The topological insulator with strong correlation effects

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Lu et al, PRL 110, 096401 (2013)

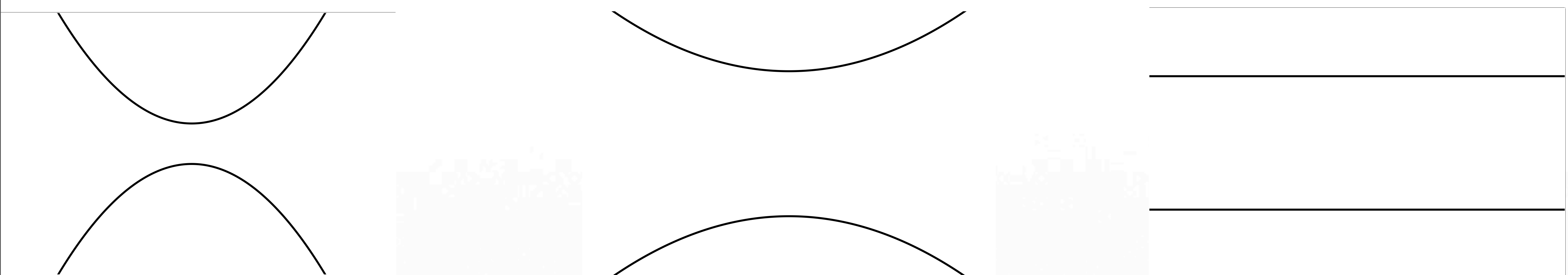
outline

- Band inversion and TI
- Mix valence compound: Band inversion between d and f bands; the important role of e-e interaction
- SmB6 and PuTe
- Conclusion

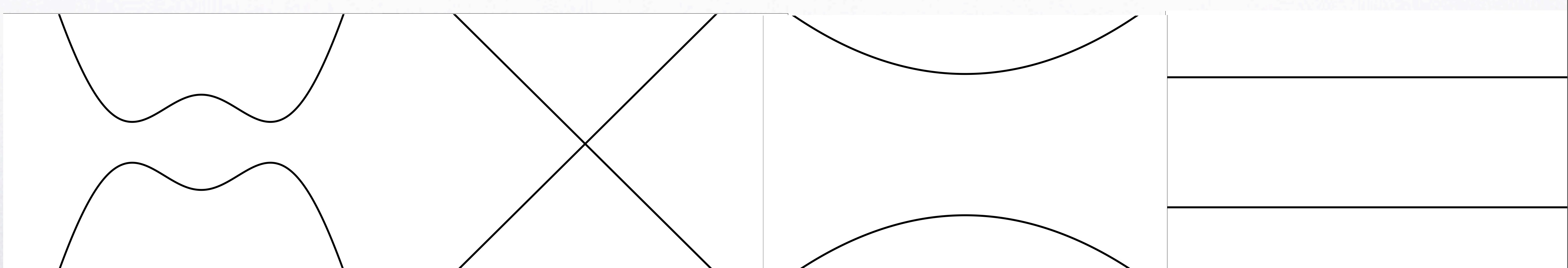
Topological classification of band insulators

- normal insulator: the electronic structure can be smoothly transformed to isolated atoms
- can not be smoothly transformed to isolated atoms without going through a phase transition, Z2 invariance defined for non-interacting TI
- TI with interaction can be defined by the Theta angle of of topological magneto-electric effect

Evolution of band structure from solid to isolated atoms



Normal Insulator



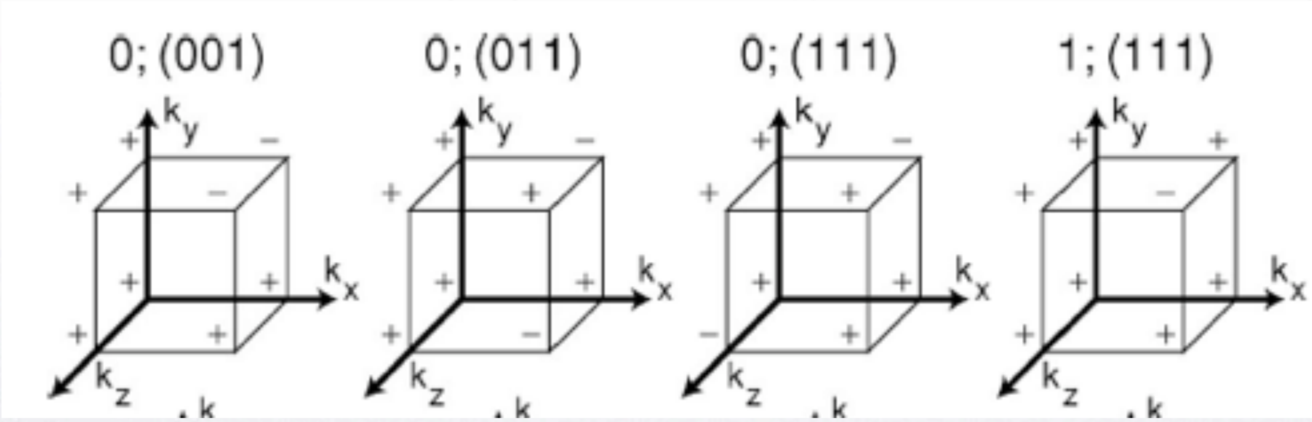
Topological Insulator

Z2 invariance for non-interacting TI with inversion symmetry

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

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

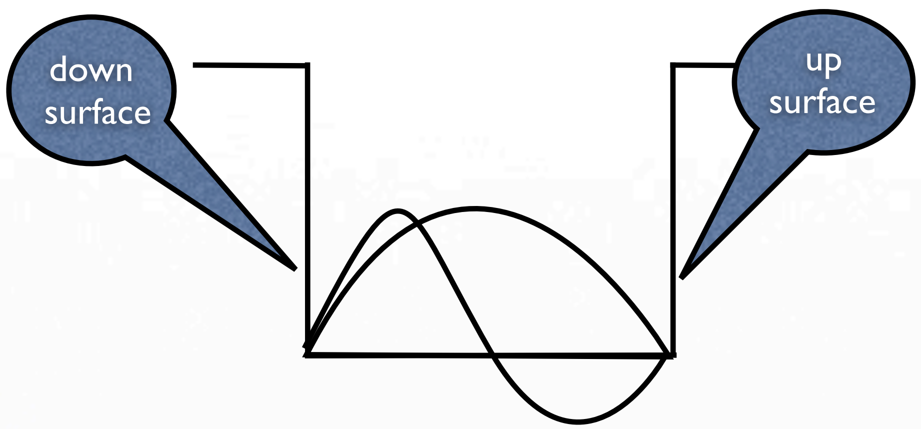
$$\delta_i = \prod_{m=1}^{N} \xi_{2m}(\Gamma_i) .$$



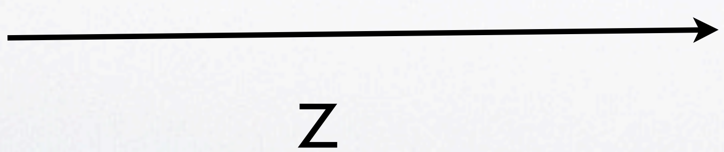
L. Fu and C. Kane, PRB 76,045302

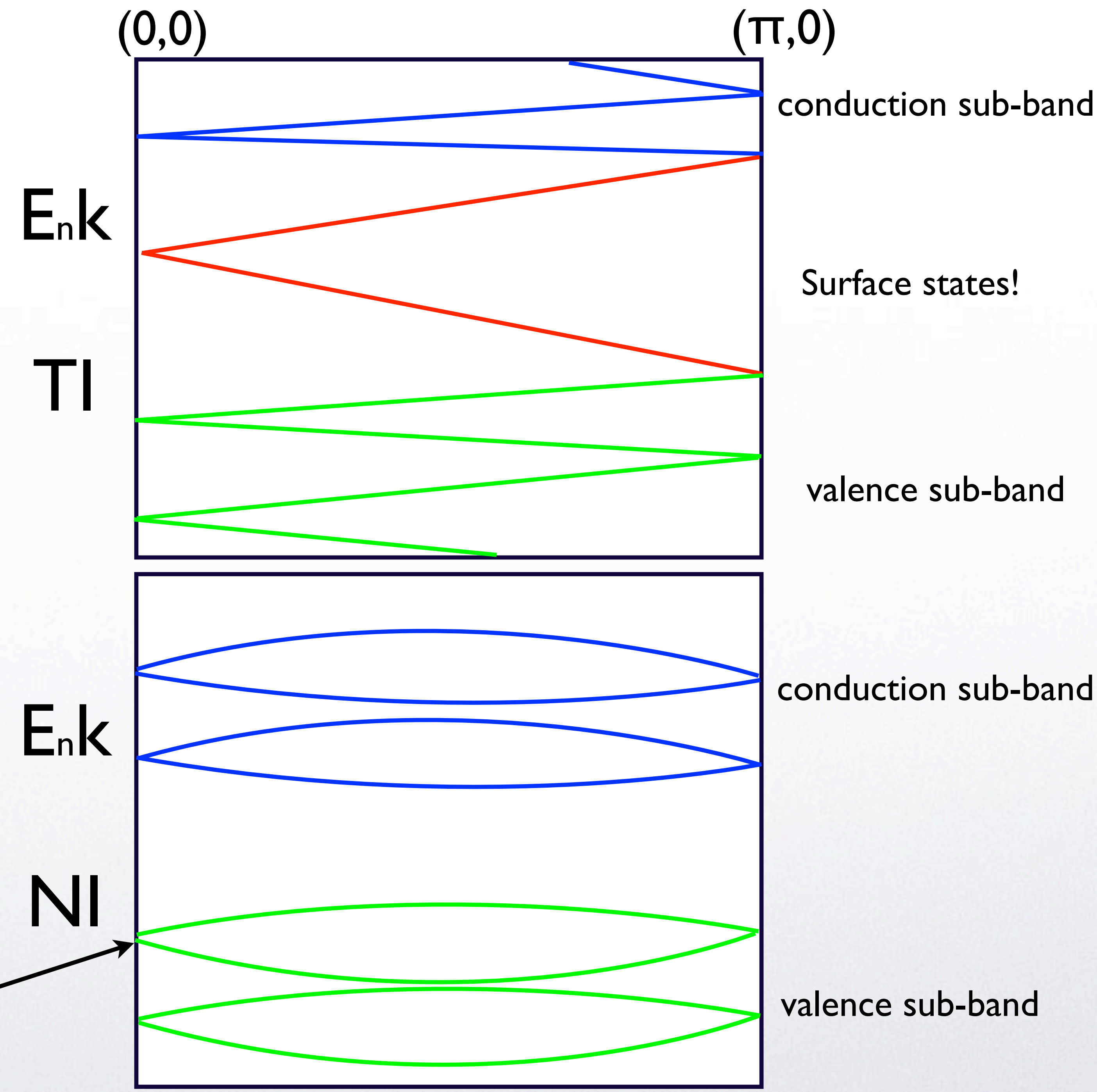
TI and surface states

Consider a slab of TI



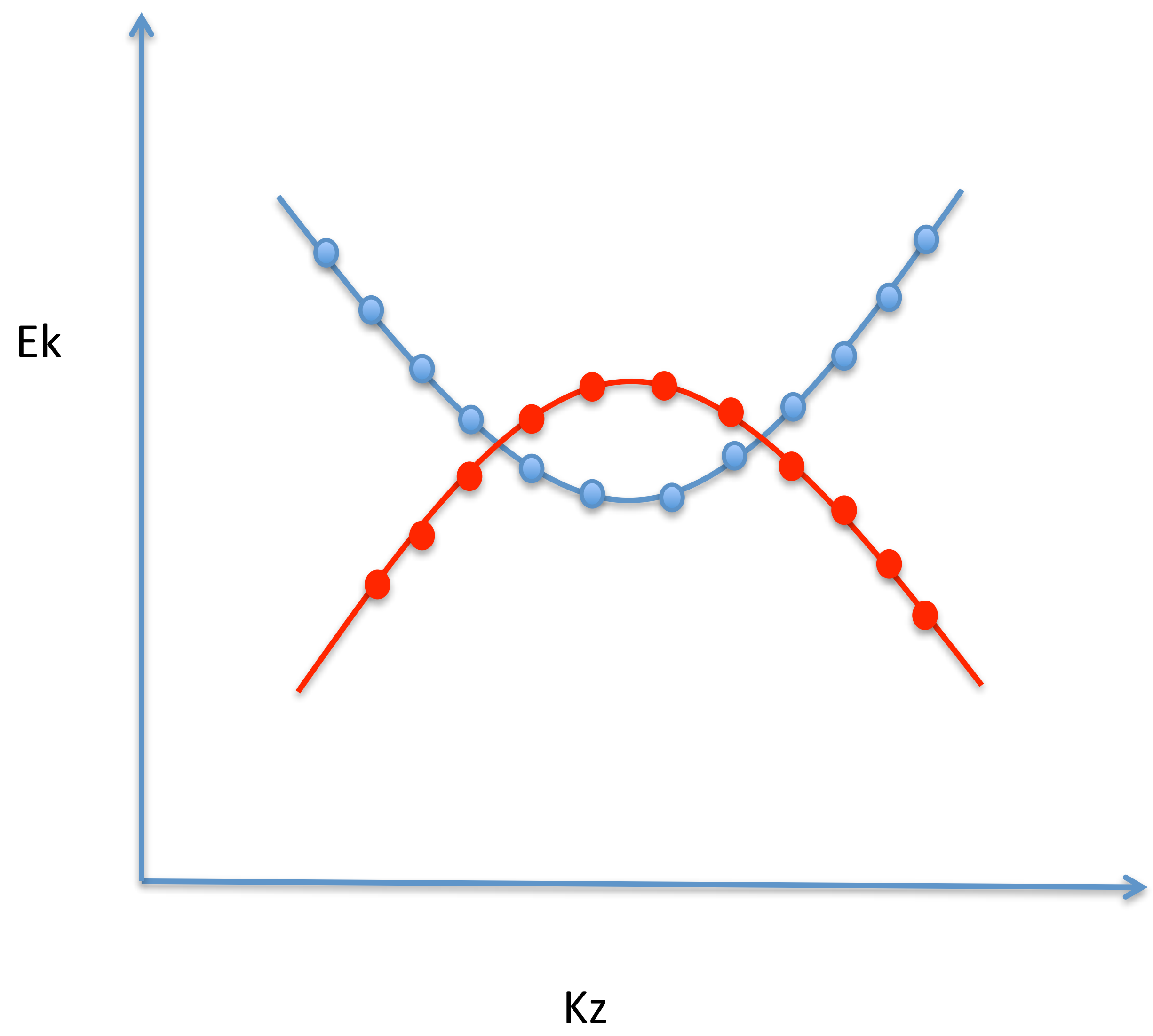
$\psi_n(kx,ky)$





k= − k+G; Kramers degeneracy

Introduction: Band Inversion and TI



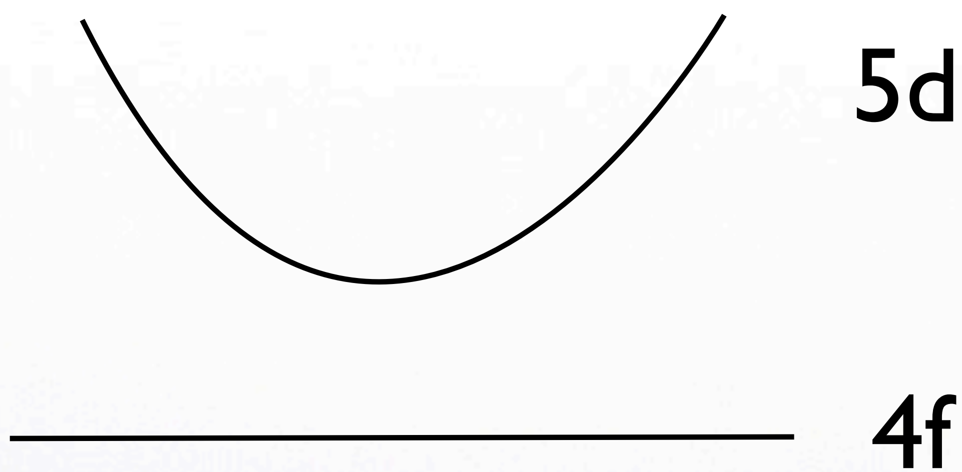
The different types of band inversion

- Band inversion between s and p bands: HgTe
- Band inversion between bonding and anti-bonding p-bands: $Bi2Se3$, Sb
- Band inversion generated by valence fluctuation of 4f/5f bands
- Very strong correlation effects in f-electron materials:
- Does these materials topologically non-trivial?

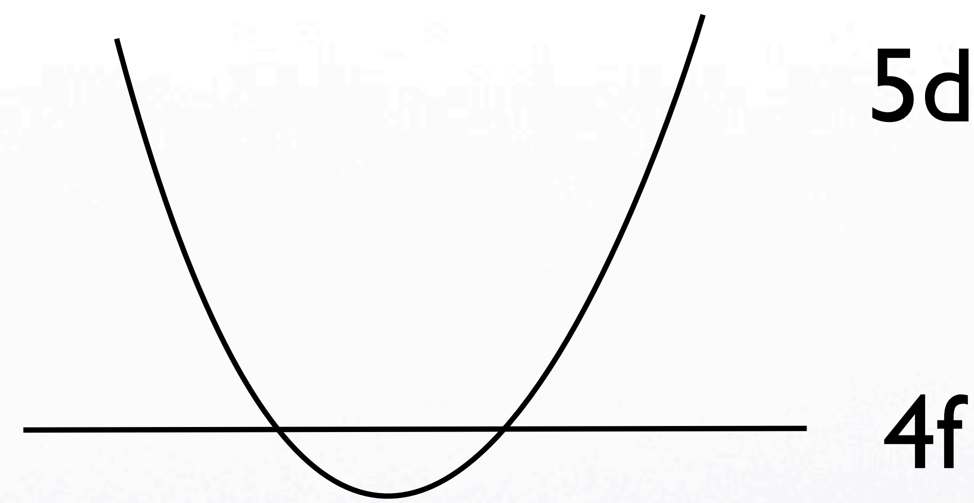
4f/5f compounds with intermediate valence

- golden phase of SmS
- SmB_6
- PuTe and PuSe
- Yb
- Are these materials topological Kondo insulator? M. Dzero et al, Phys. Rev. Lett. **104, 119901,2010**

Intermediate Valence and band inversion: from the band theory point of view



Rare earth compounds with divalence (not very stable), Sm, Eu, Yb......



intermediate valence state band theory point of view

Is the band description correct for these compounds?

- from non-interacting band insulator to strong coupling "Kondo insulator"
- how to capture the correct electronic structure?
- how to describe its topological nature?

How to compute the Z2 invariance for interacting system?

Formula derived from the topological 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 dependence PRB **85**, 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 function
- Combined with first principle code
- Suitable for the study of f-electrons
- Has been applied to many correlated system: LaOFeAs; NaxCoO2; Ce; Pu....PHYSICAL REVIEW B **79**, 075114 ,2009

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 Gutzwiller Trial wave function 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_U
Ψ_0: uncorrelated wave function (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 truncation respect to the occupation number, for SmB6, we keep all the atomic states with nf=5,6,7, about 8000 variational parameters!

Effective Hamiltonian in Gutzwiller approximation

- Under Gutzwiller approximation, we can define

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

It can be easily proved that Heff is equivalent to $H0+\Sigma(0)$ by comparing the Green's function in low frequency limit

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

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

The double counting problem

- The total Hamiltonian treated in LDA+Gutzwiller

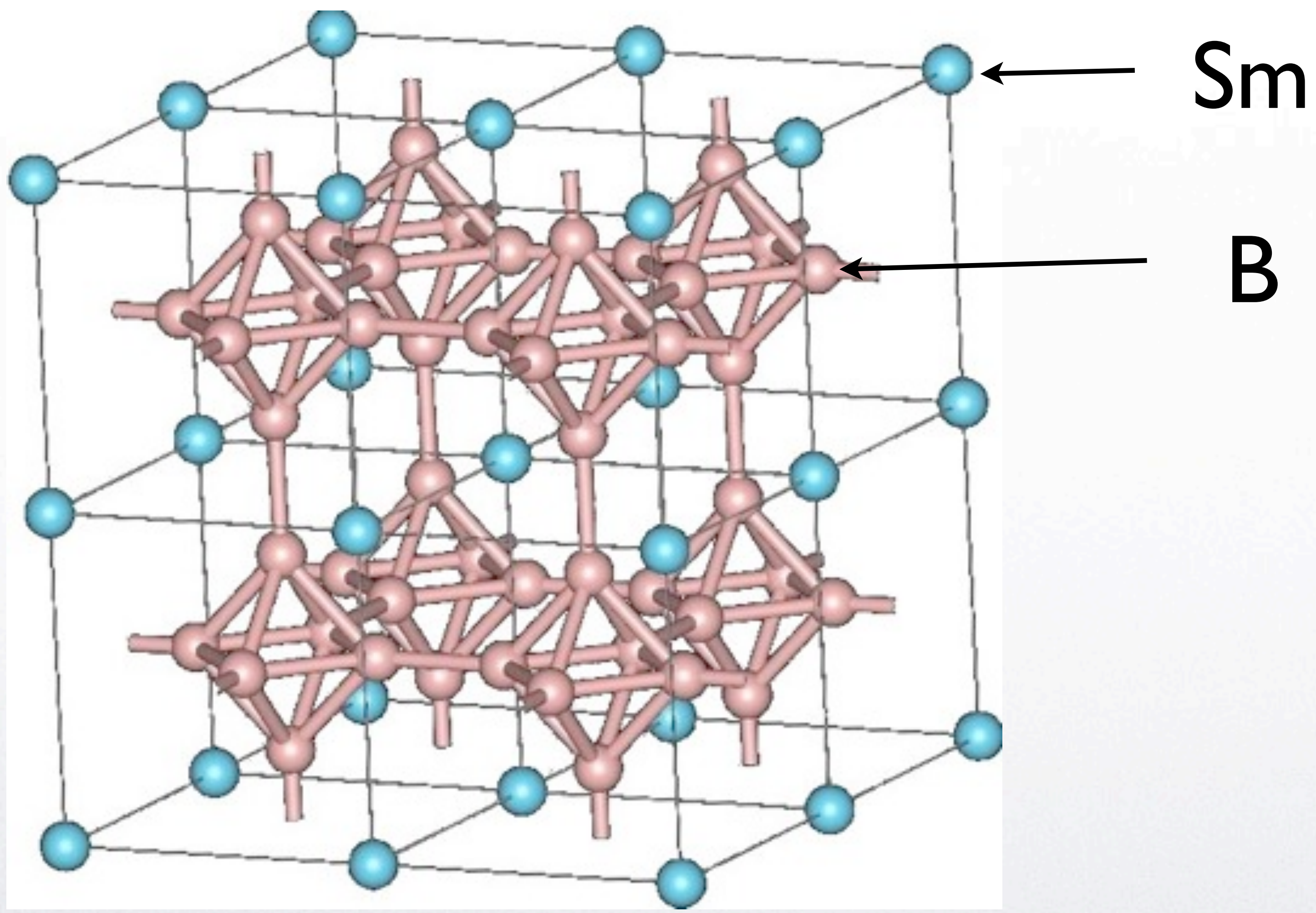
$$H_{total} = H_{LDA} + H_U + H_{DC}$$
$$H_{DC} = V_{DC} \sum_{k\sigma} f^{\dagger}_{k\sigma} f_{k\sigma}$$

- A commonly used form for DC term:

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

- Kotliar et al, RMP78, 865,2006

The structure of SmB6



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

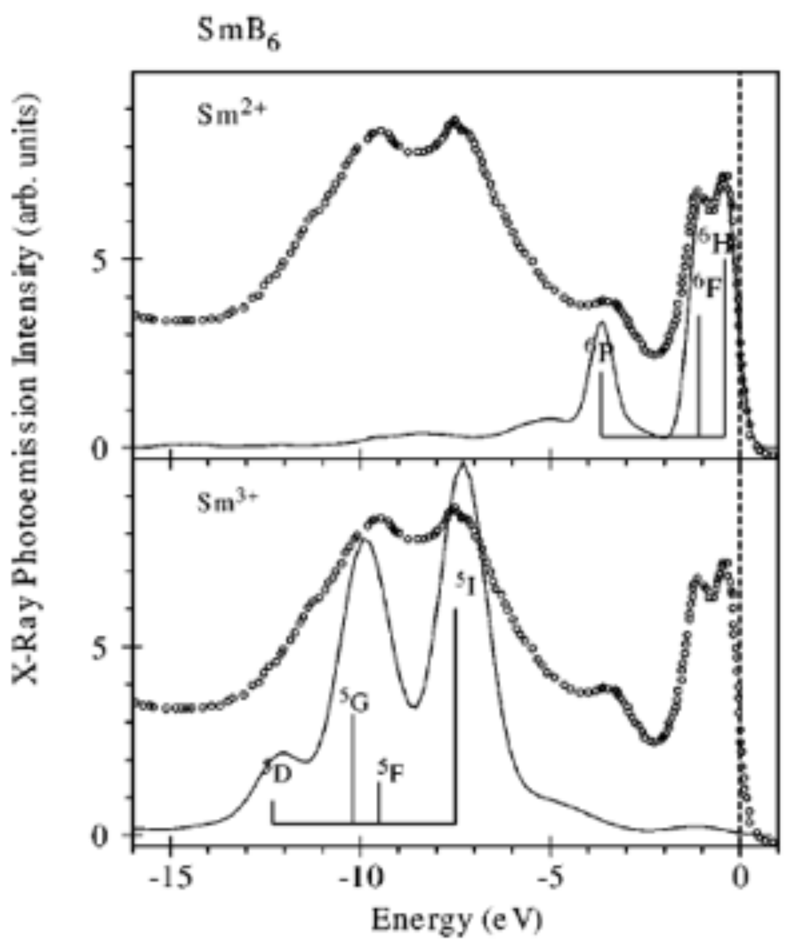
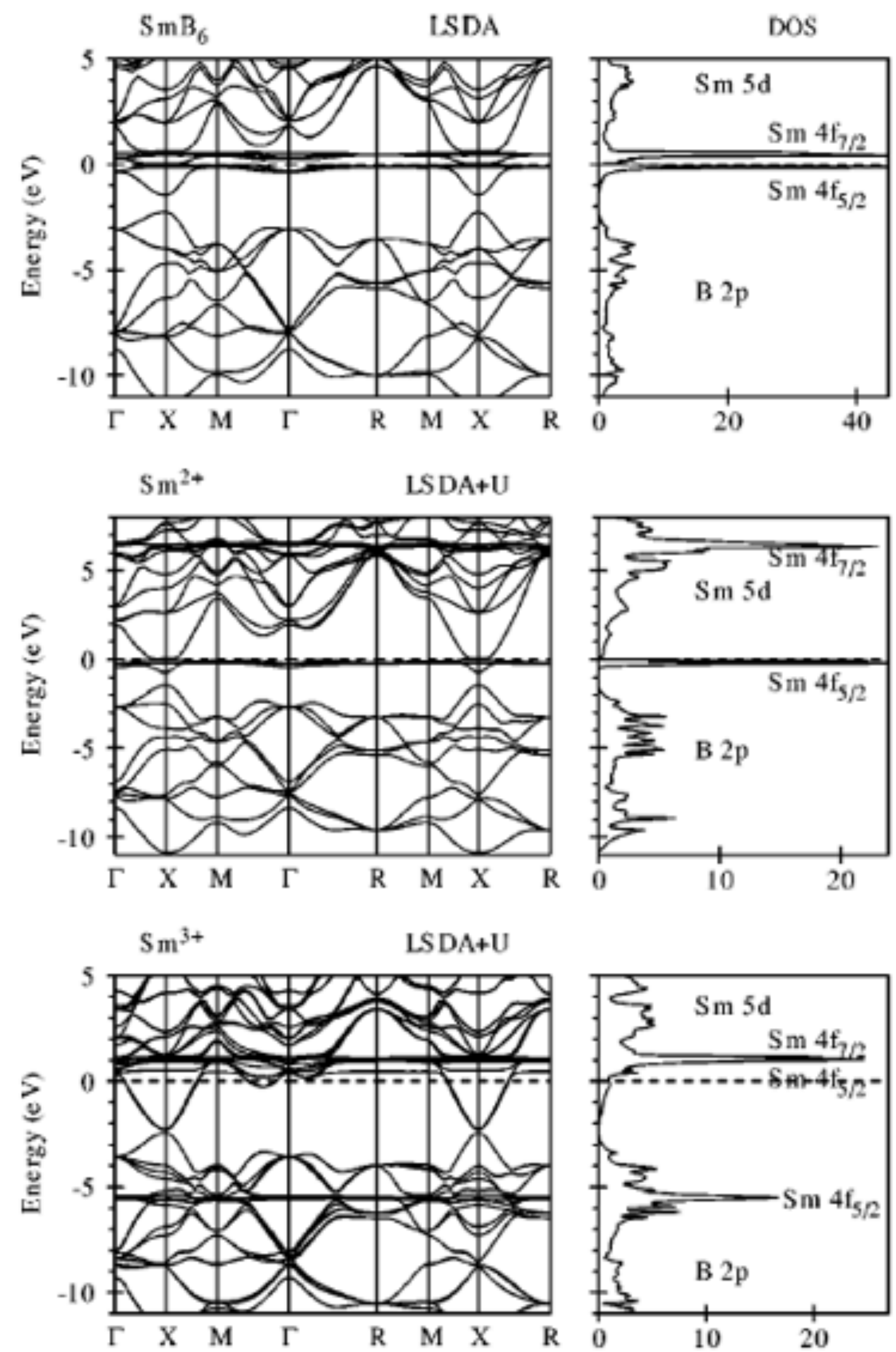


FIG. 3. Comparison of the calculated $4f$ DOS of SmB_6 using the LSDA+U approximation with the experimental XPS spectra from Ref. 18, taking into account the multiplet structure of the $4f^5$ and $4f^4$ final states (see explanations in the text).

compare to XPS

The valence determined by XPS is 2.54



band structure obtained by LDA and LDA+U

Assuming some kind of orbital ordering from Sm3+

phase

Valence of Sm determined by exp

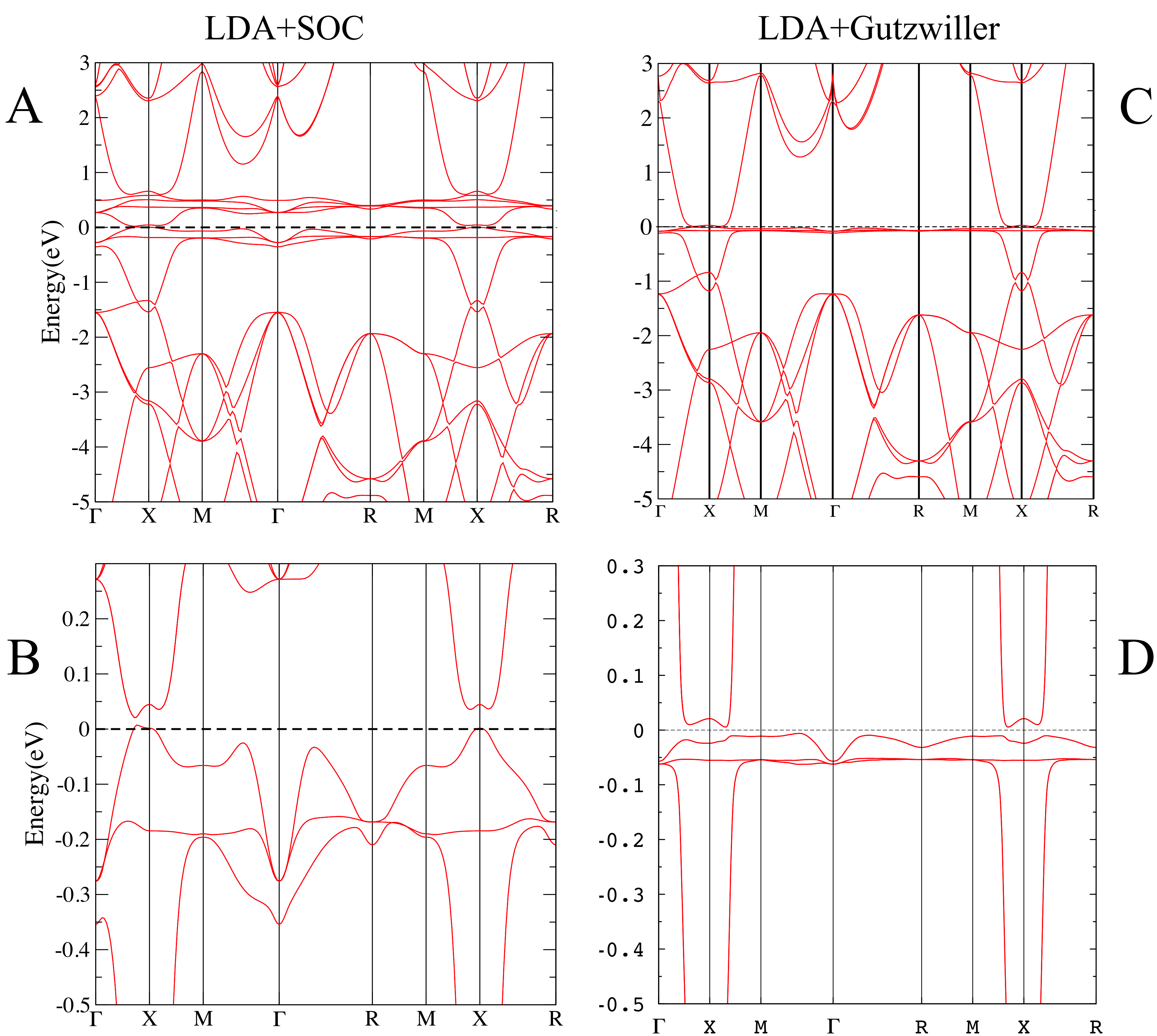
	paper	experiment	nf	Average valence
SmB_6	PRB: 1976 14 , 4586	XPS	5.3	2.7
SmB_6	JAP: 1970 41 , 898	Mossbauer effect	5.4	2.6
SmB_6	Physica B: 1995 215, 99	neutron experiments	5.44	2.56
SmB_6	JPCS: 2009 176, 012034	XAS	5.47	2.53

SmB6: Z, nf, Gap vs Parity

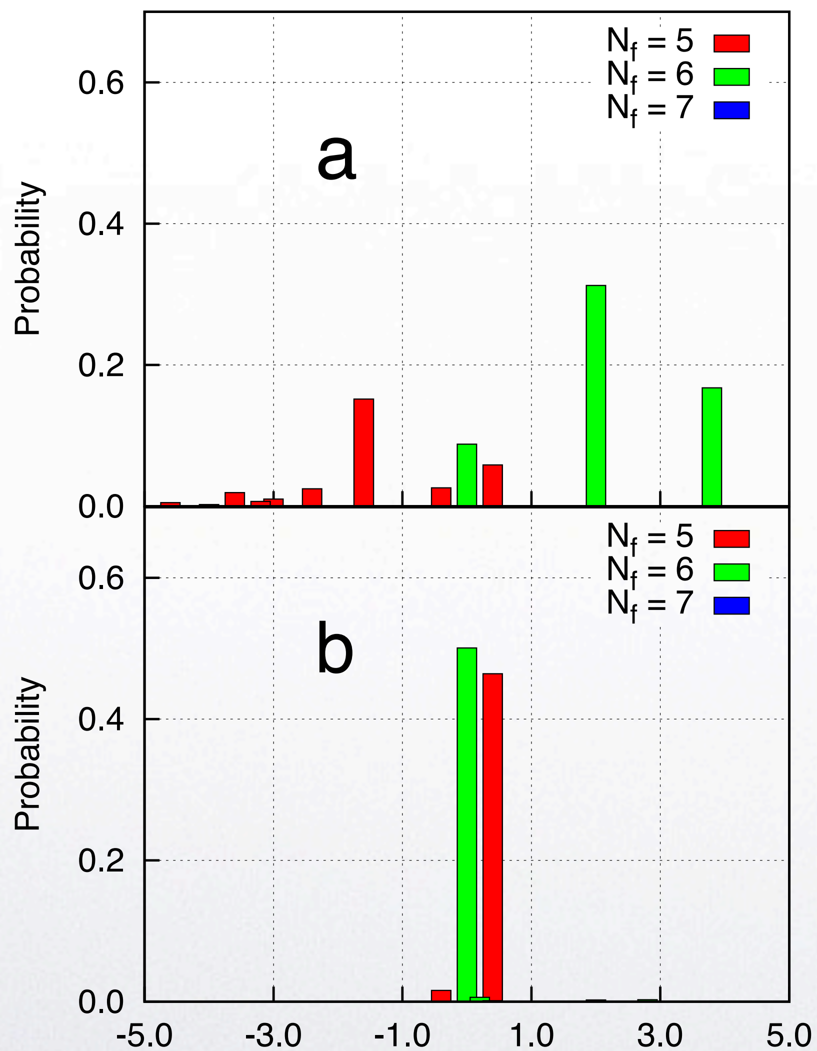
		E_g	Γ	3X	R	3M	ToI
SmB6	LDA	25mev	+	-	+	+	-
SmB6	**LDA + G**	**10mev**	**+**	**-**	**+**	**+**	**-**

Vdc	n_f		$Z(R^2_{mat})$	
			5/2	7/2
	5.35			
26.4	**5.45**		**0.18**	**0.59**

Band structure obtained by LDA and LDA+G



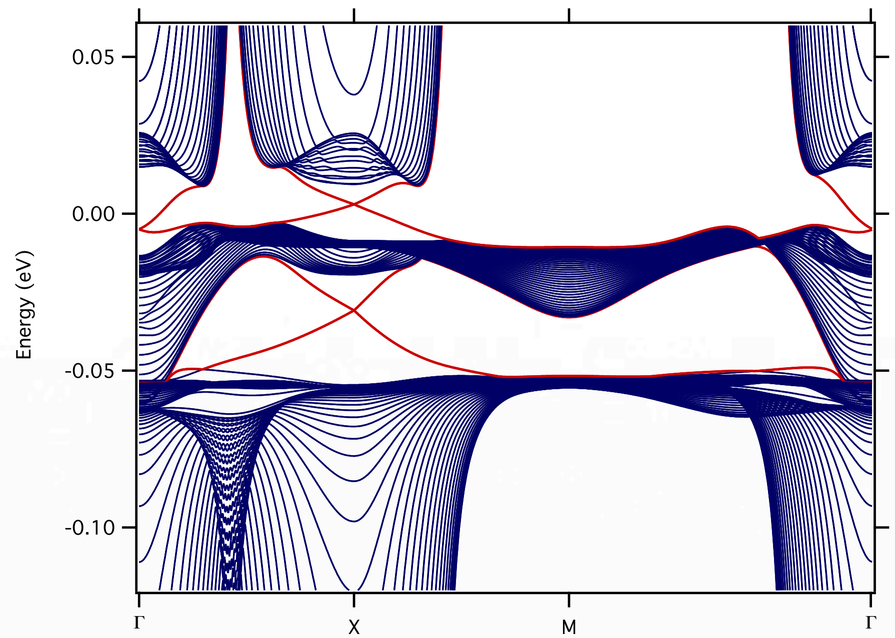
The probability of atomic eigenstates for SmB6

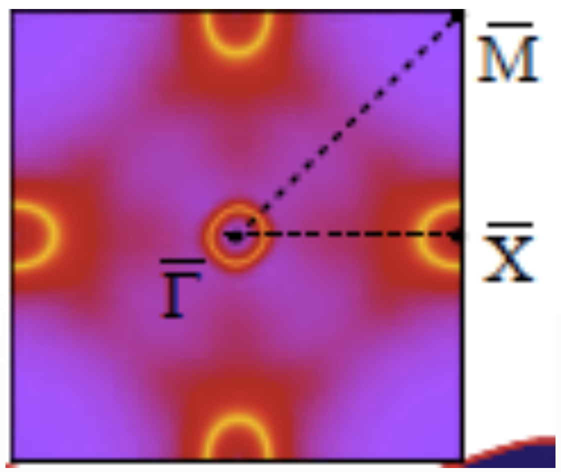


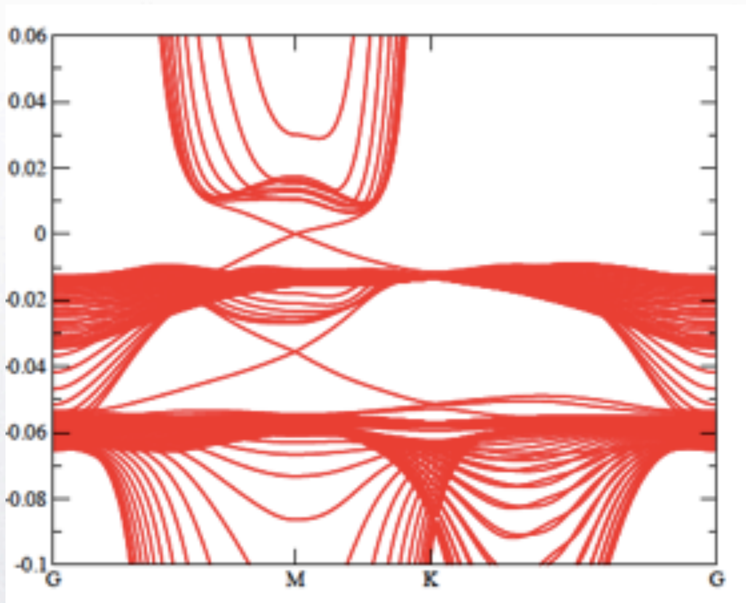
LDA

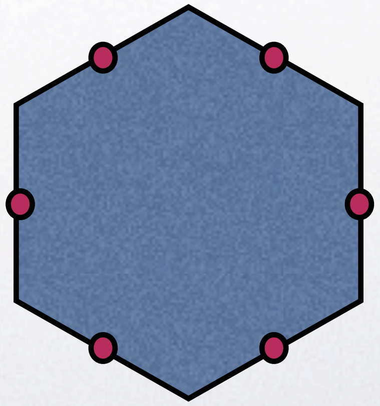
LDA+G

The unique surface states of SmB6 on (001) surface

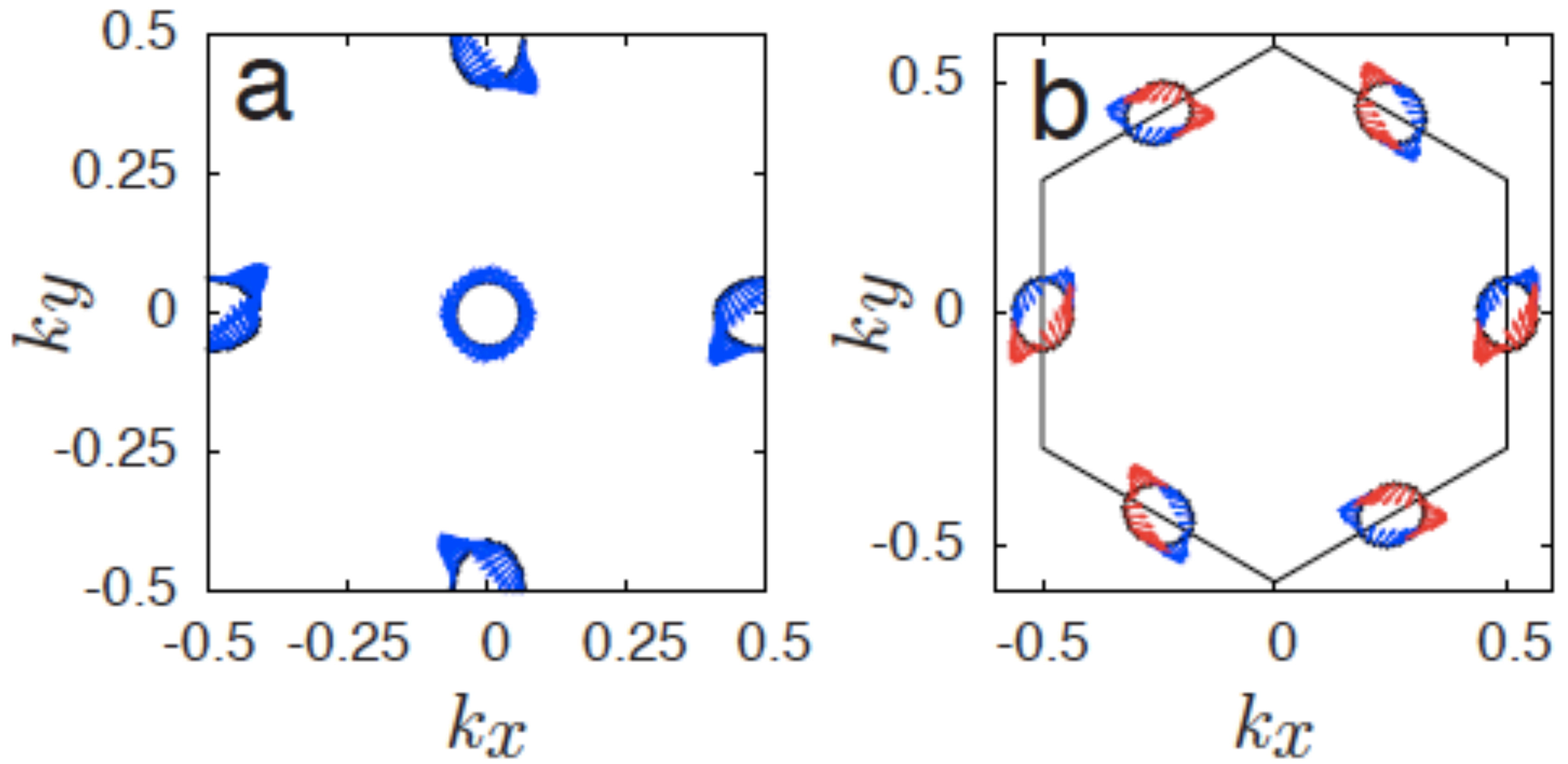






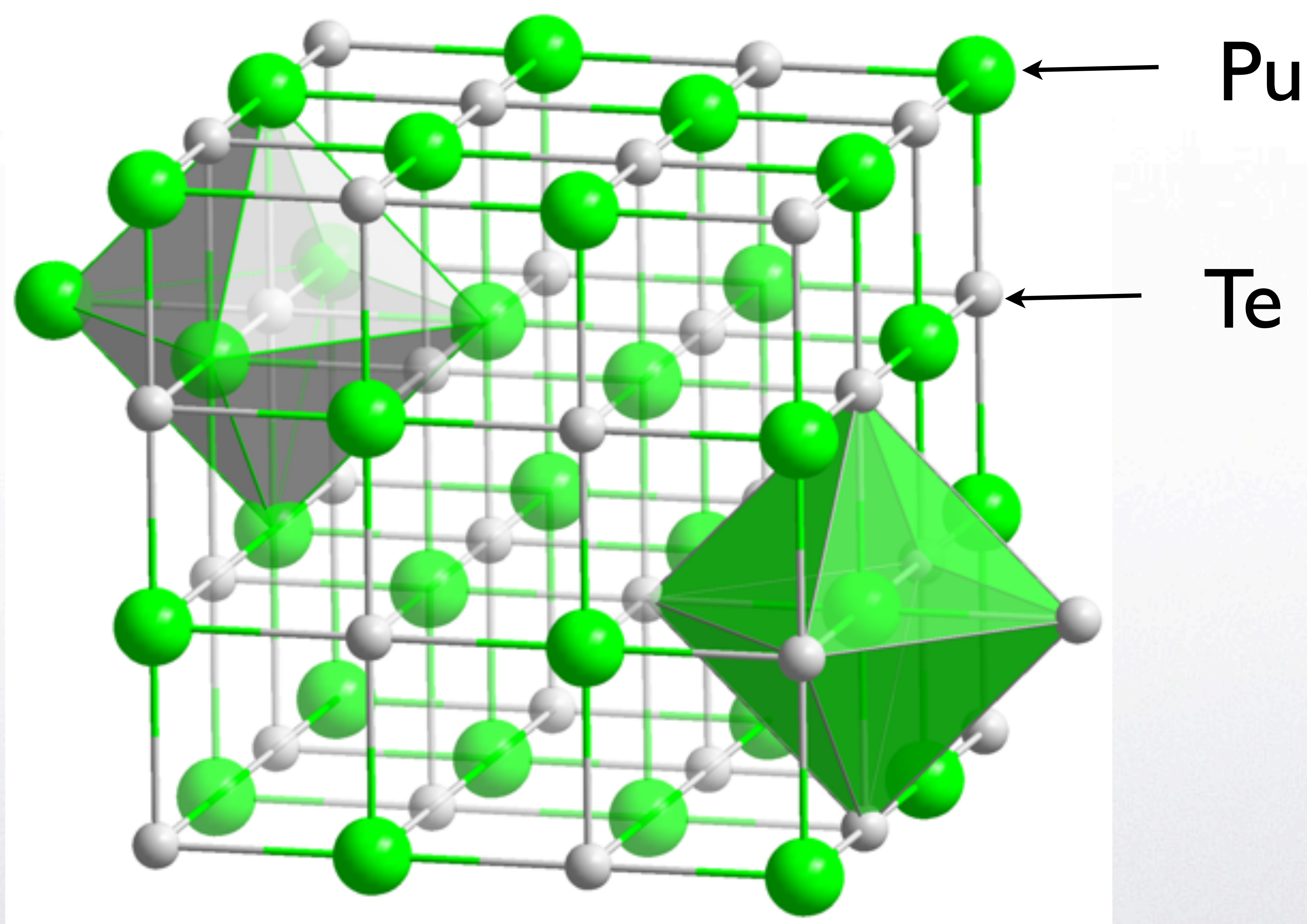


Spin texture for surface states

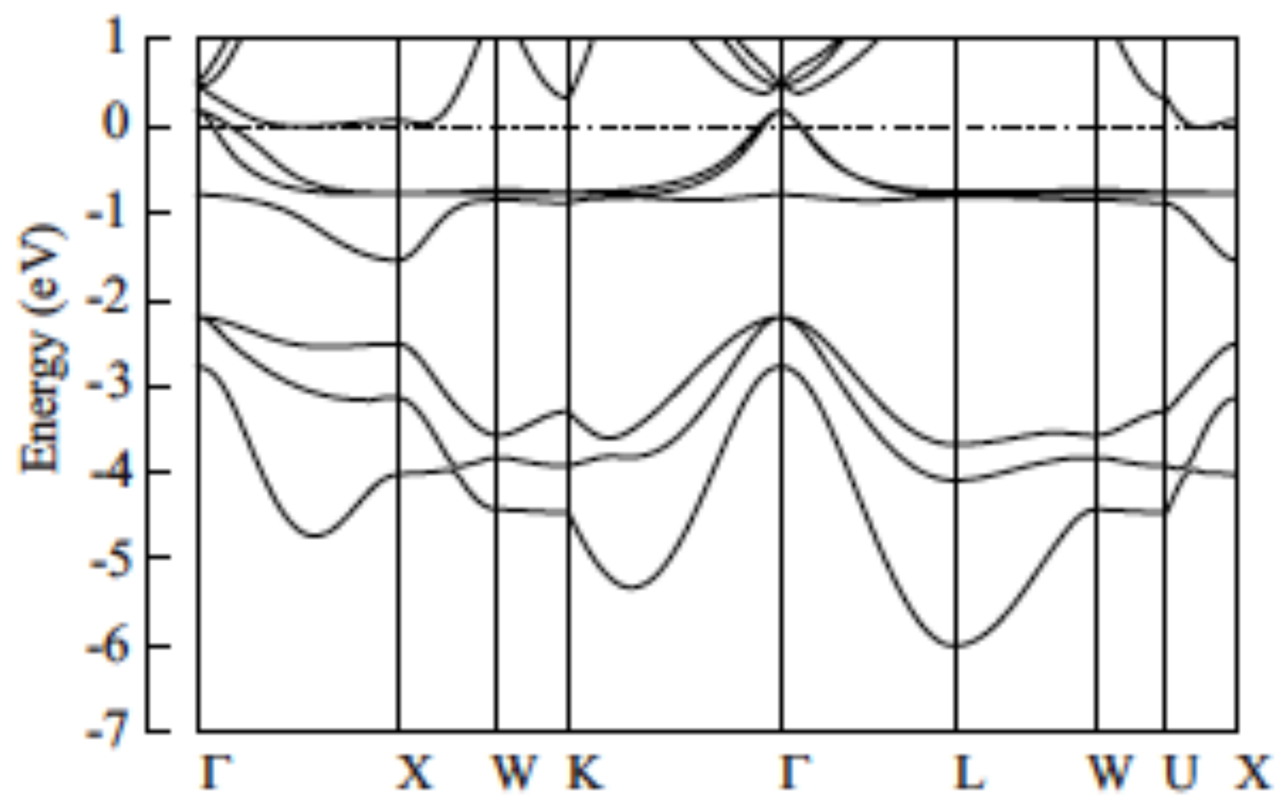


001 surface   111 surface

PuTe

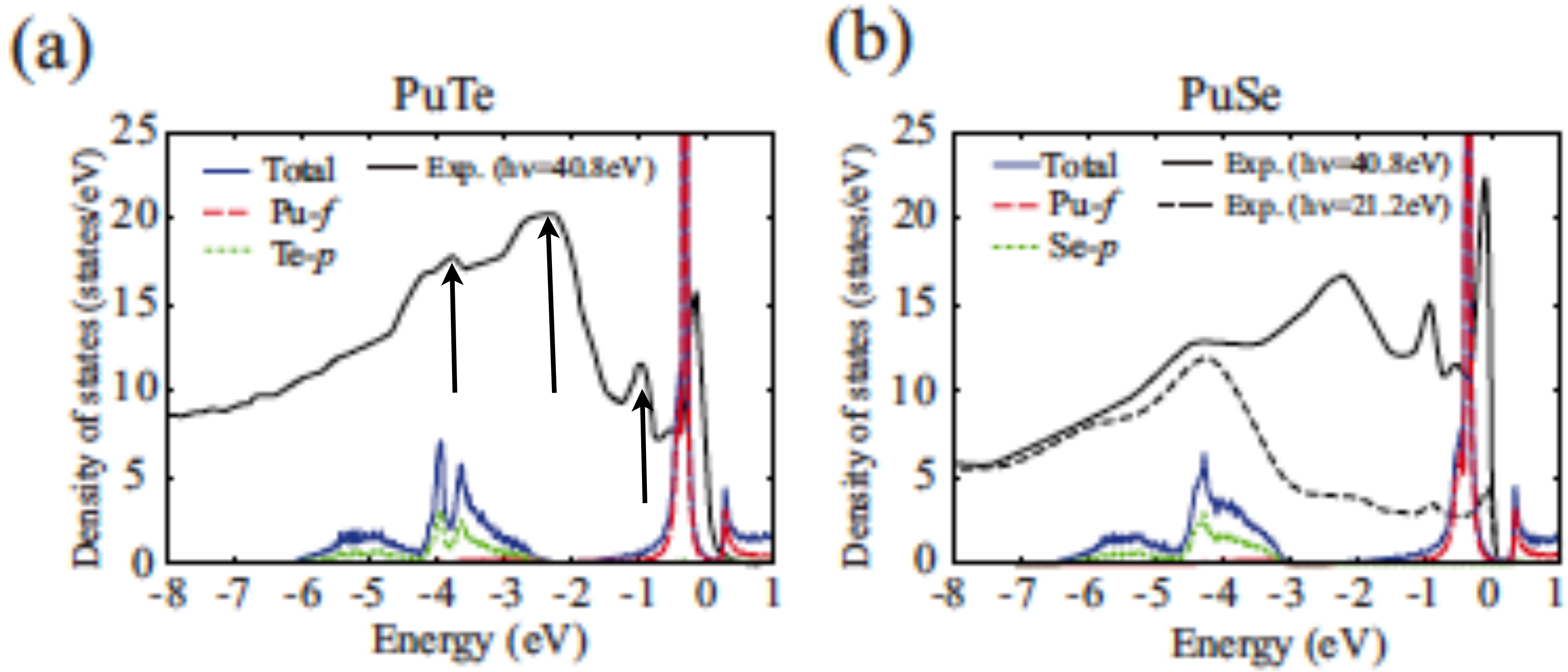


The results obtained by LDA+U



PHYSICAL REVIEW B **80**, 161103，2009

Clear multiplet structure in XPS



PHYSICAL REVIEW B **80**, 161103(R) (2009)

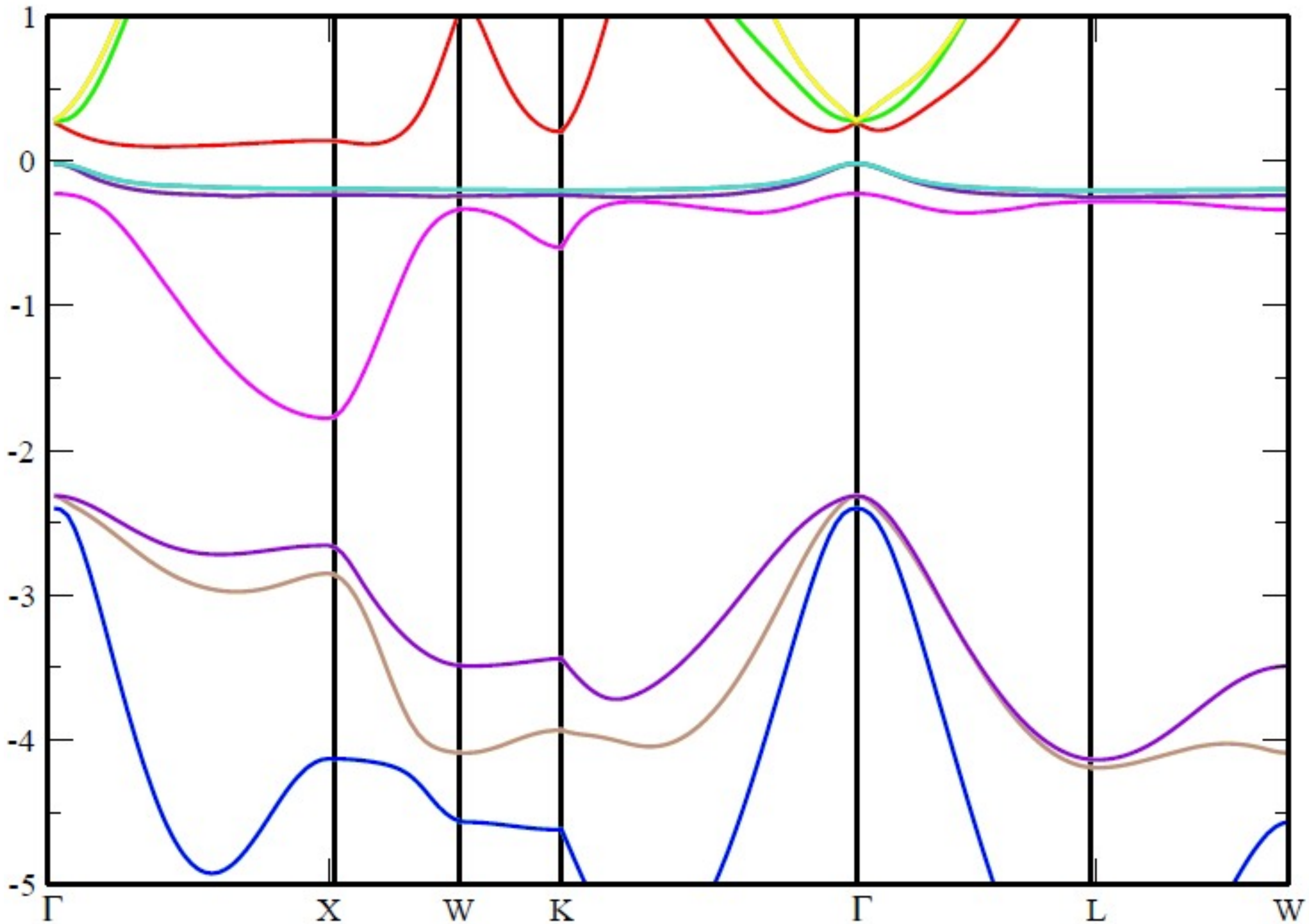
PuTe: Z, nf, Gap vs Parity

Udc	n_f	E_g	$Z(R^2_{mat})$	
			5/2	7/2
20.5eV	5.11	0.12ev	0.51	0.67

		E_g	Γ	3X	4L	Tol
PuTe	LDA		-	+	-	-
PuTe	GW	0.12ev	-	+	-	-

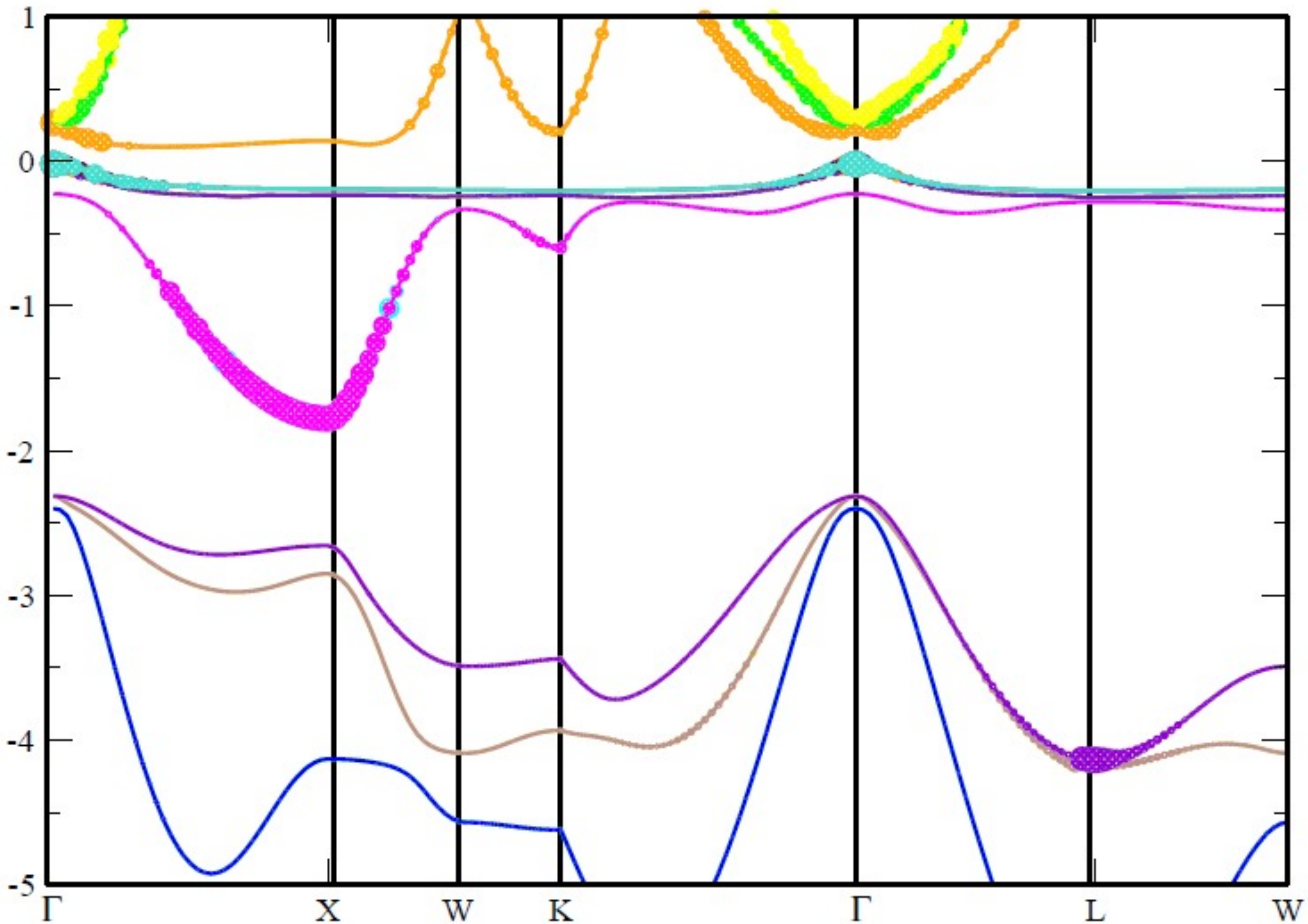
PuTe

Band structure: GW method



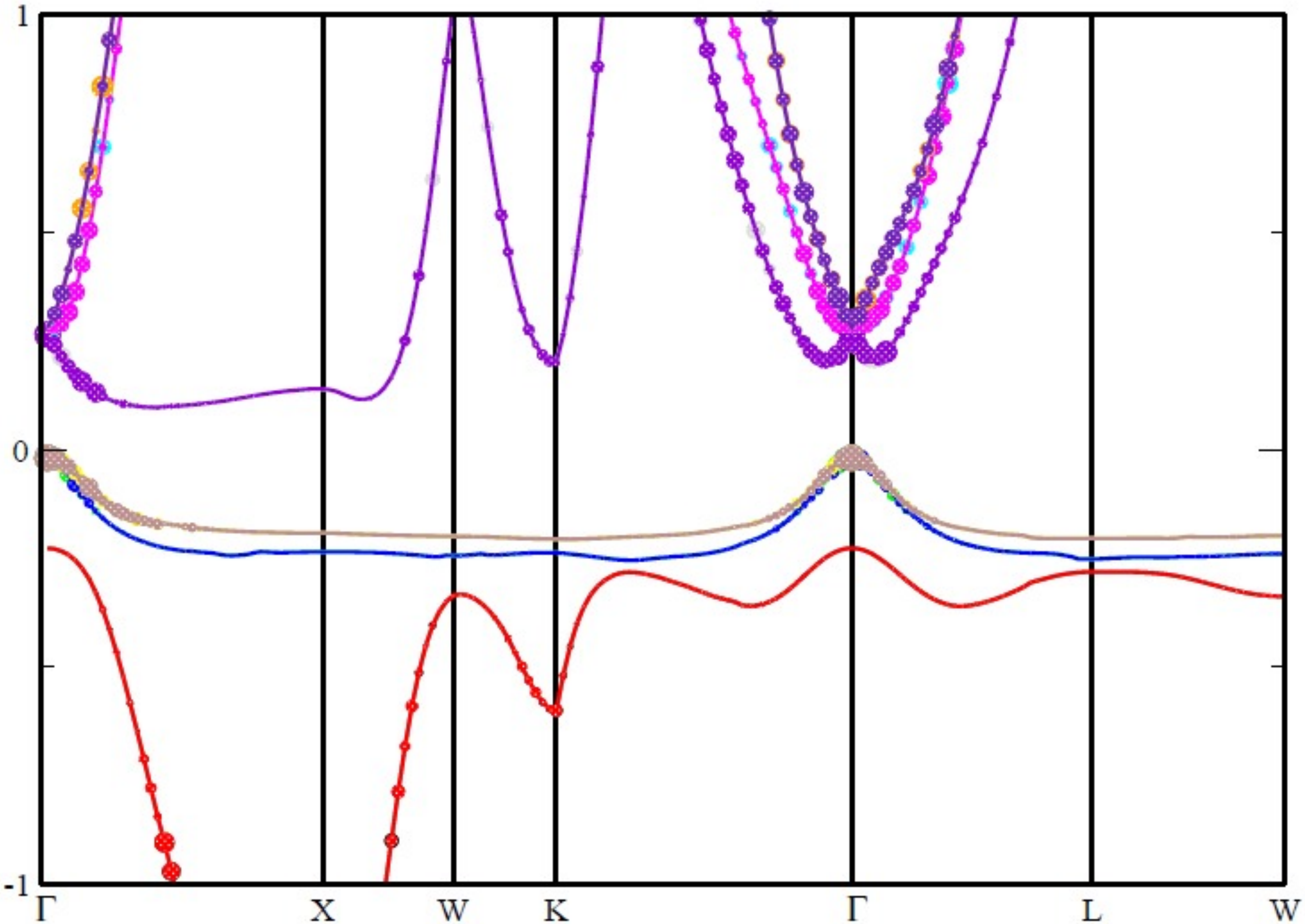
PuTe

Fat Band structure: GW method

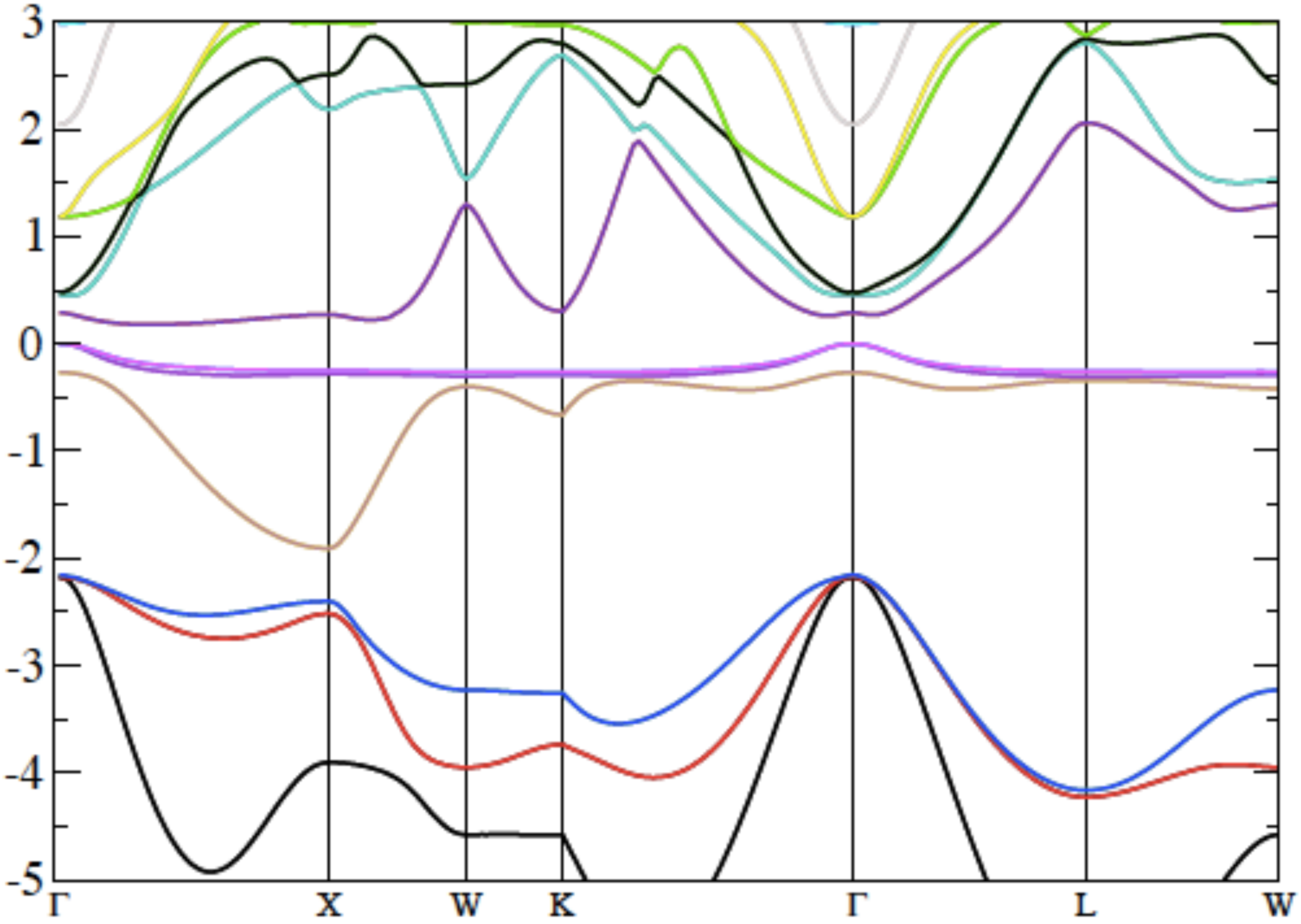


PuTe

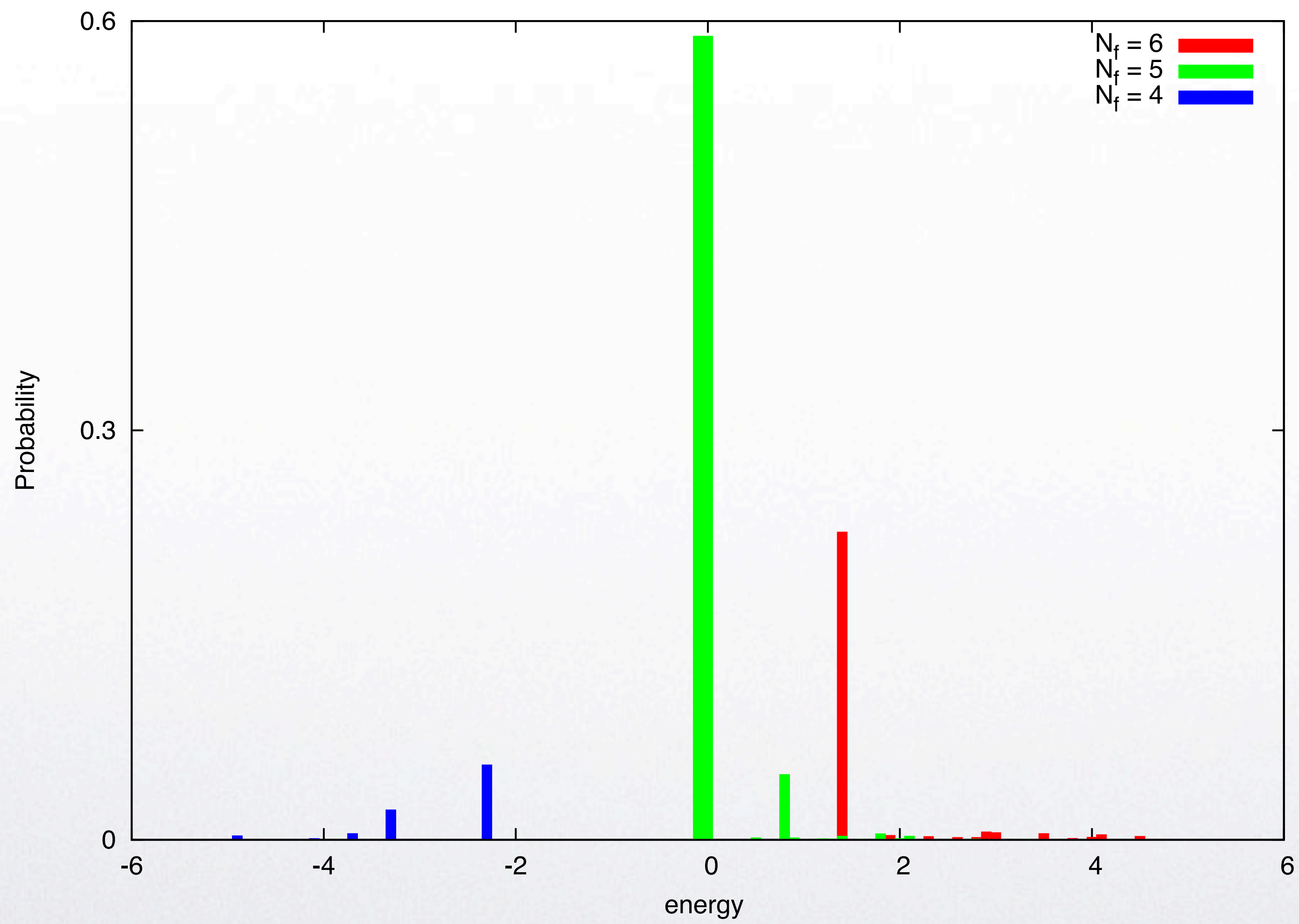
Fat Band structure: GW method



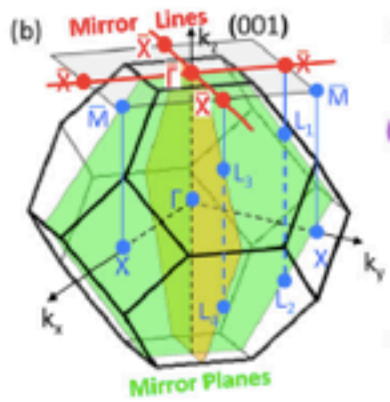
Electronic structure of PuTe at 5.5GPa gap=0.21eV



The probability of atomic eigenstates for PuTe

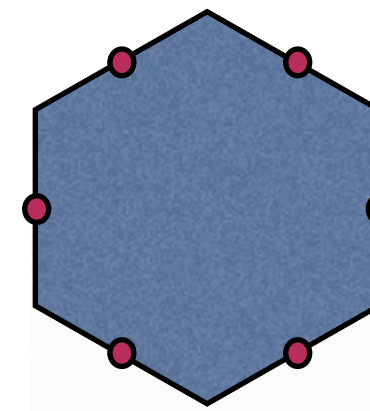


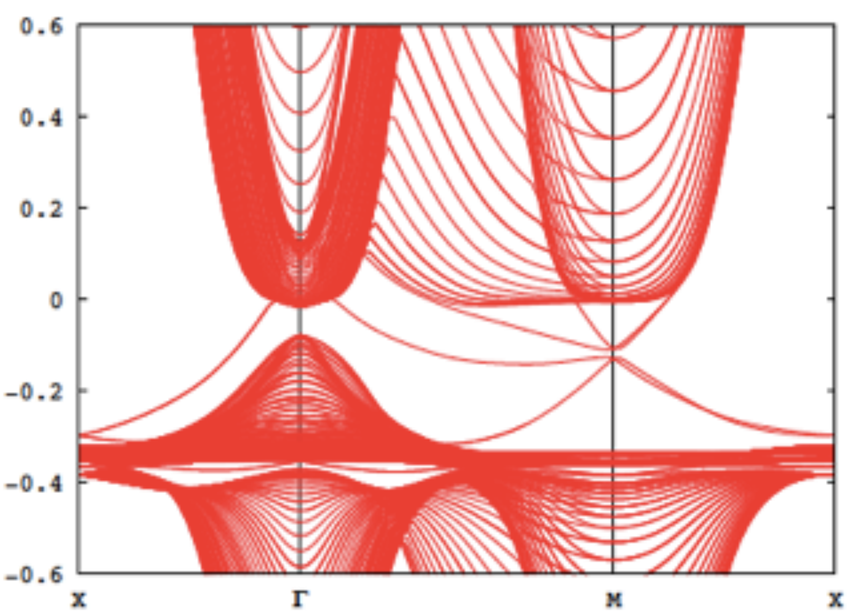
Surface state

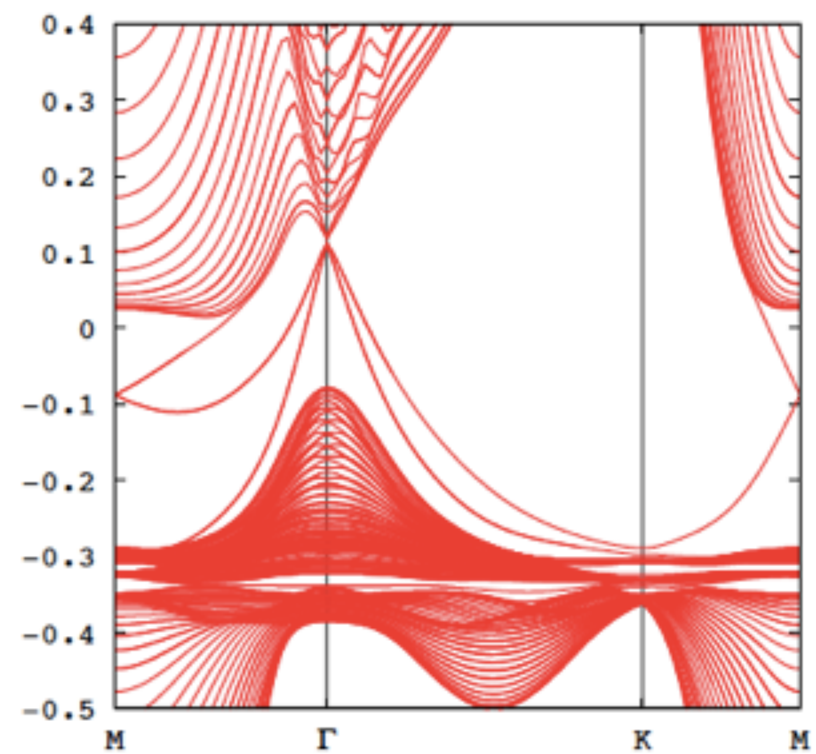


(0 0 1)

(1 1 1)







Conclusions

- Mix valence TIs, SmB_6 and PuTe
- The topological phase survives from the Strong e-e interaction among f electrons
- The Z_2 invariance can be computed by the green's function in low frequency
- More similar materials!