependan e of the spe tral fun tion



Surfa e states for YbB6

Surfa e states for YbB12



Con lusions

- Mix valen e TI SmB6, and YbB6
- Topologi al Crystalline Kondo Insulator with mirror Chern number 2 :YbB12
- The topologi al phases survive from the Strong e-e intera tion among f ele trons
- More similar materials!