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Topological Materials Science
トポロジーが紡ぐ物質科学のフロンティア

Magnetic states in a strongly correlated topological insulator

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Topological Materials Science
トポロジーが紡ぐ物質科学のフロンティア

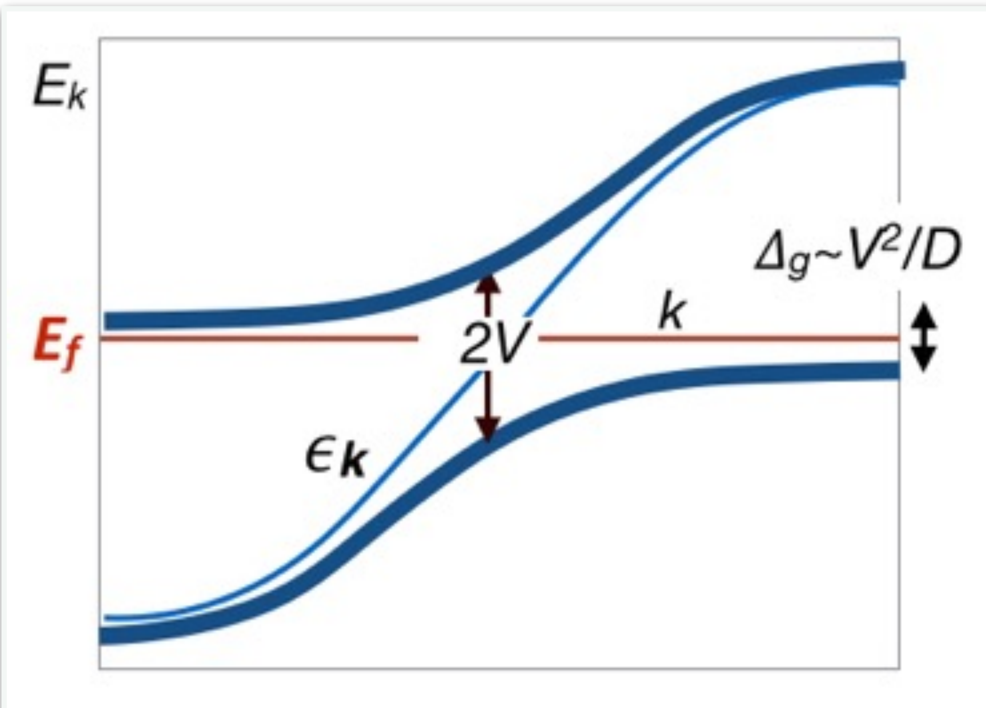
- Correlation effects in topological Kondo insulators
- Magnetic states

"Coexistence of light and heavy surface states in a topological multi-band Kondo insulator"

RP, T Yoshida, H Sakakibara, and N Kawakami
Phys. Rev. B 93, 235159 (2016)

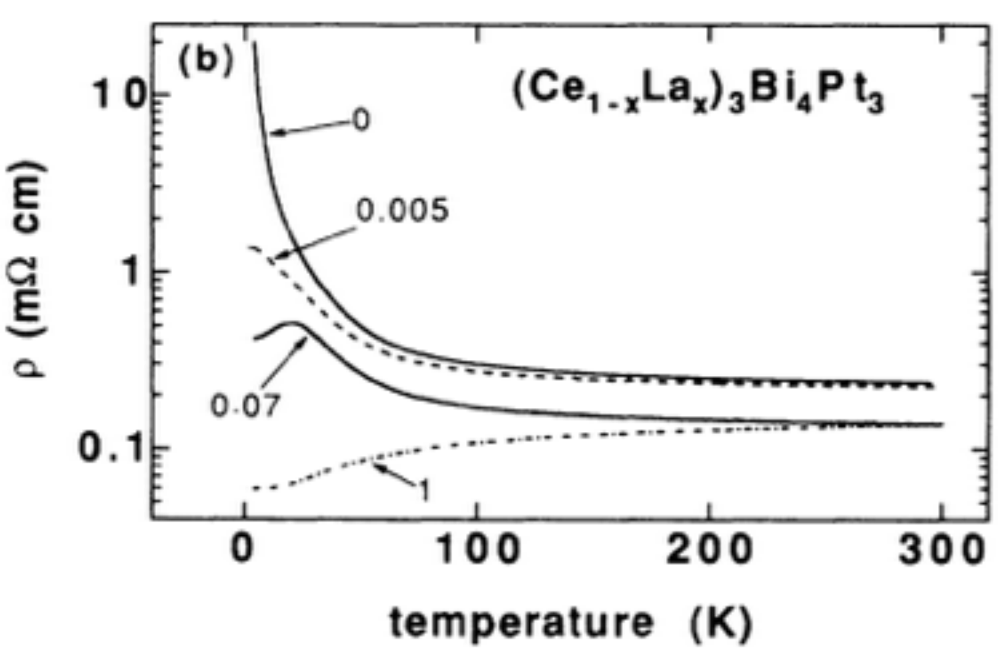
"Magnetic states in a strongly correlated topological Kondo insulator"
in preparation

Kondo insulator



Dzero et al.; Annual Review of Condensed Matter Physics, Volume 7 (2016)

- Due to a hybridization between two bands a gap opens
- **In f-electron systems: Due to a strong correlation effect in the f-orbital, the Kondo effect becomes important and the gap is renormalized.**

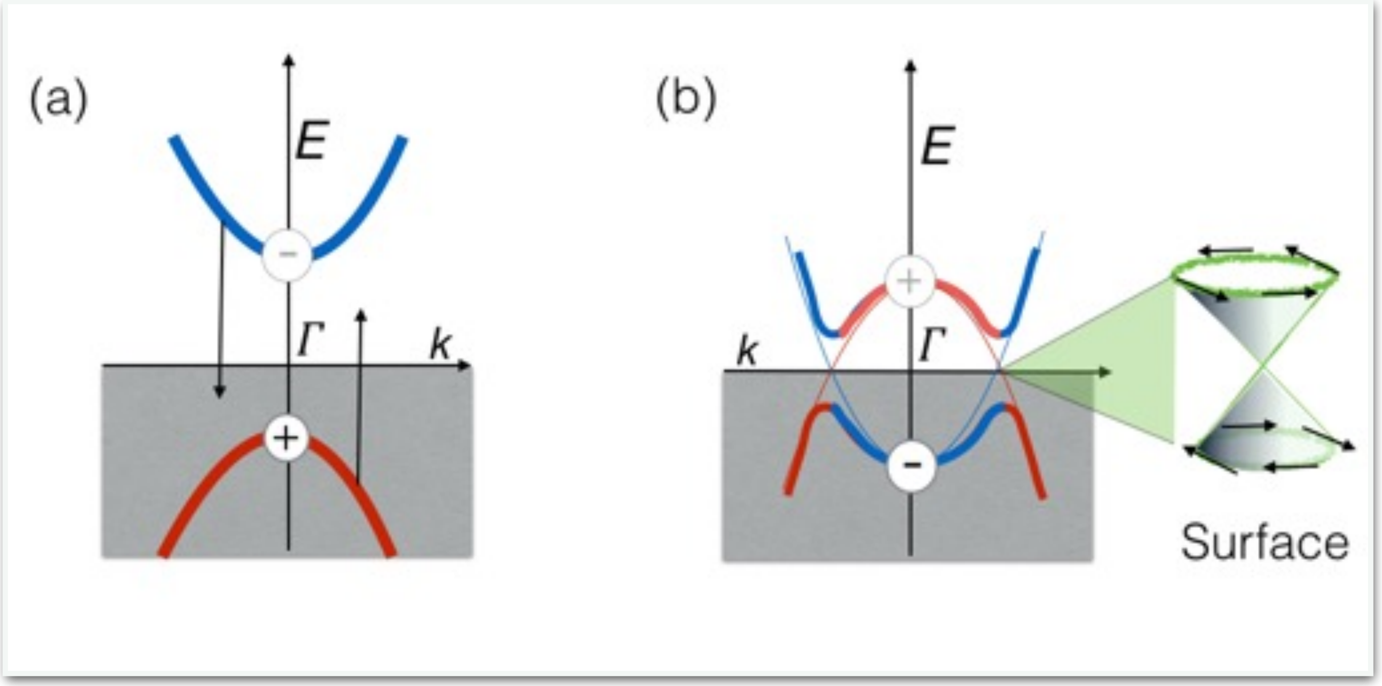


resistivity strongly increases at low temperature

Hundley, et al. PRB 42 6842 (1990)

from a Kondo insulator to a topological Kondo insulator

topological Kondo insulator

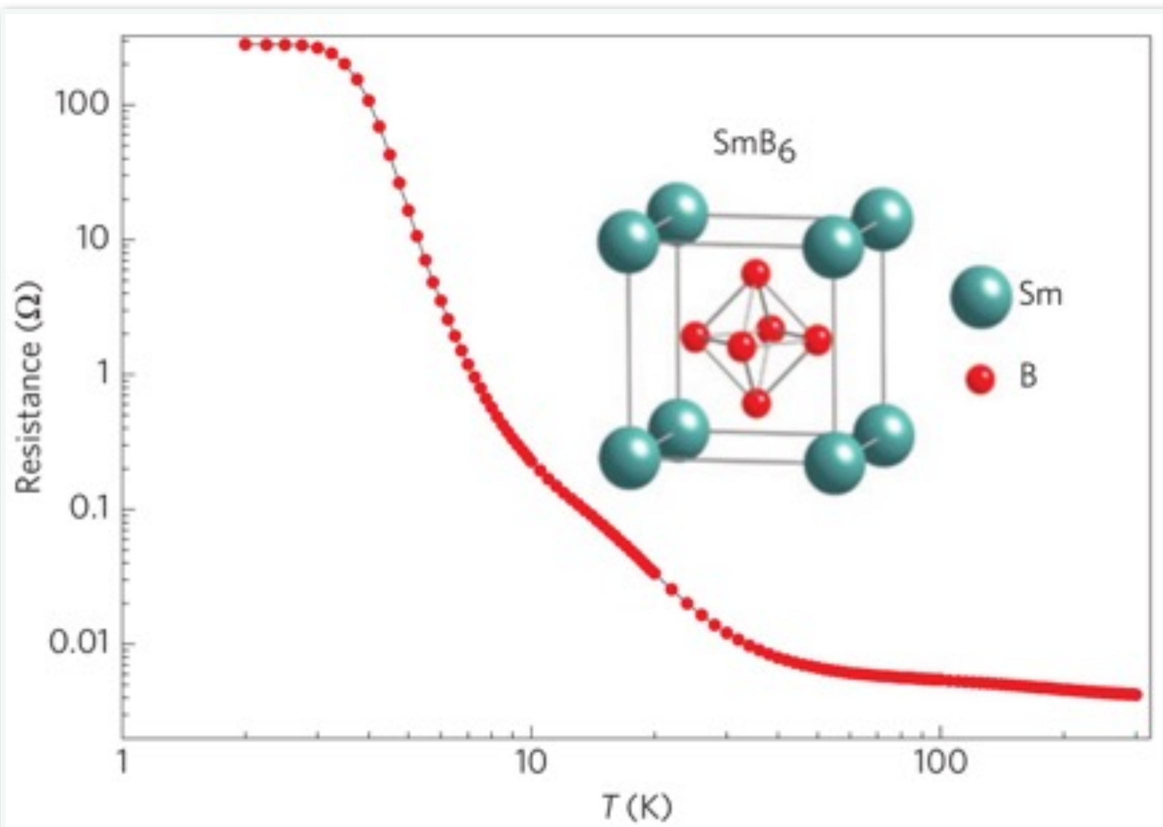


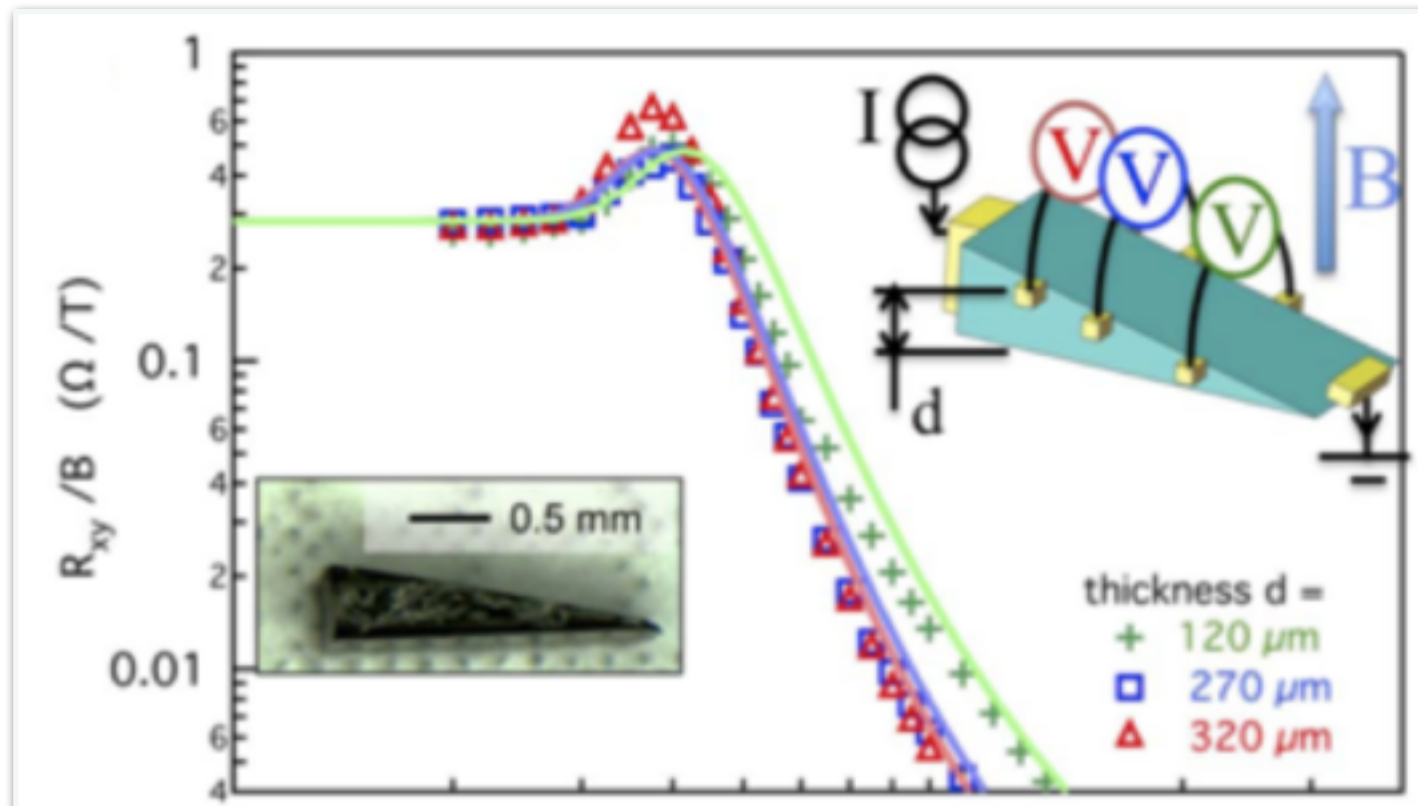
Dzero et al.; Annual Review of Condensed Matter Physics, Volume **7** (2016);

Dzero et al PRL **104** 106408 (2010)

topological Kondoinsulator

candidate SmB_6



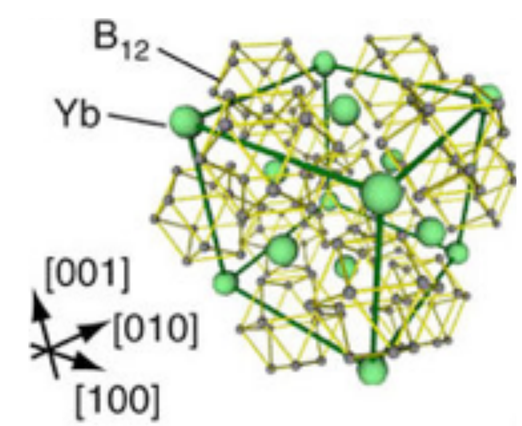


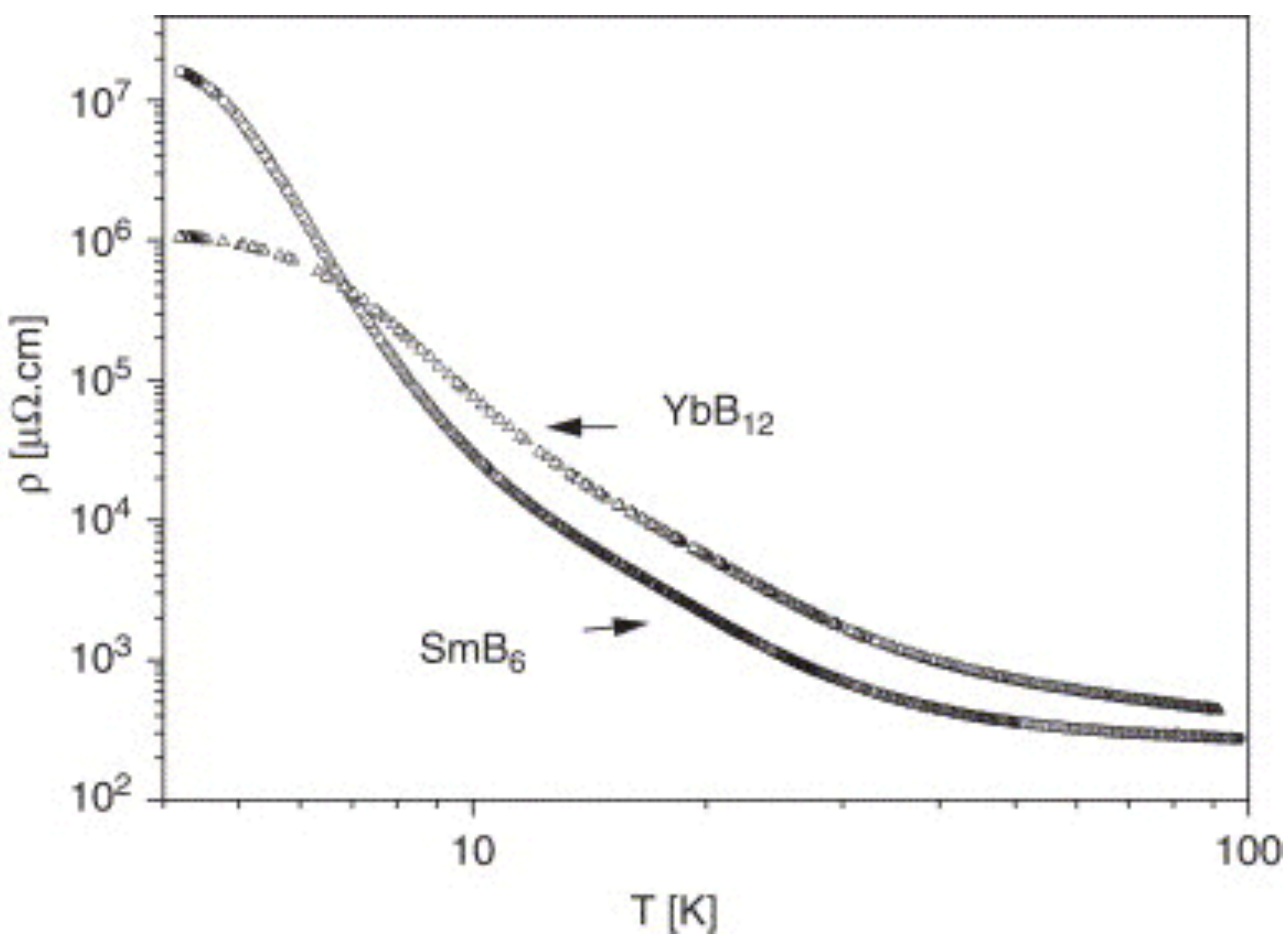
Kim et al., Nature Materials 13 466 (2014)

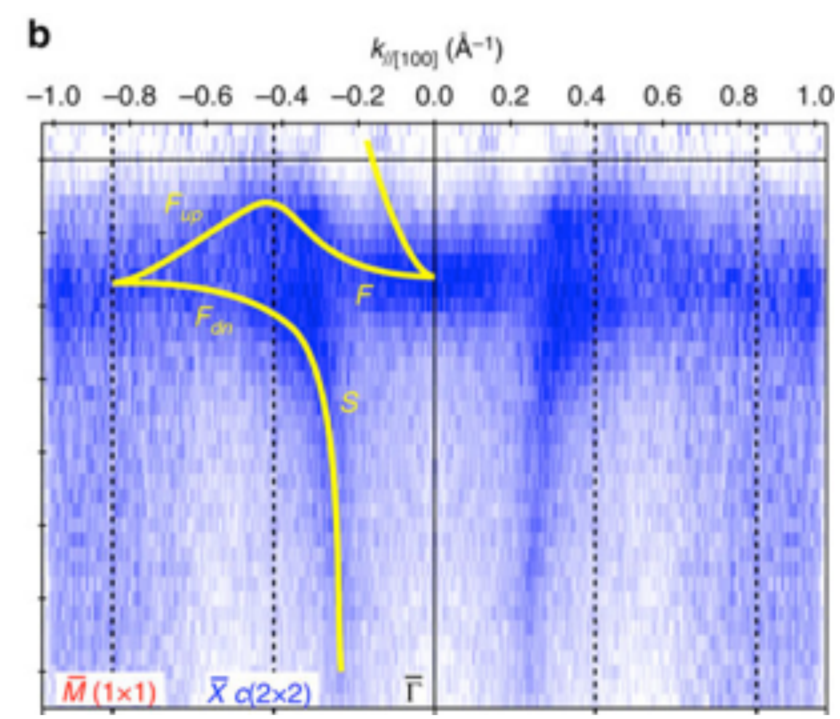
Kim et al., Scientific Reports **3**, 3150 (2013)

topological Kondoinsulator

candidate YbB_{12}





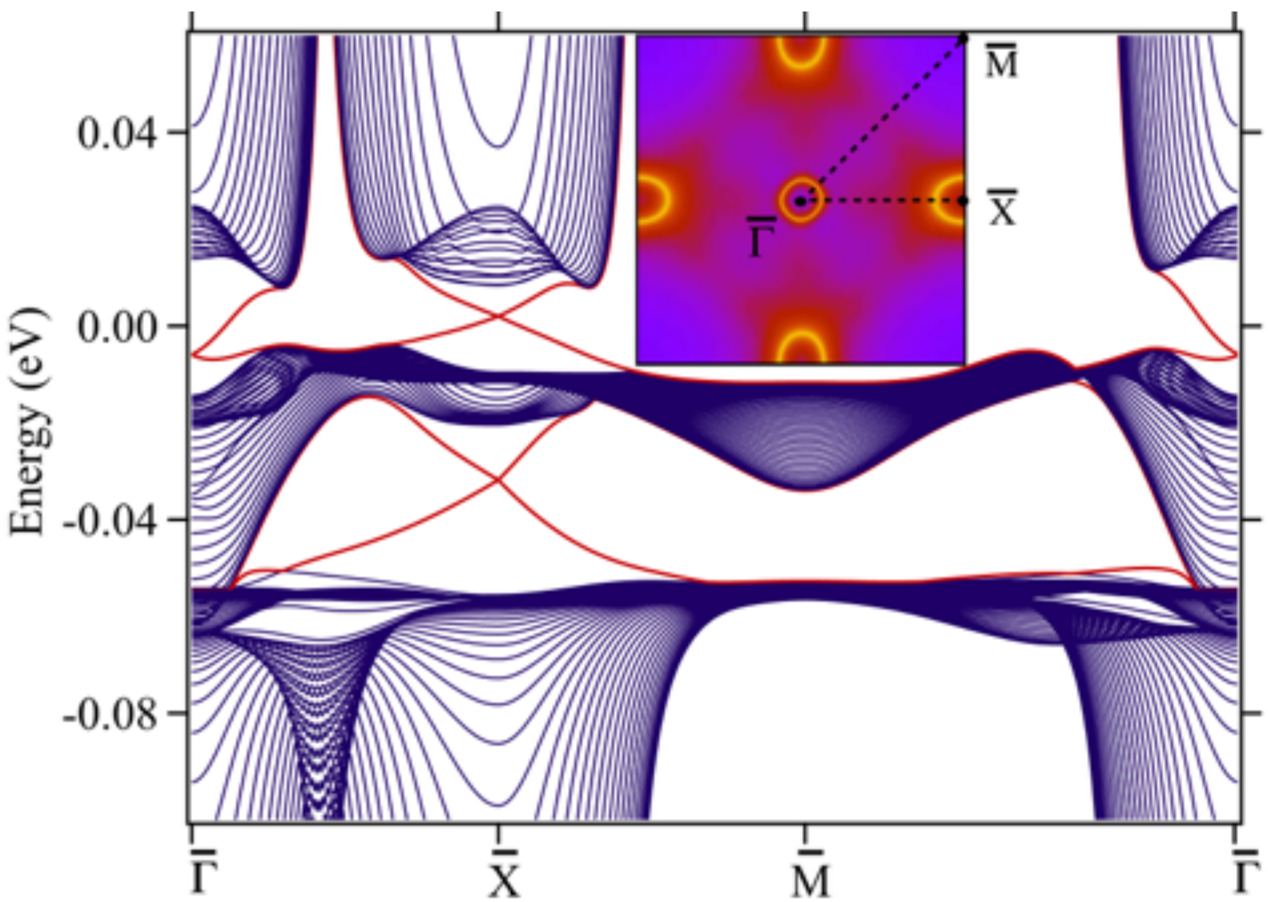


M.Bat'ková Proceedings SCES 2005

Hagiwara et al. Nature Comm. **7**, 12690 (2016)

LDA for SmB_6

LDA + Gutzwiller



Lu et al PRL 110 096401 (2013)

surface states due to the topology

SmB_6 a three dimensional strongly correlated topological insulator

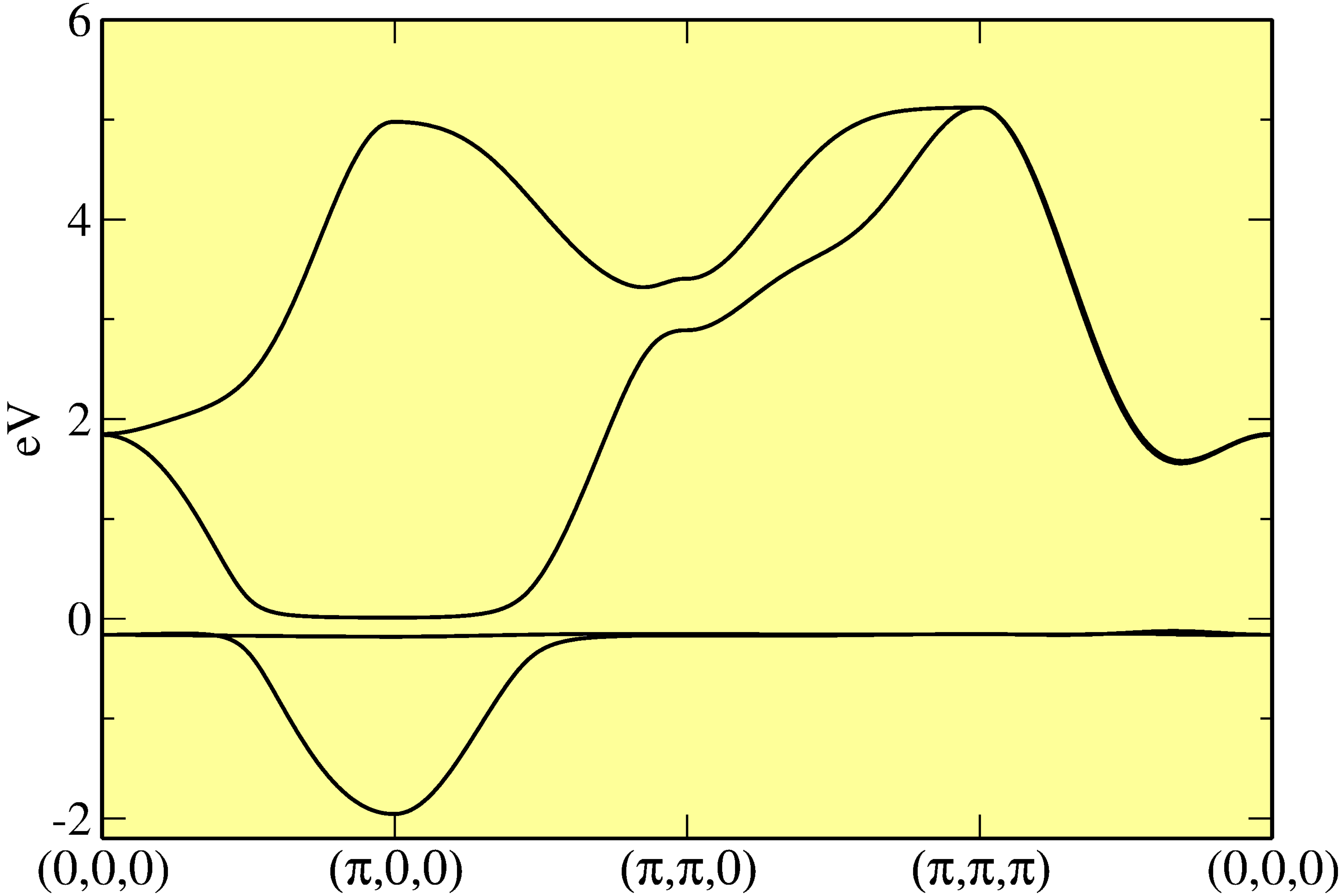
heavy surface states

first LDA calculation T. Takimoto JPSJ 2011

topological Kondoinsulator

Interplay between topology and strong correlations

band structure of SmB_6



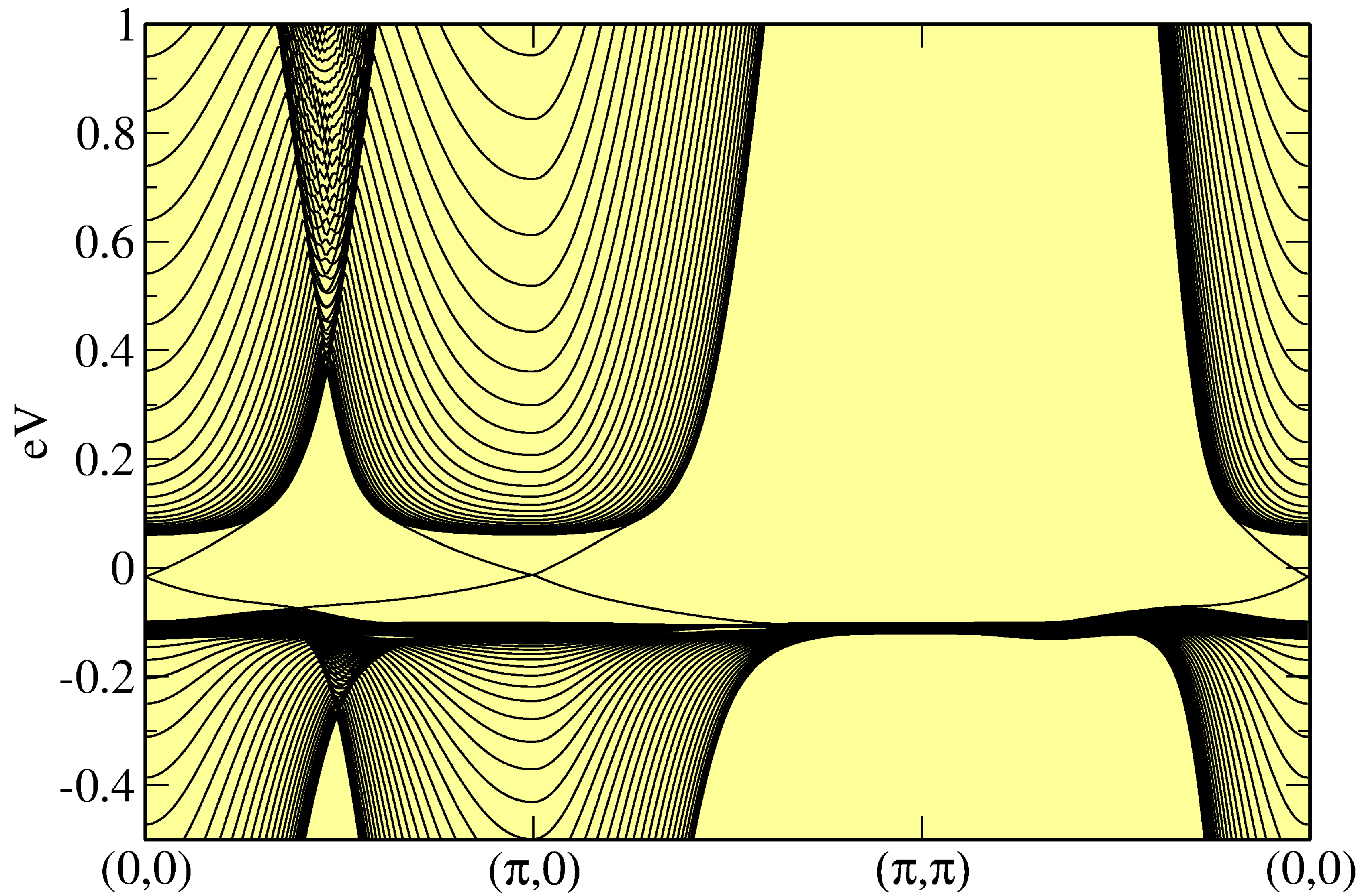
d-electrons

f-electrons

strong topological insulator

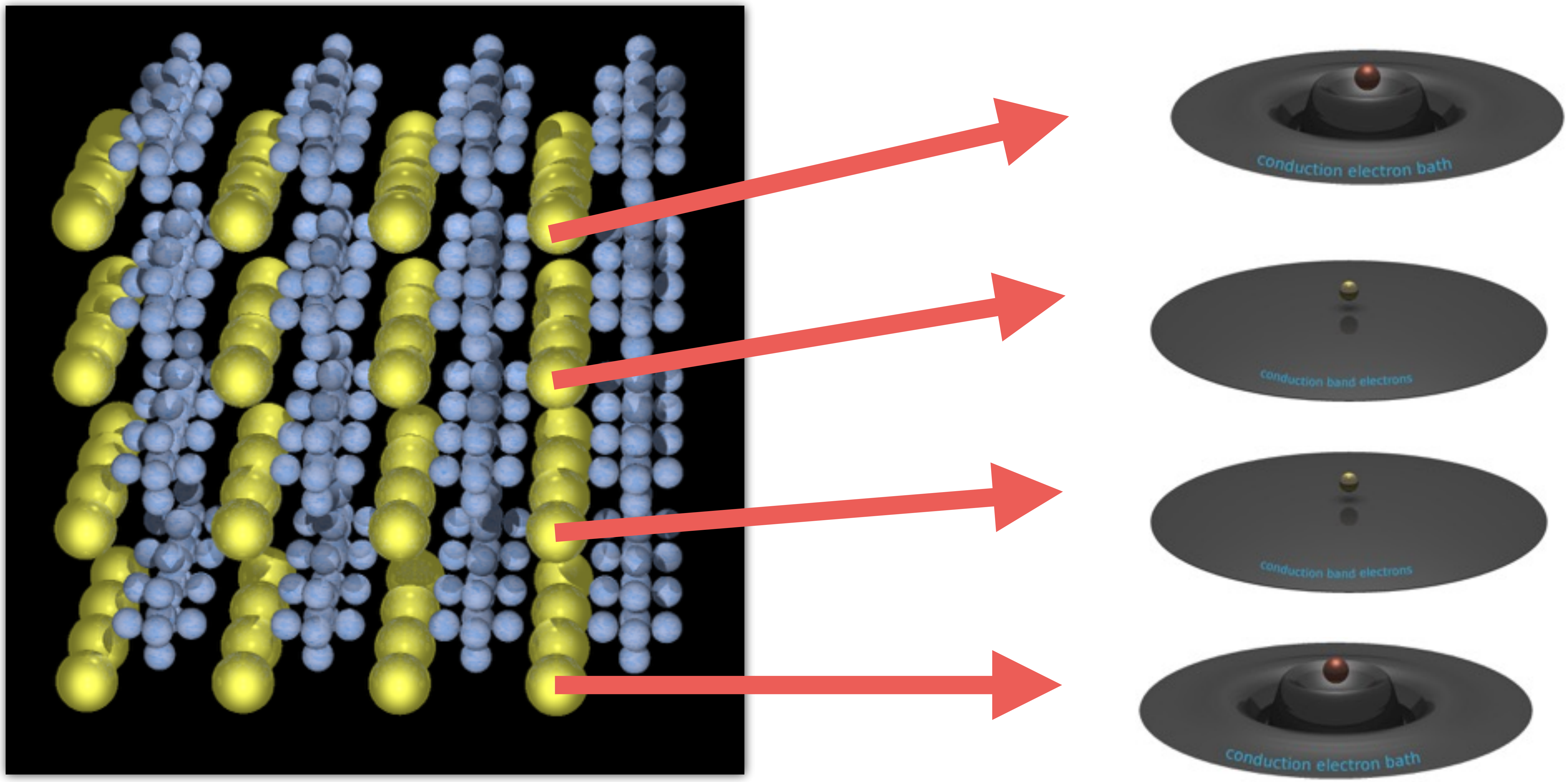
band structure of SmB_6

open surface in z-direction

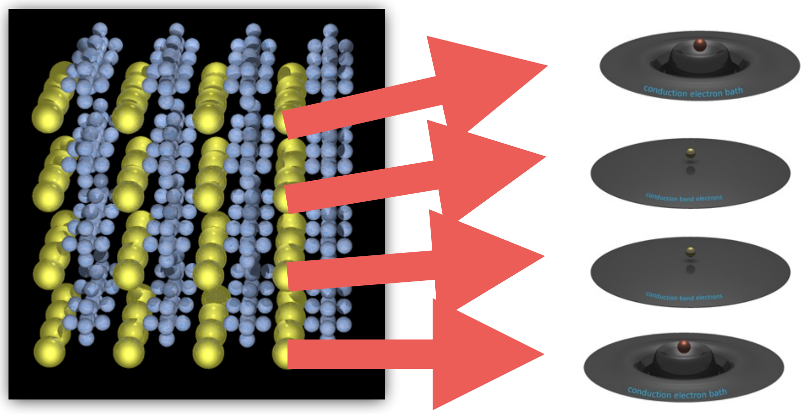


surface states at Γ and X

Study effects of strong correlations on topological surface states.



Study effects of strong correlations on topological surface states.

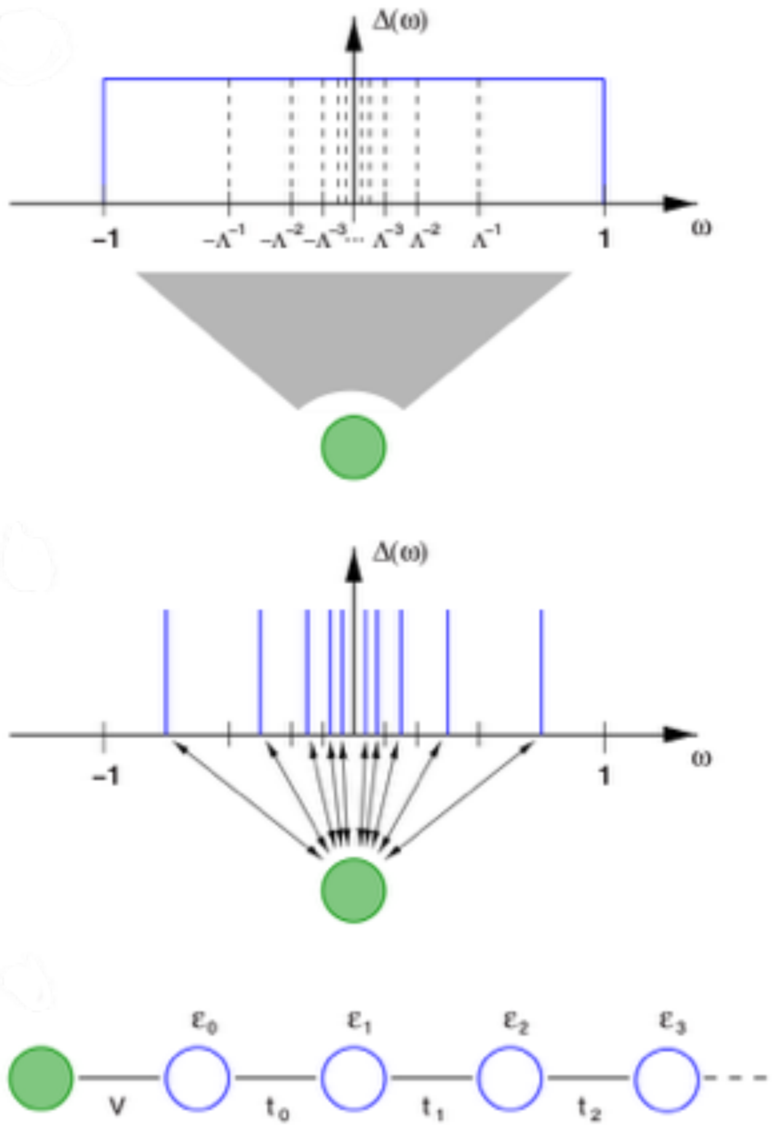


$$G^{-1} = \begin{pmatrix} z - \Sigma_1 & & & \cdots \\ & z - \Sigma_z & & \cdots \\ & & z - \Sigma_3 & \cdots \\ & & & \ddots \end{pmatrix}$$

we use 20-50 layers

open boundaries in z-direction

Study effects of strong correlations on topological surface states.



NRG

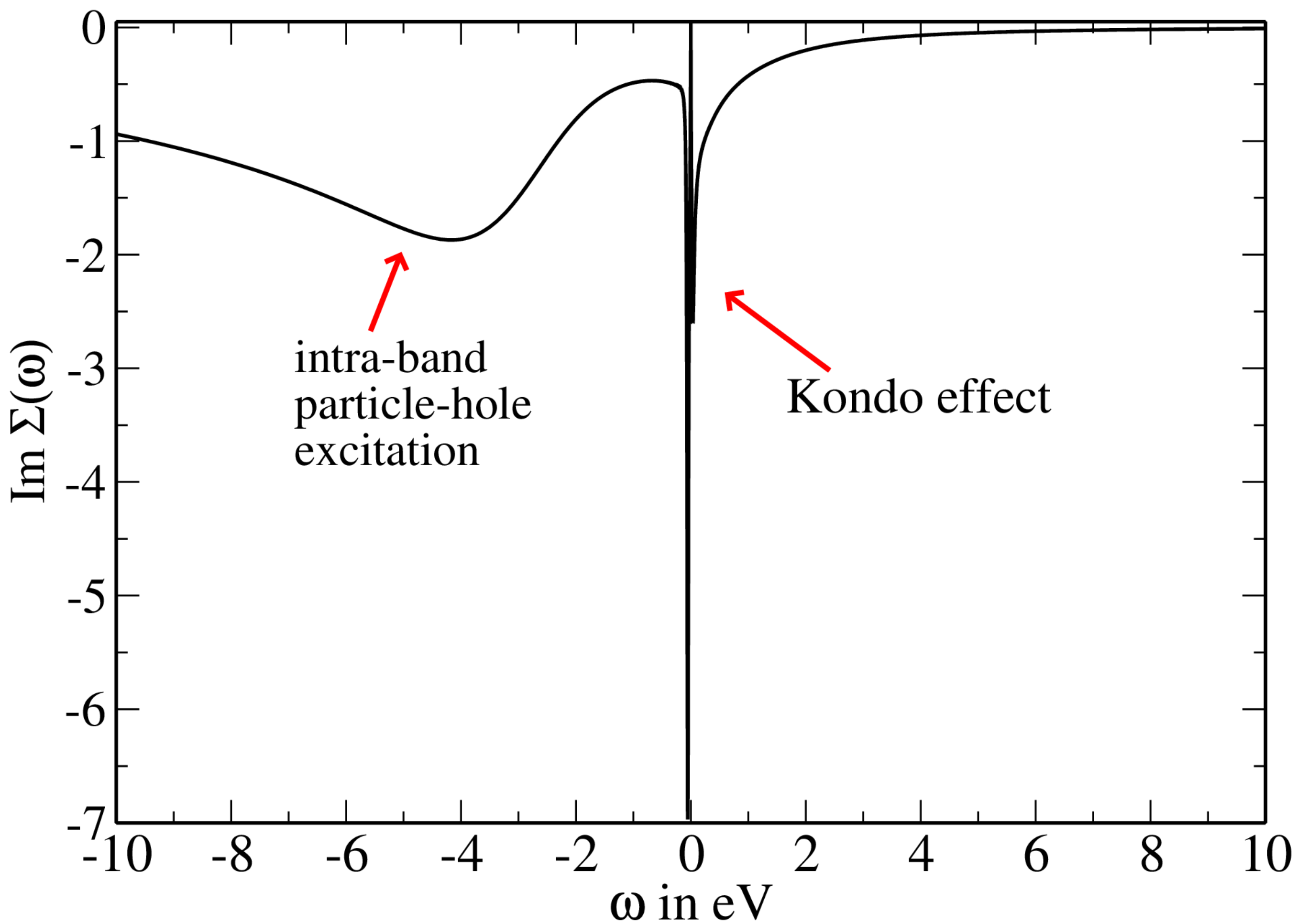
- Logarithmic discretization of the energy band
- Iterative Diagonalization
- Able to calculate **real frequency spectral functions**
- We resolve **details** around the Fermi energy down to **0.00001eV**

Ralf Bulla, Theo A. Costi, and Thomas Pruschke

Rev. Mod. Phys. 80, 395 (2008)

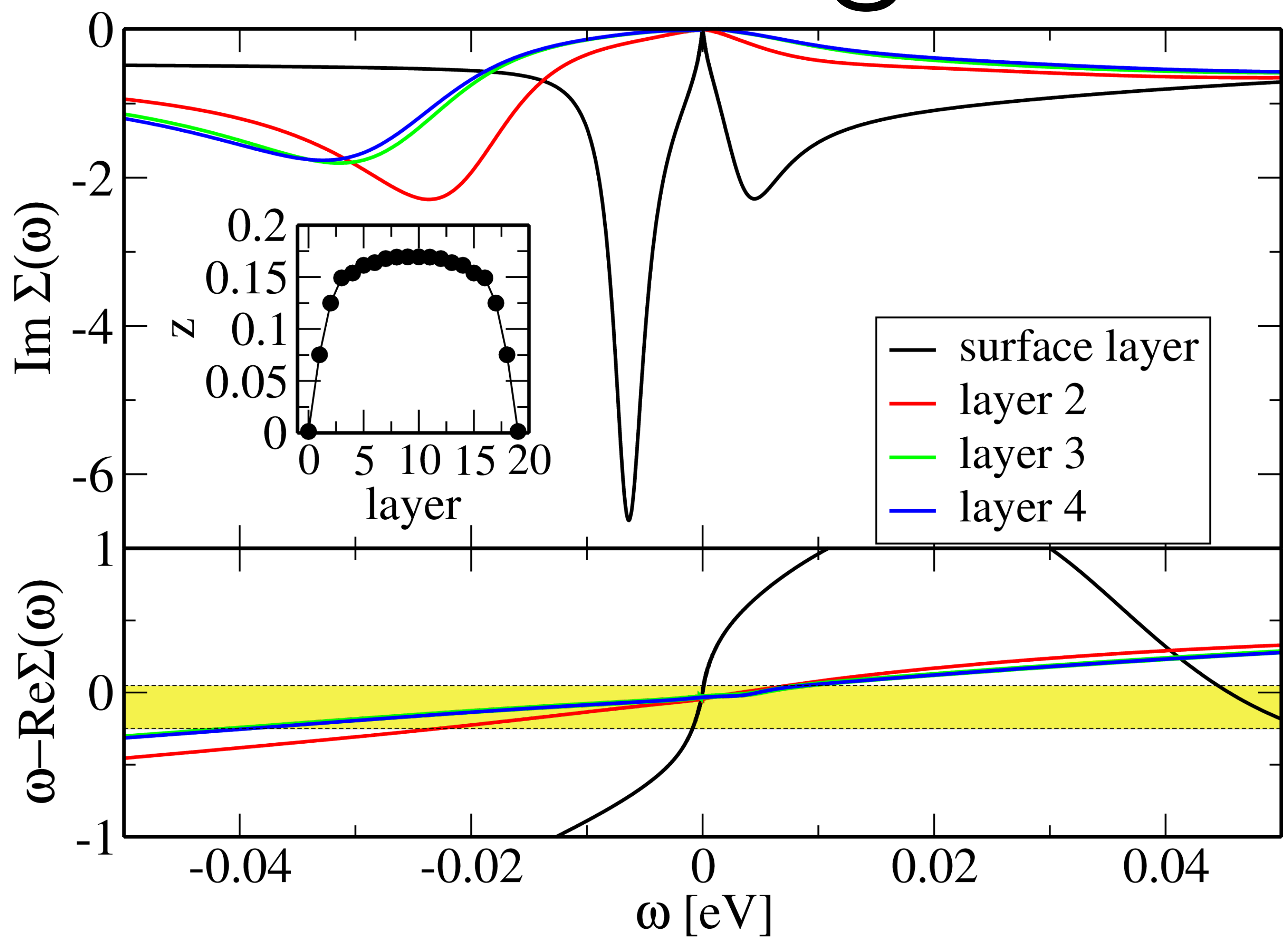
Study effects of strong correlations on topological surface states.

general self-energy for these parameter



- This self-energy results in a renormalization of the band structure.
- The gap becomes smaller!

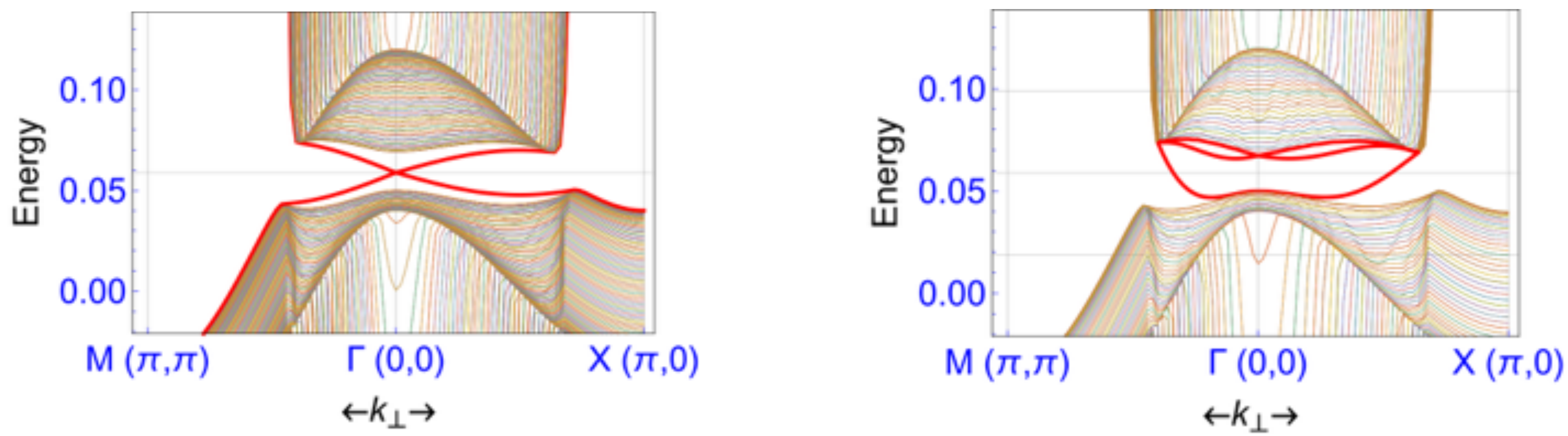
layer dependent self energies



The surface layer are much stronger correlated than the bulk

Kondo breakdown at the surface

$T = 0$

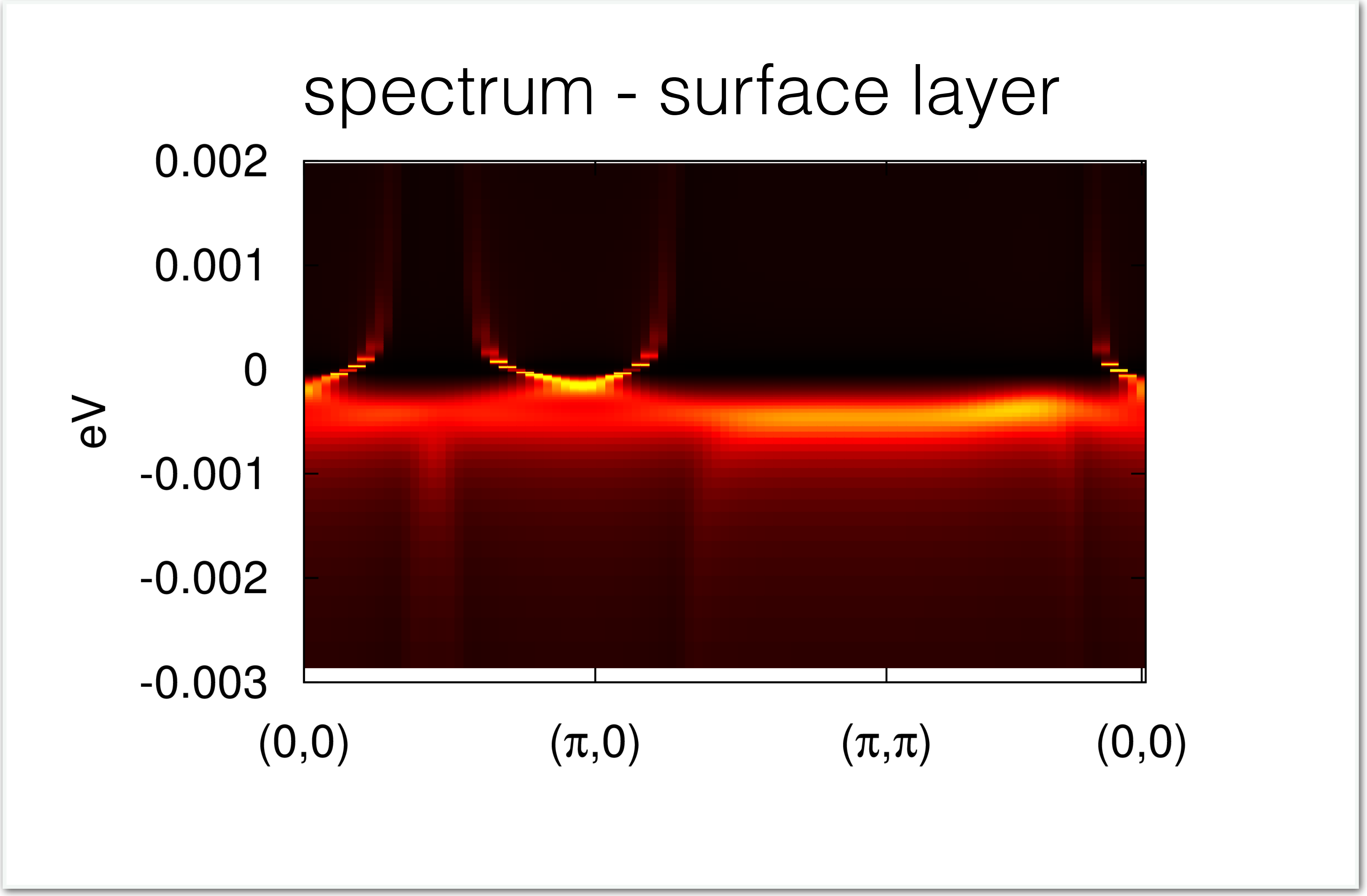


$T > T_K$

Victor Alexandrov, Piers Coleman, and Onur Erten
Phys. Rev. Lett. 114, 177202

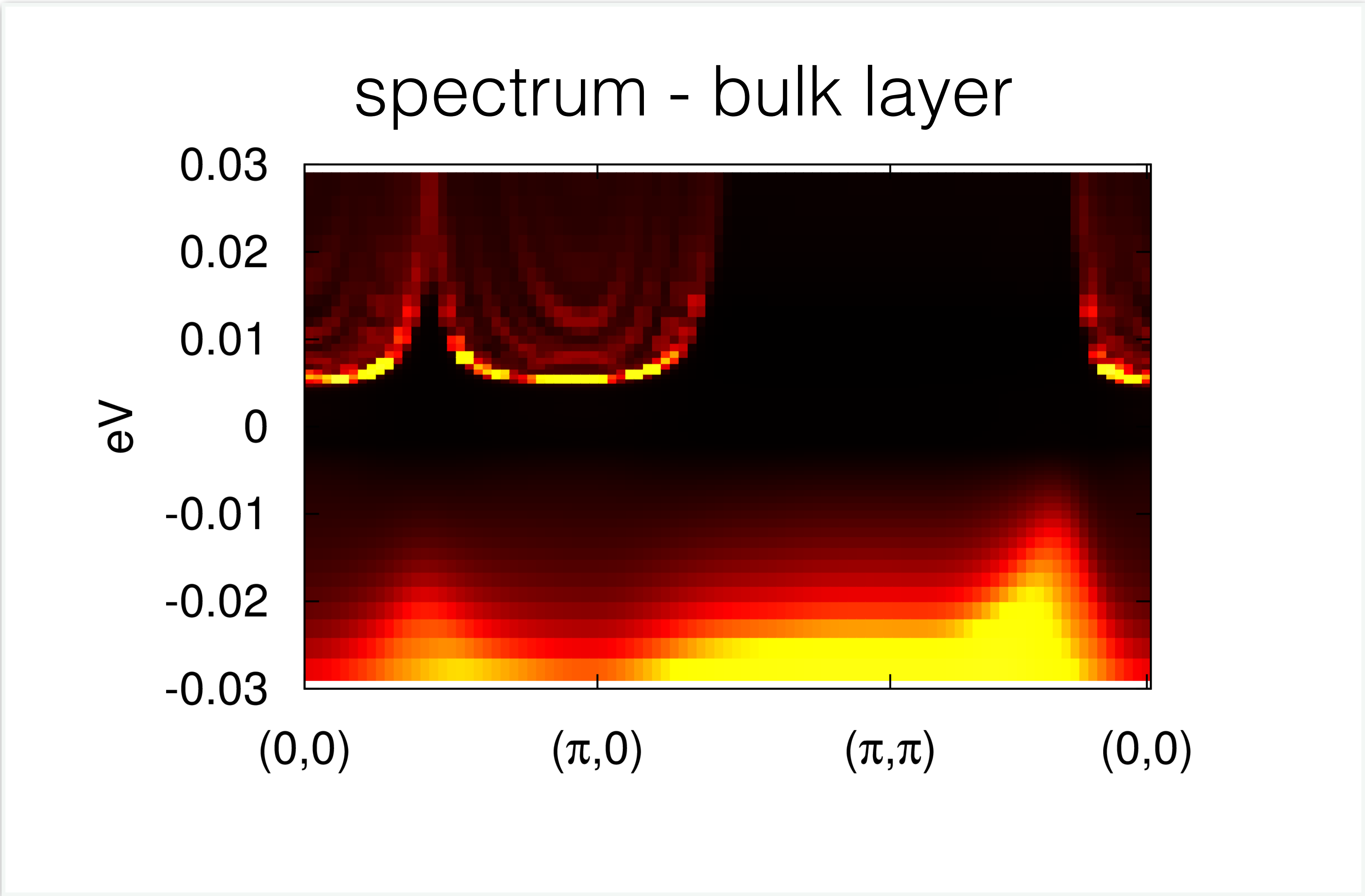
The surface states change their behavior depending on the temperature

Strongly correlated surface states



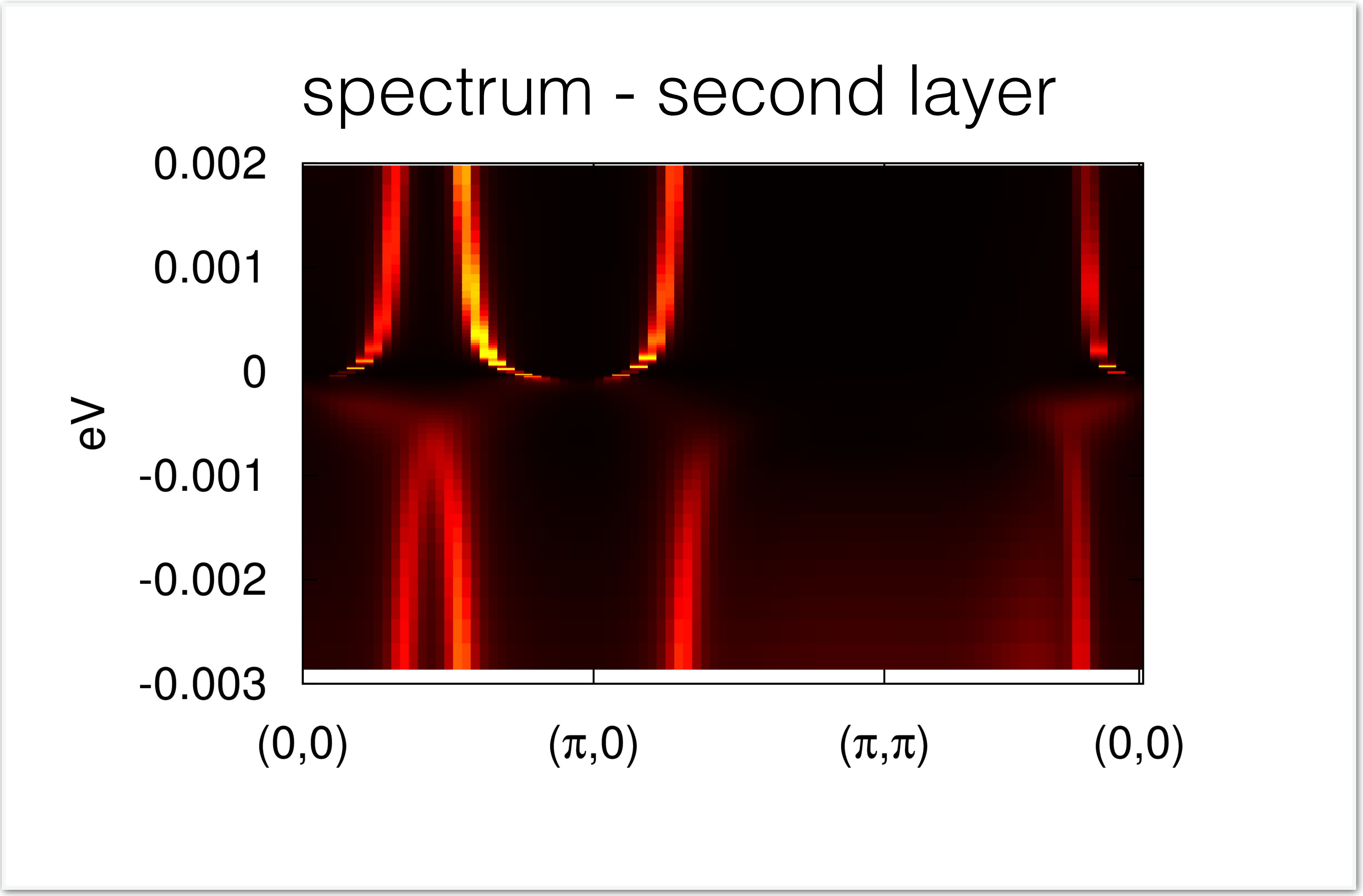
at T=0, surface electron are strongly confined to the Fermi energy and form heavy Dirac cones

Strongly correlated surface states



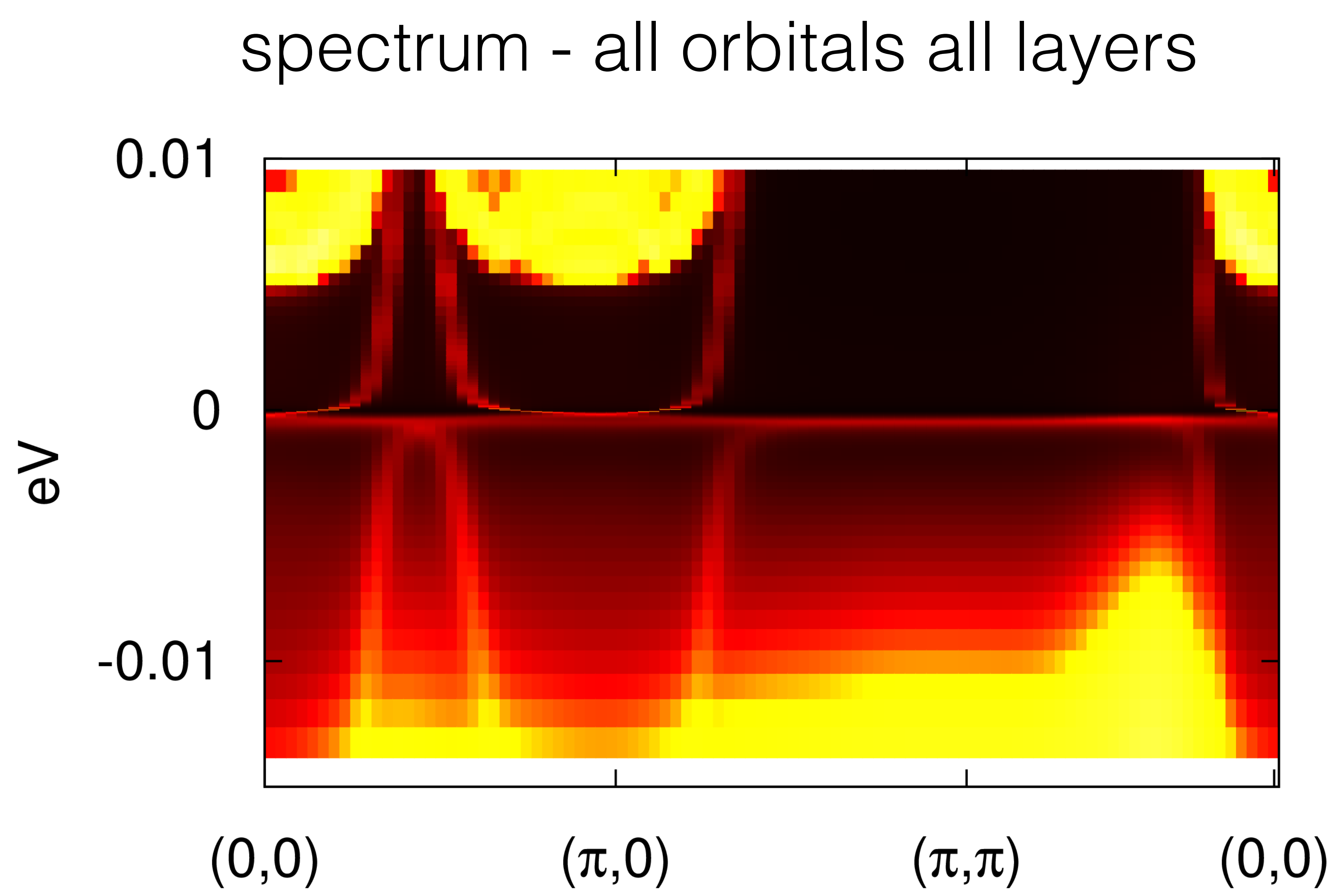
the bulk gap is larger than band width of the surface electrons

Strongly correlated surface states

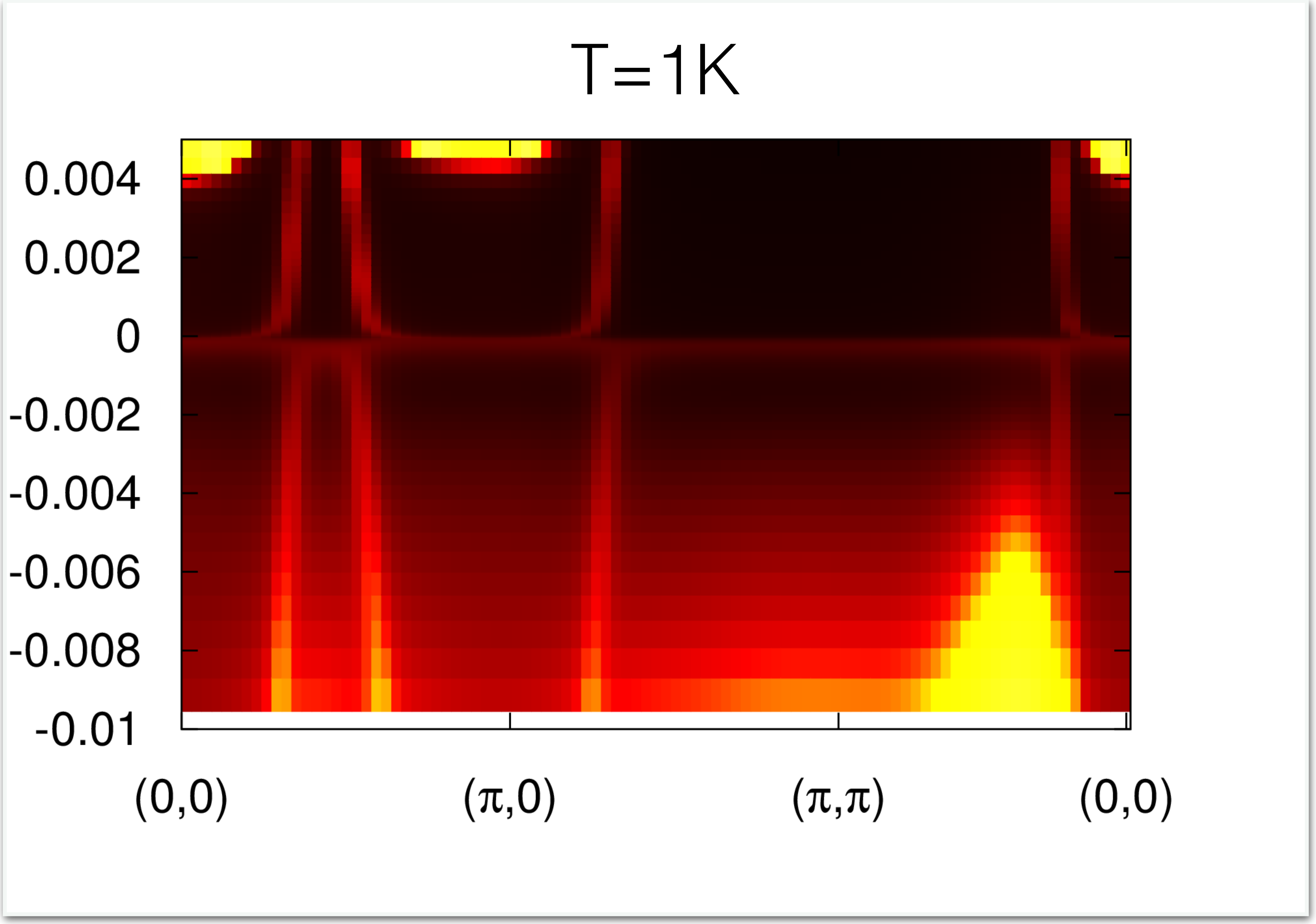


As a consequence there are light electrons in the second layer connecting the heavy electron bands of the surface and the bulk electrons.

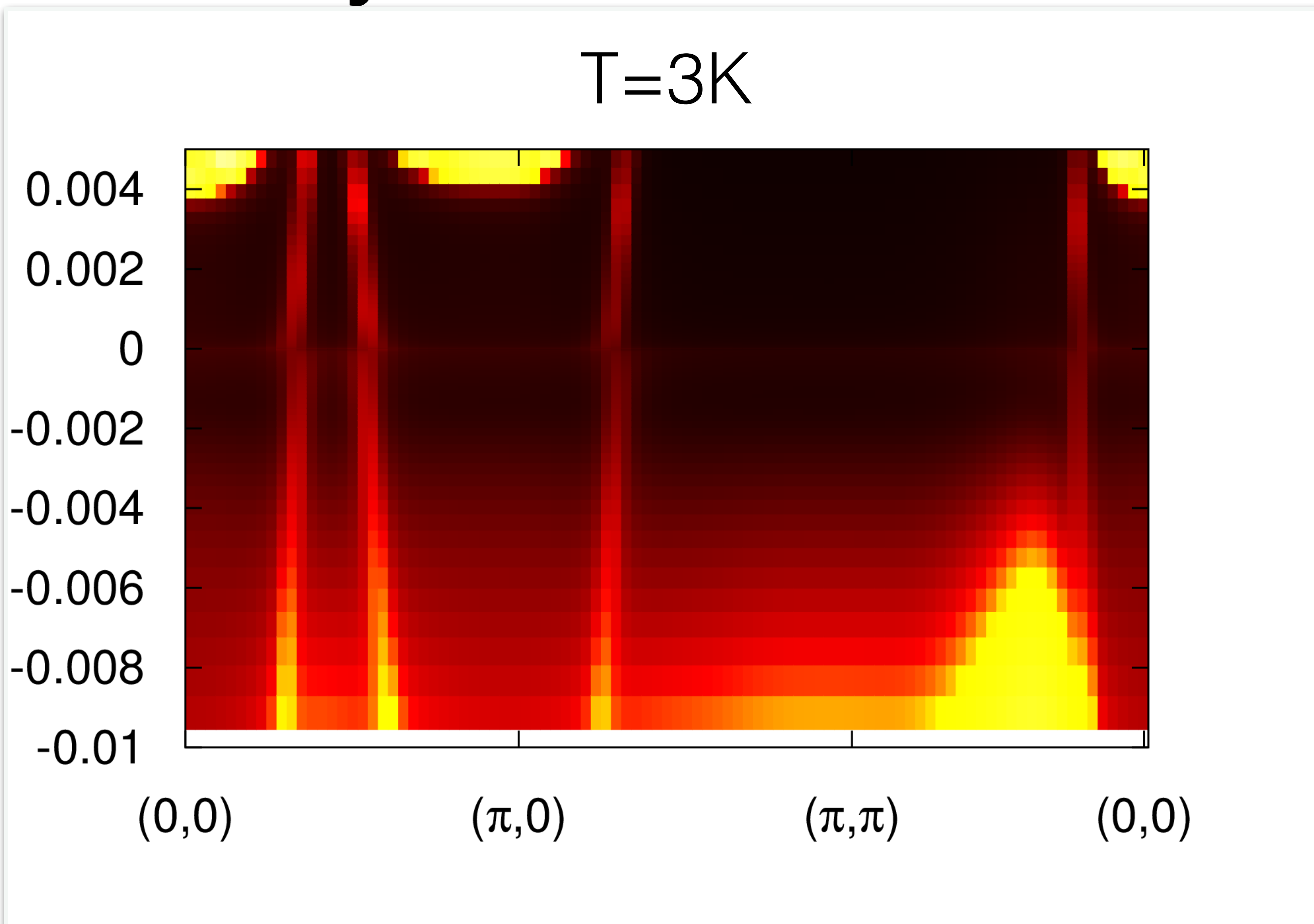
Strongly correlated surface states



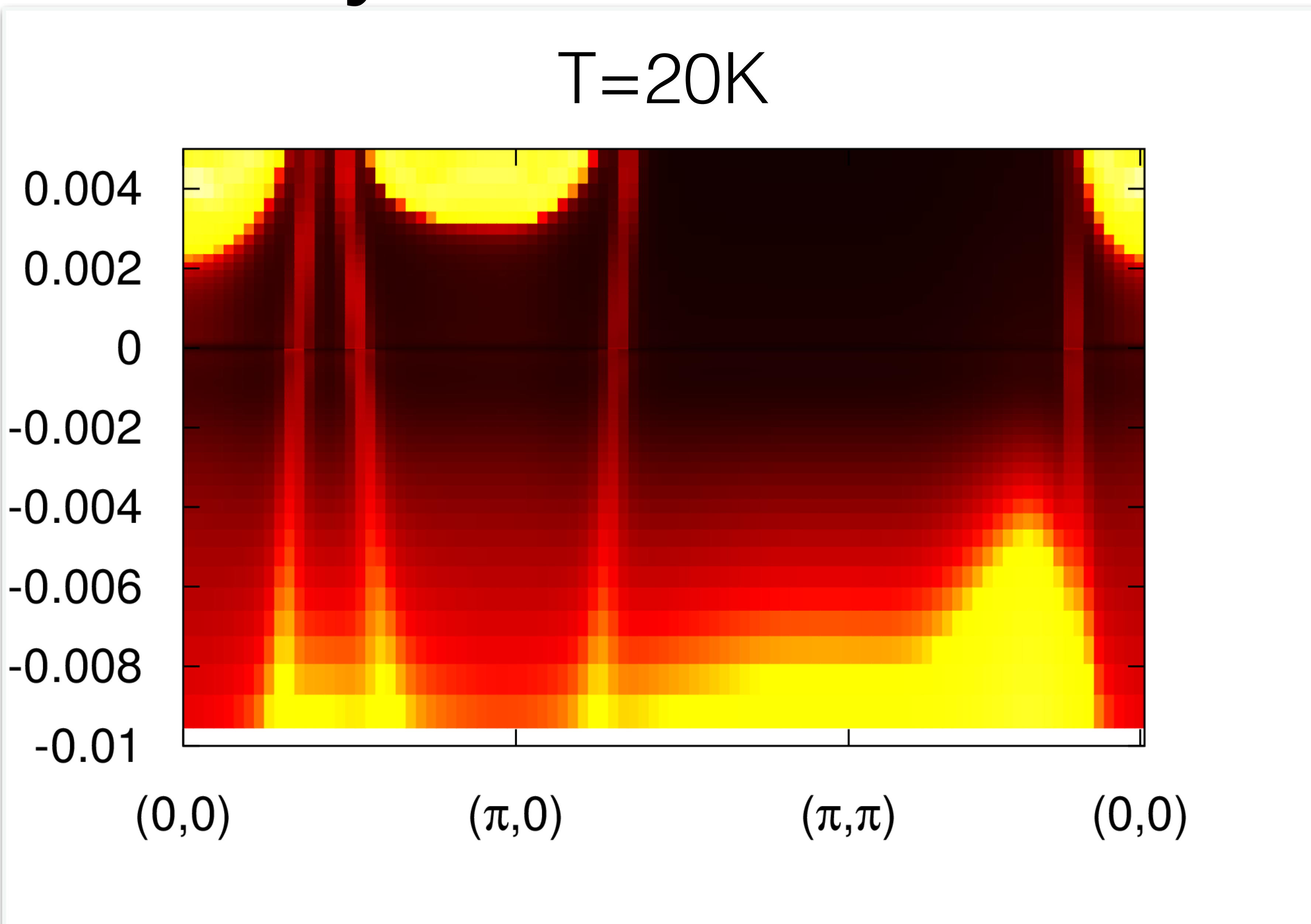
Coexistence of light and heavy surface states



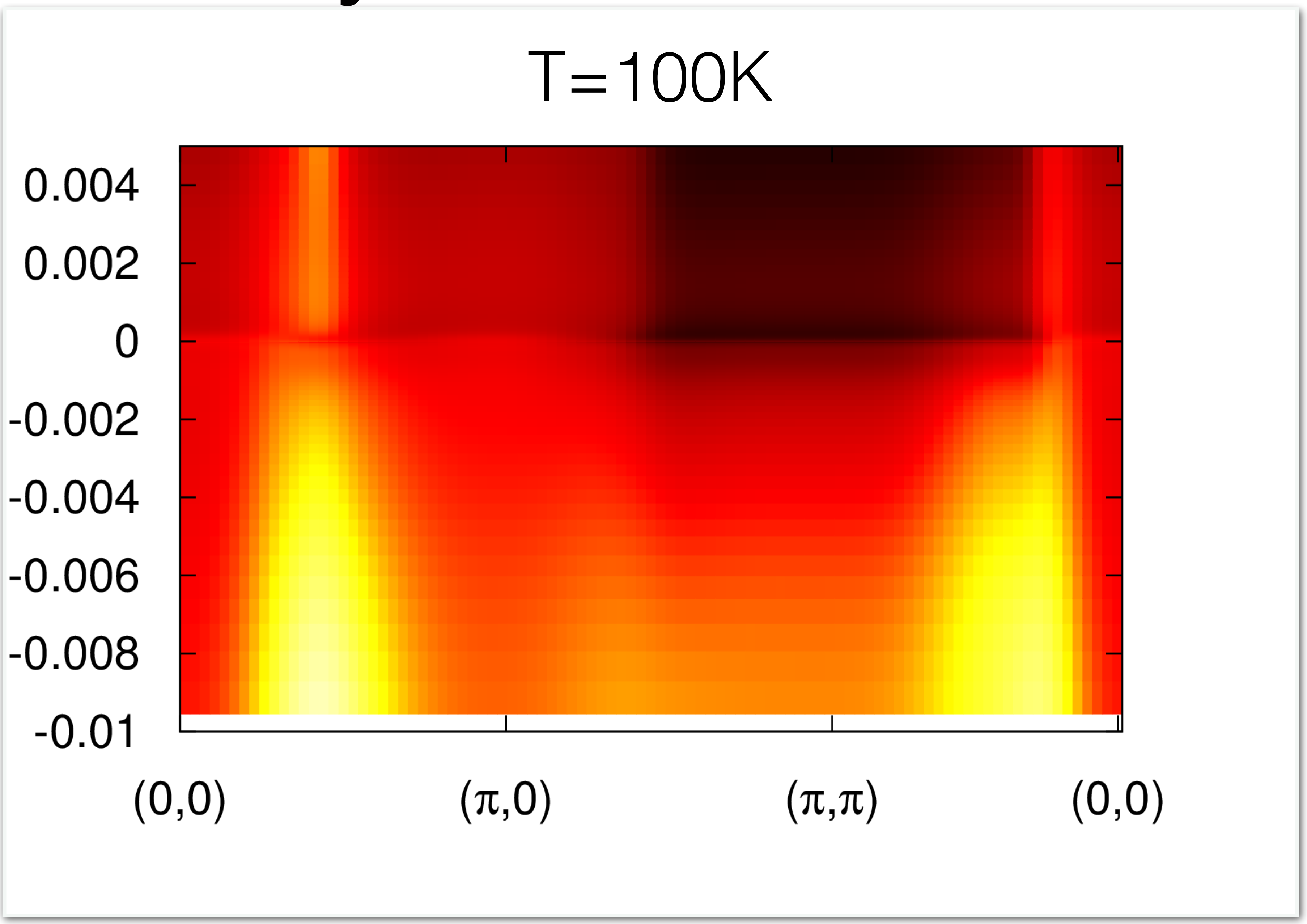
Coexistence of light and heavy surface states



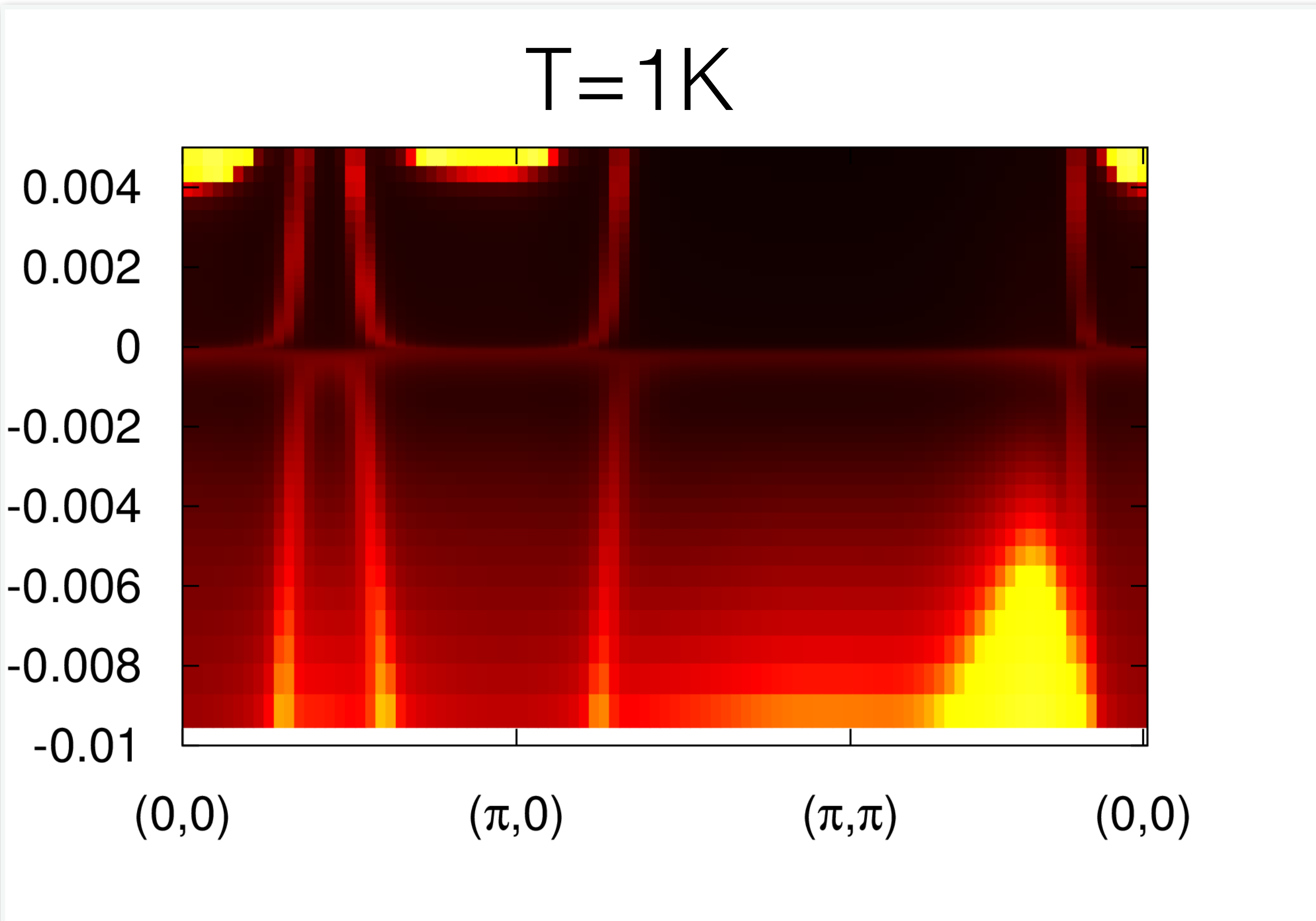
Coexistence of light and heavy surface states



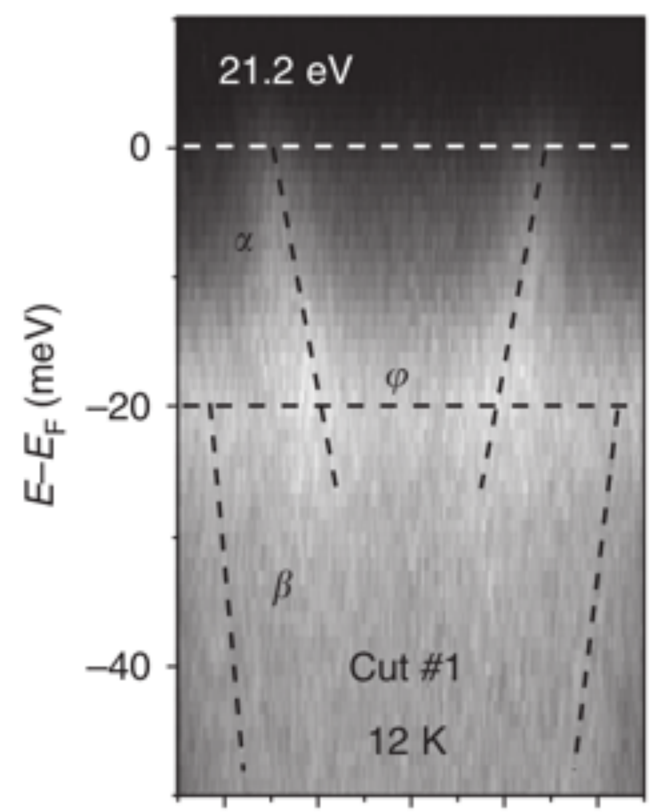
Coexistence of light and heavy surface states



Coexistence of light and heavy surface states

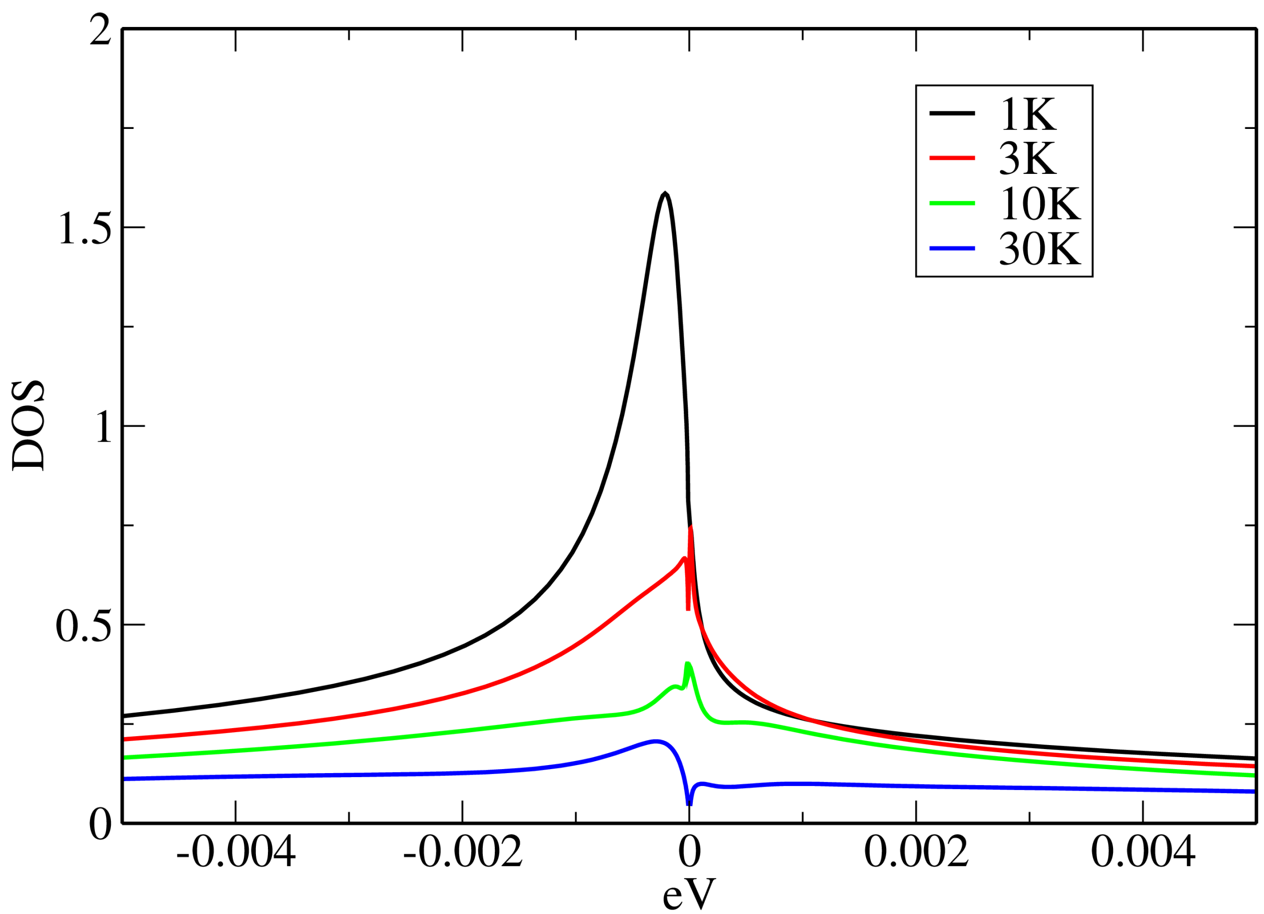


ARPES

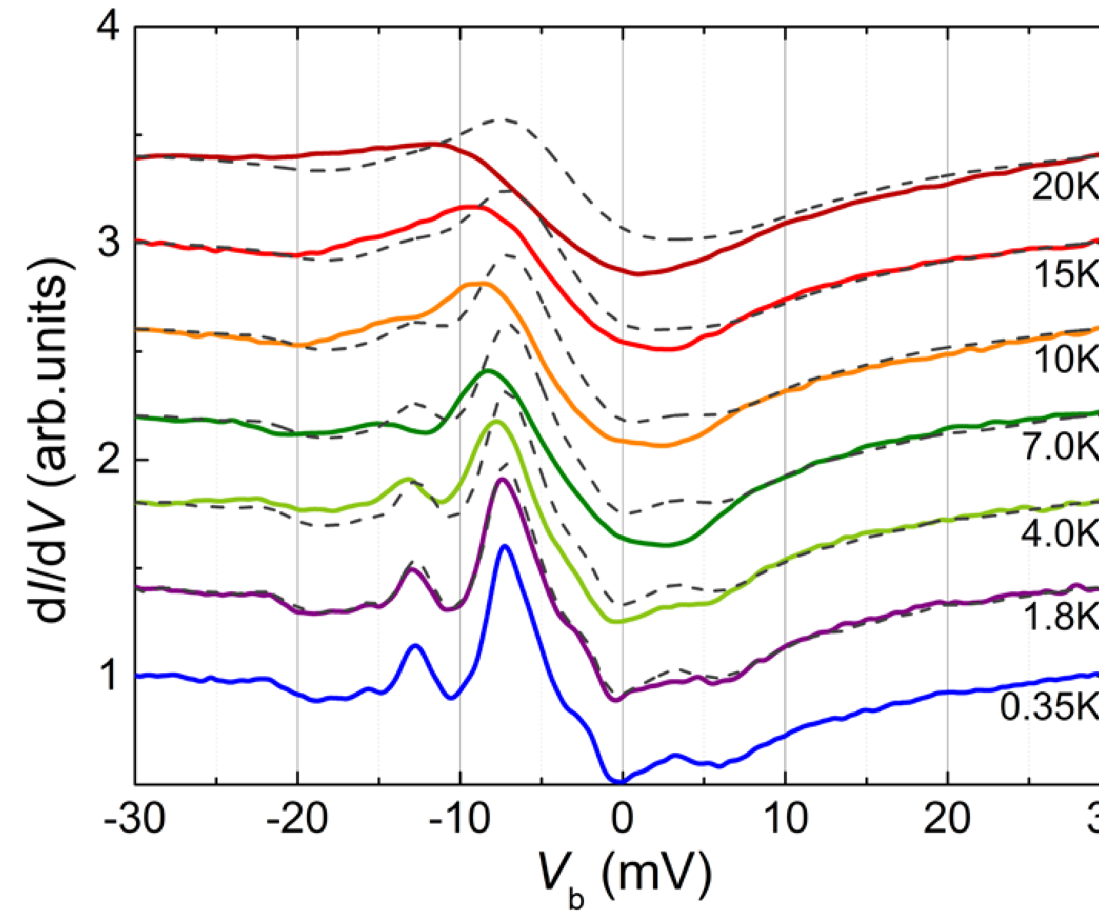


Jiang et al. Nature Comm. 4 1 (2013)

Coexistence of light and heavy surface states



surface DOS
this calculation



STM spectra of SmB_6

L. Jiao,

Nature Communications 7, 13762 (2016)

Discussion

- strong topological insulator
- strongly correlated
- especially in the surface layer, f-electrons are strongly confined close to the Fermi energy

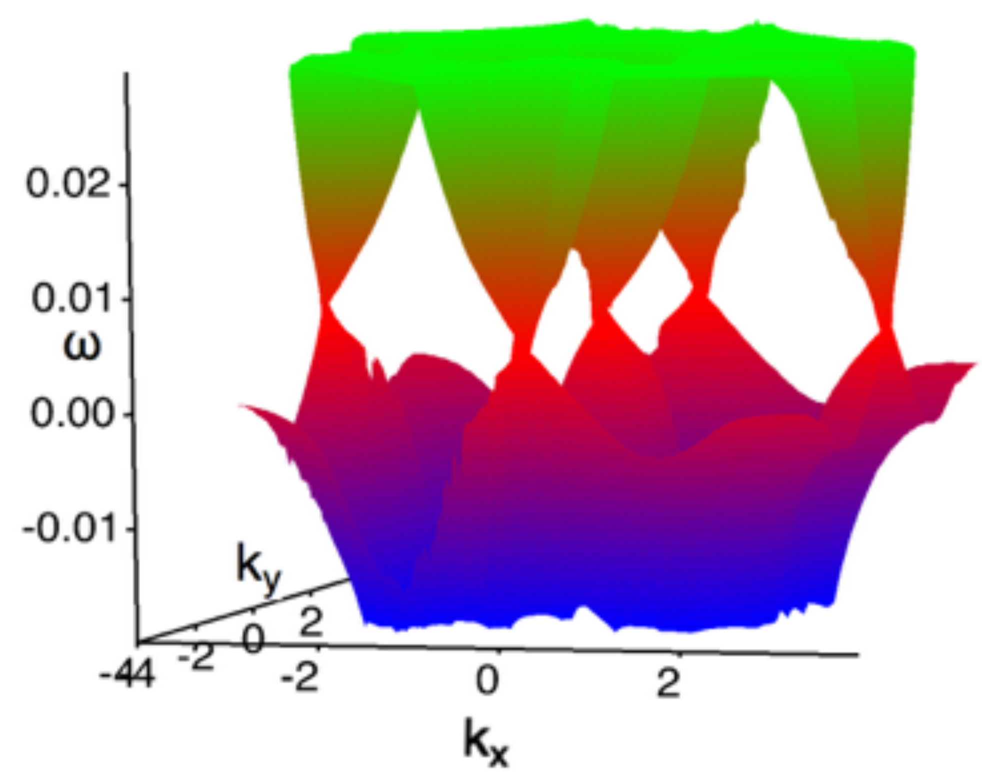
→ **The surface layer forms heavy Dirac cones at the Fermi energy**

- BUT, the topology demands/protects surface states penetrating the whole gap.

→ **Thus, there appear light "surface" states in the next layer**

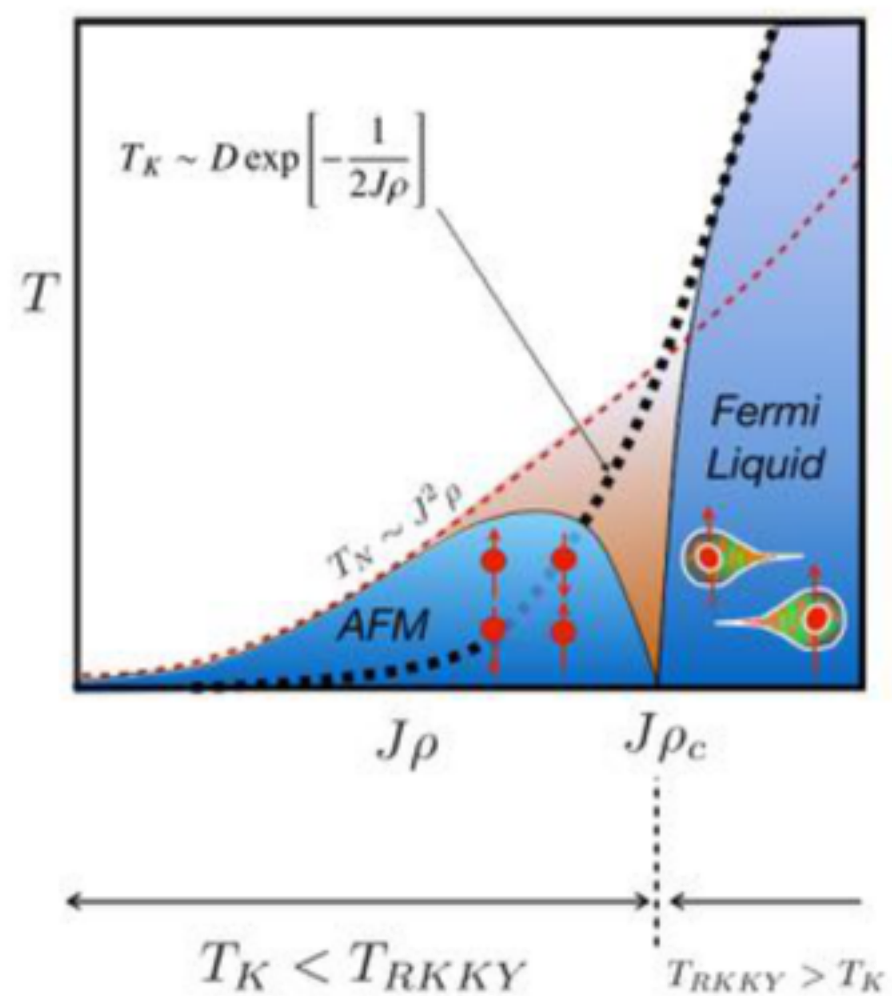
Magnetic States

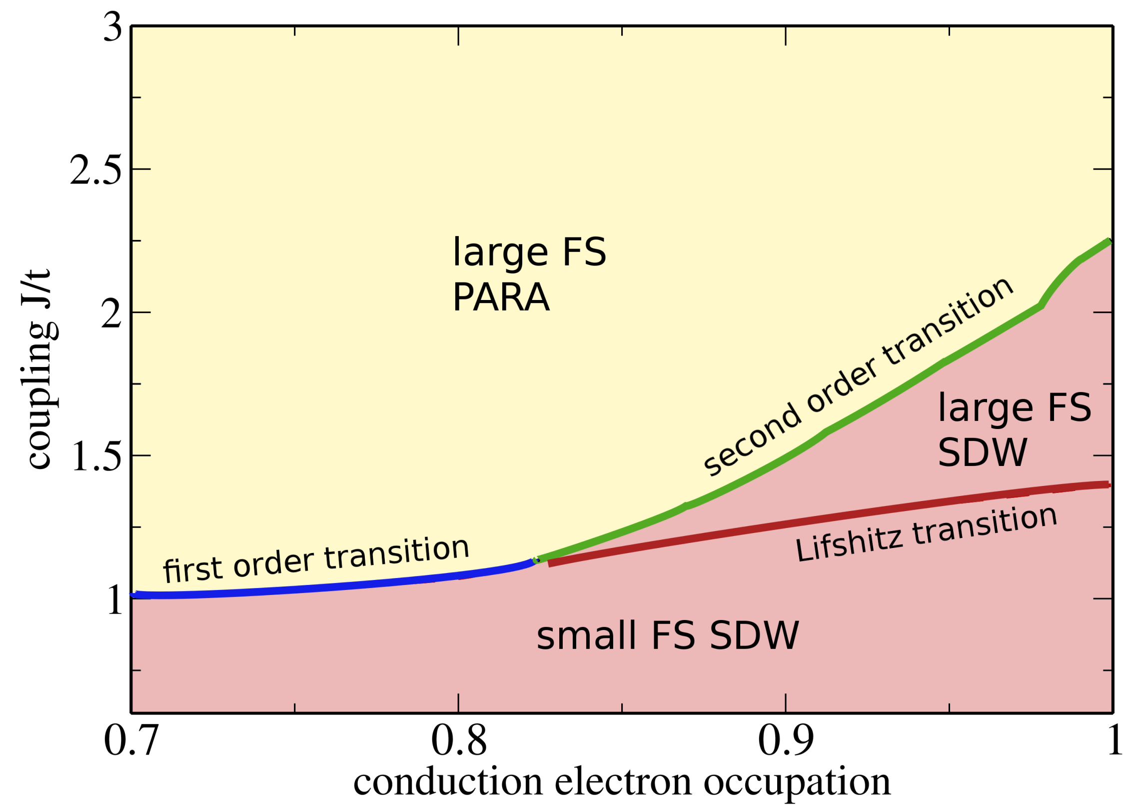
- **Are there magnetic solutions, when doping the system away from integer filling?**
- **What becomes of the surface states, which were protected by time-reversal symmetry?**



Magnetism in the Kondolattice

Doniach phase diagram



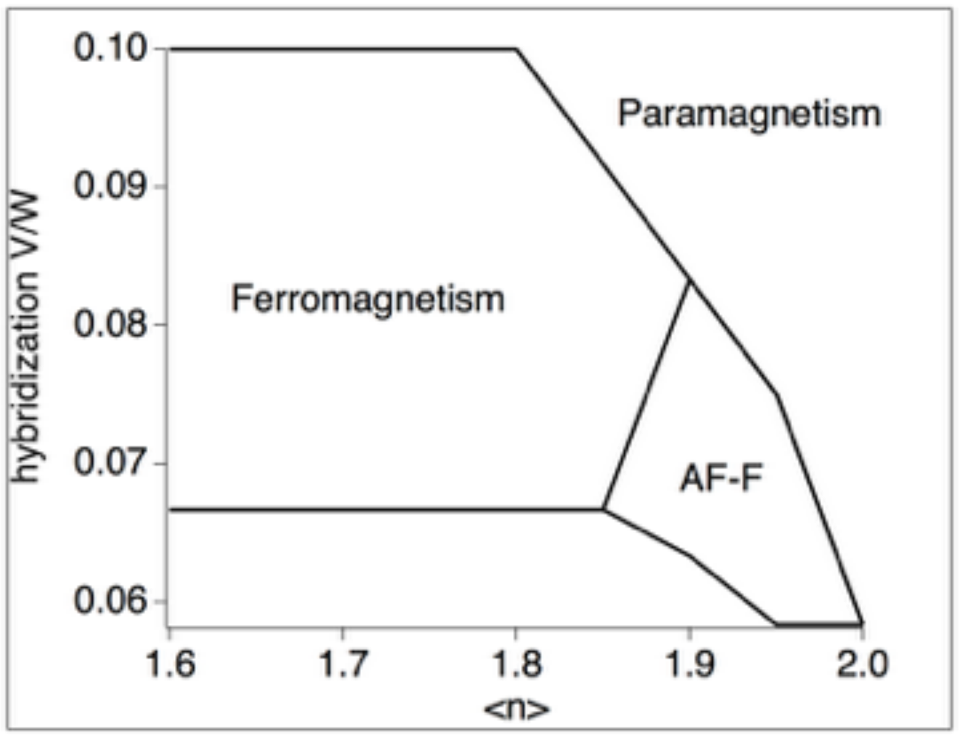


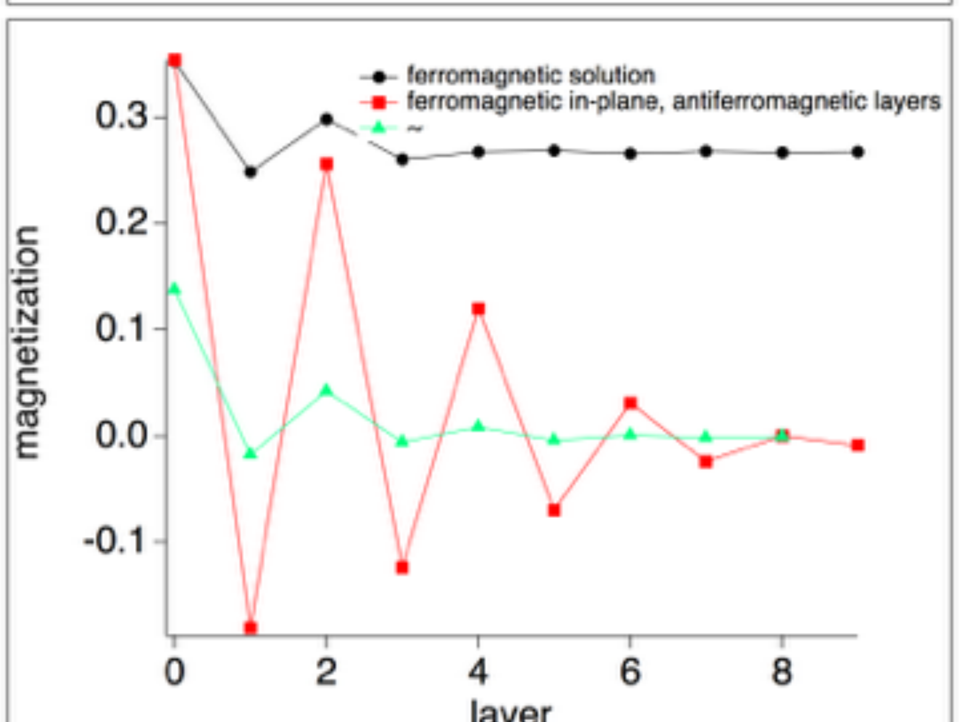
P. Coleman in
"Many-Body Physics: From Kondo to Hubbard"
(eds E. Pavarini, E. Koch and P. Coleman),

RP et al. PRB **92** , 075103 (2015)

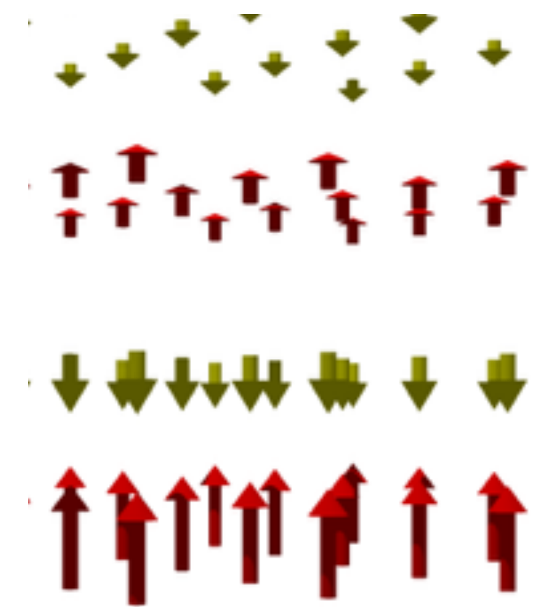
Topological Materials Science

Magnetism in a topological Kondoinsulator

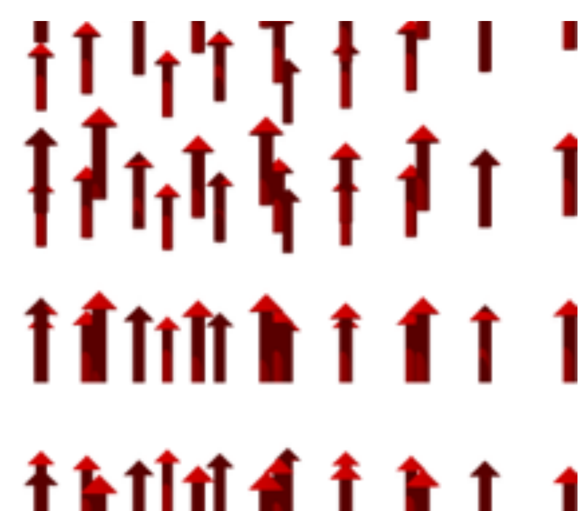




AF-F: **in-plane ferromagnetic**
out-of-plane antiferromagnetic

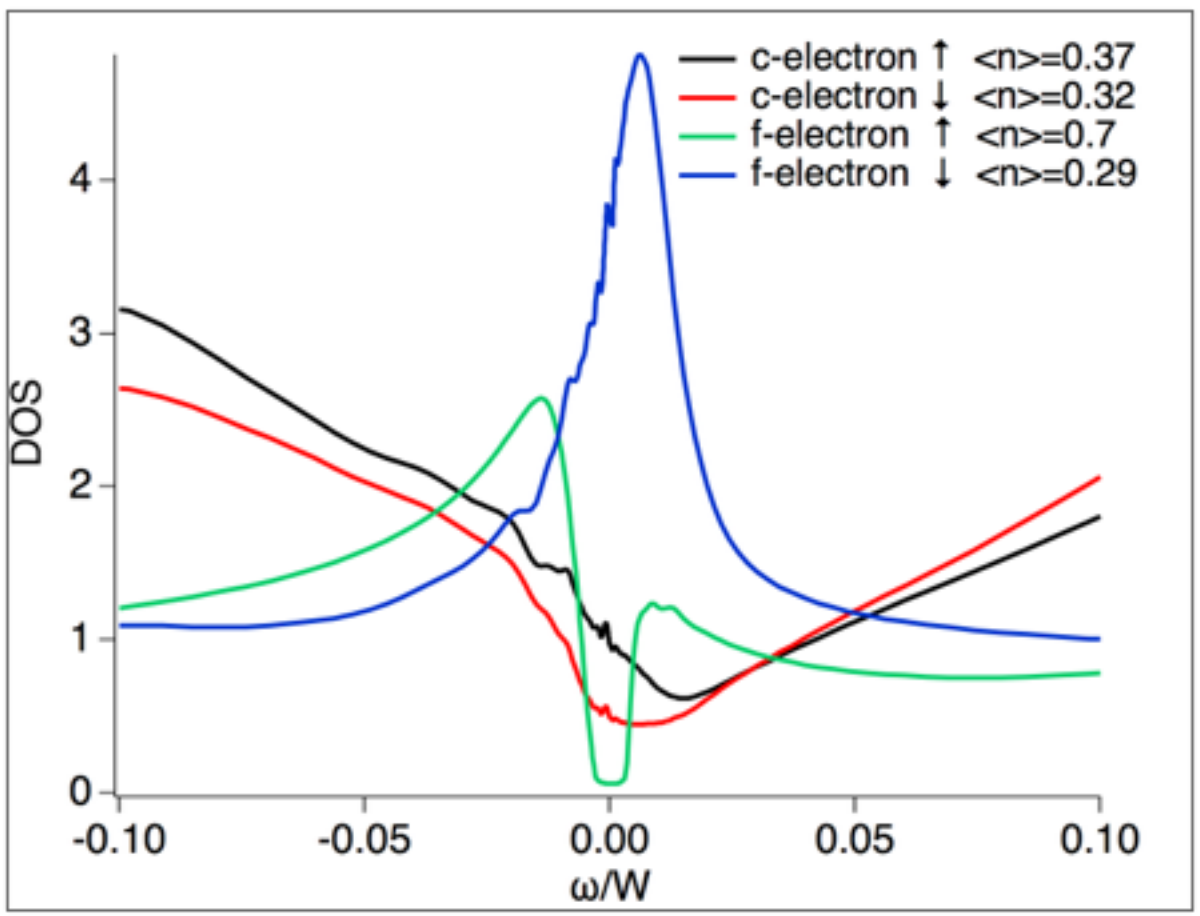


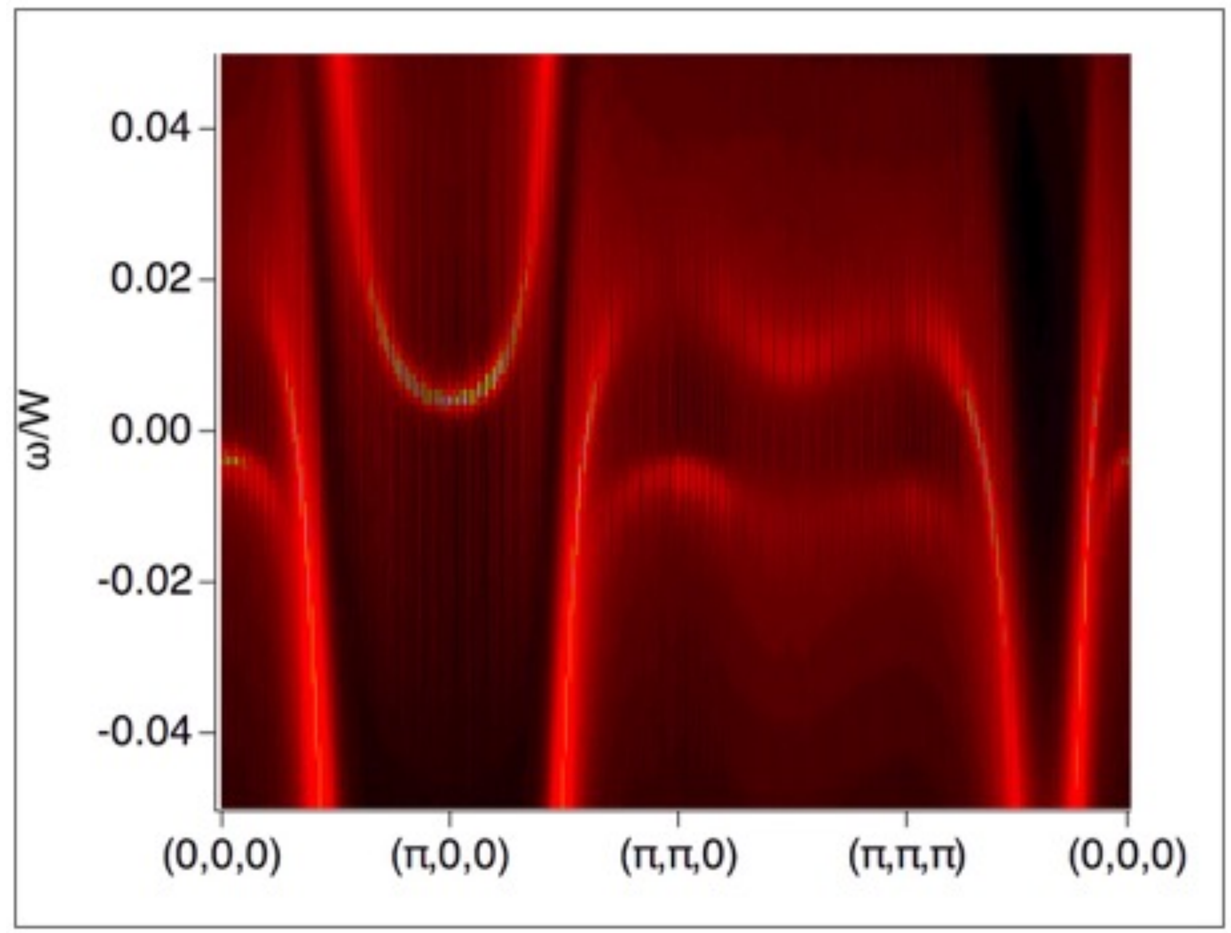
ferromagnetic



Ferromagnetism by Doping

bulk <n>=1.7





- Although there are bands crossing the Fermi energy f-electron ↑ and c-electron ↓ seems to be gapped

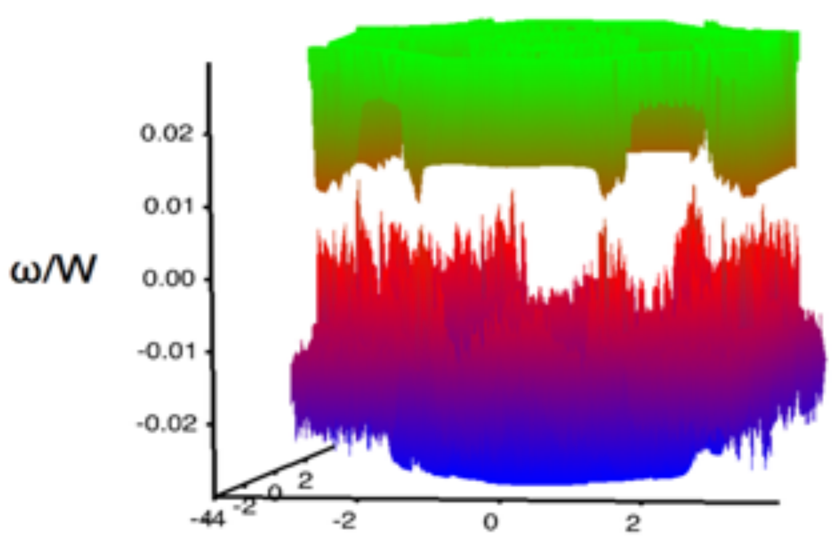
half-metal (spinselective Kondoinsulator)

RP et al. Phys. Rev. Lett. **108**, 08640 (2012)
Yoshida et al. Phys. Rev. B **87** 165109 (2013)

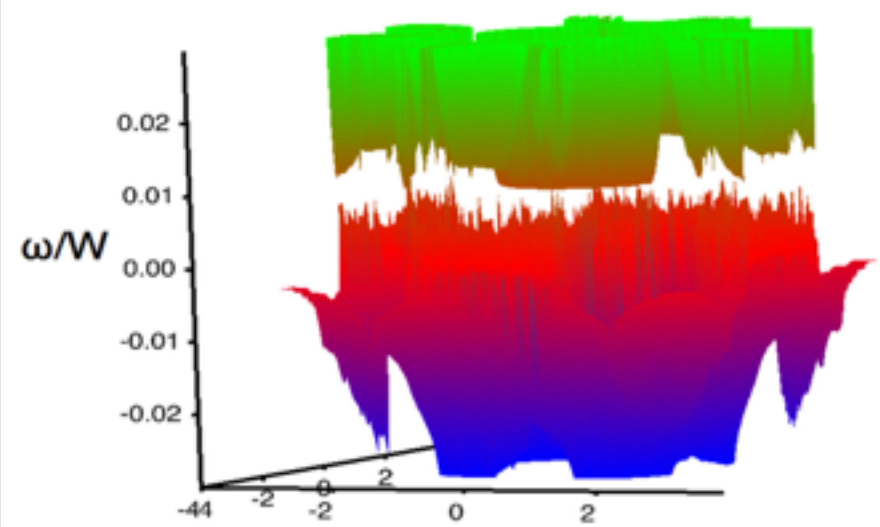
Ferromagnetism by Doping

open surface: z-direction

surface



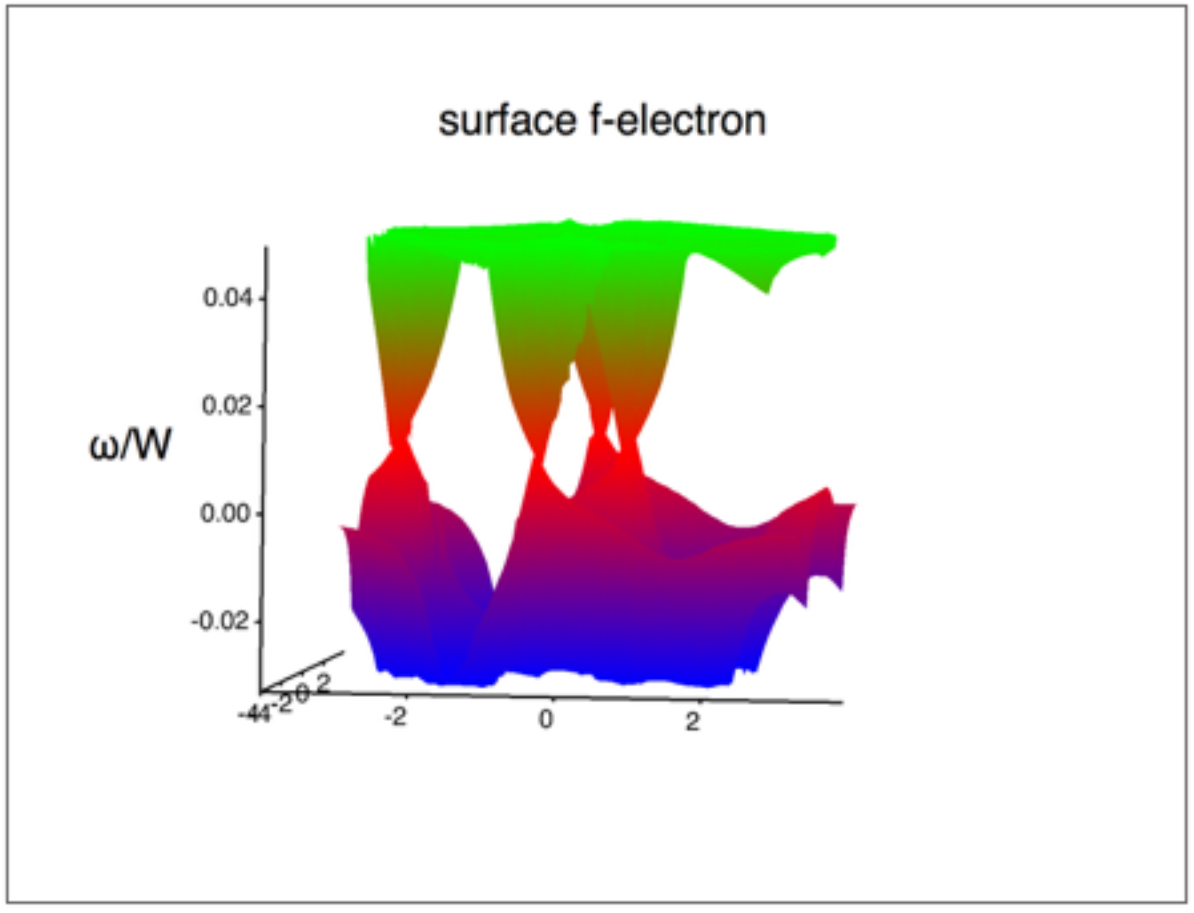
bulk

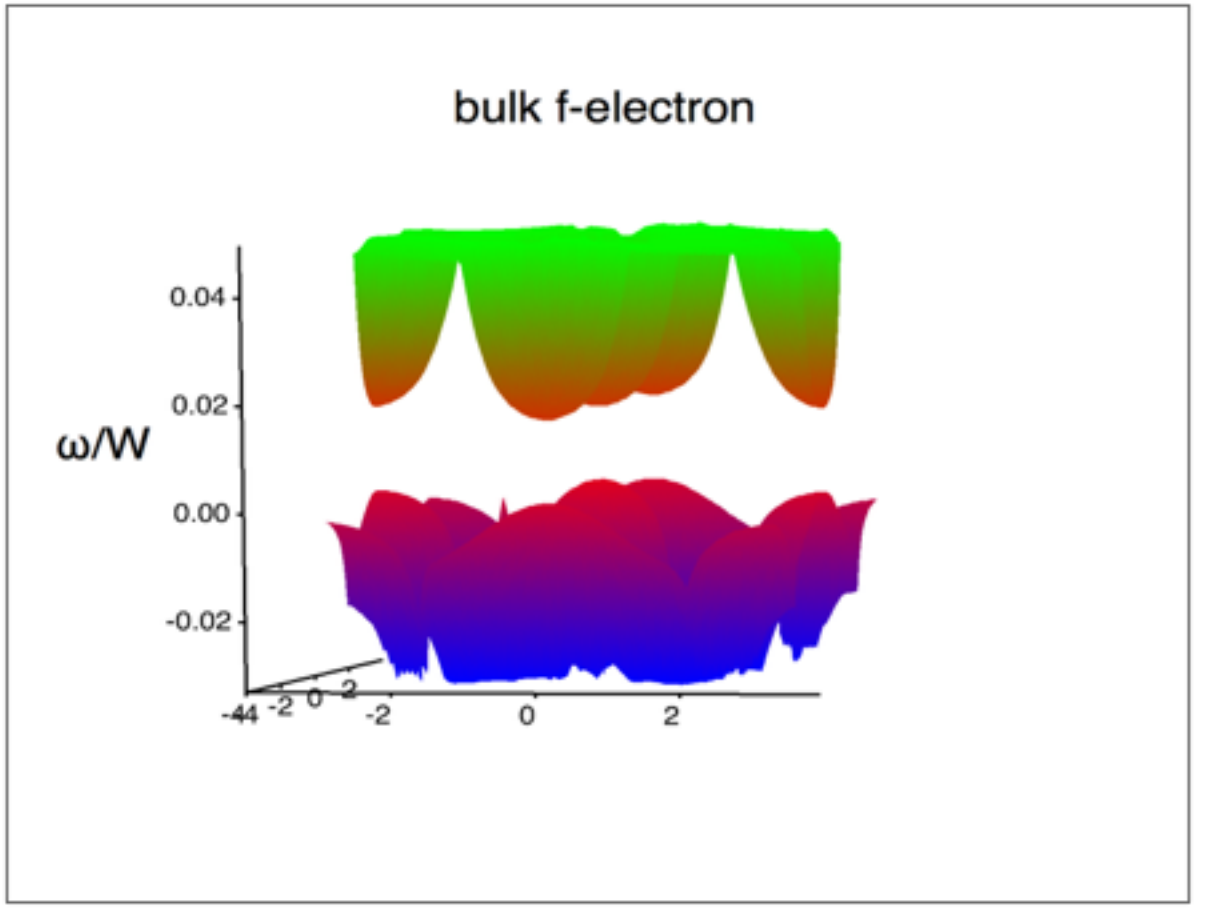


- Although this component is gapped, the surface Dirac-cones have vanished
- The surface states were protected by time-reversal symmetry, which is now broken

Ferromagnetism by Doping

open surface: x-direction

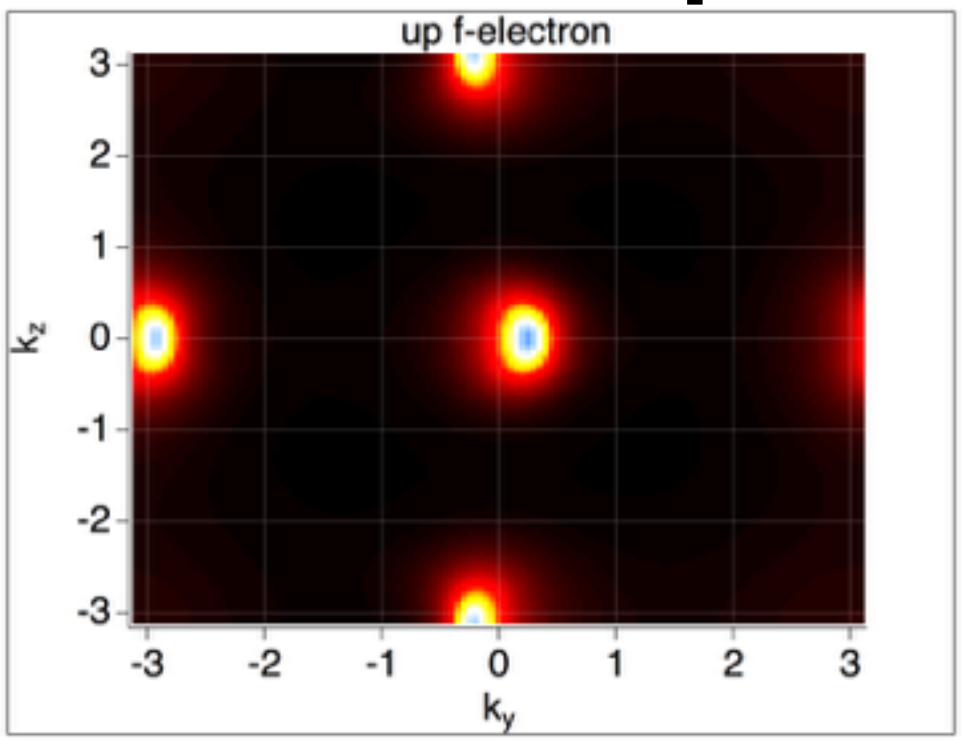


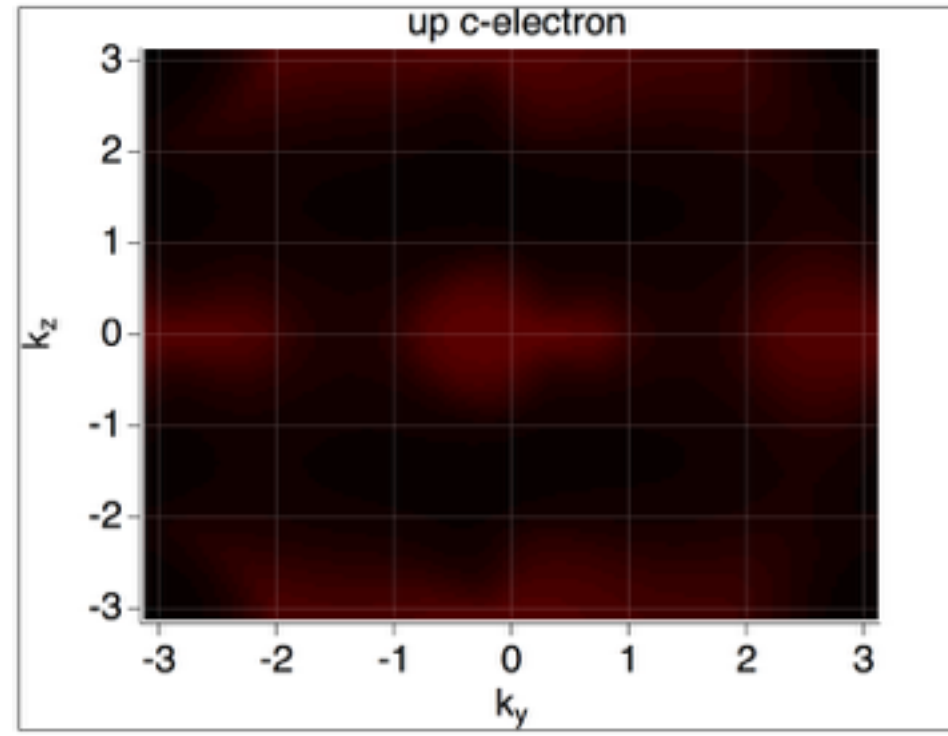


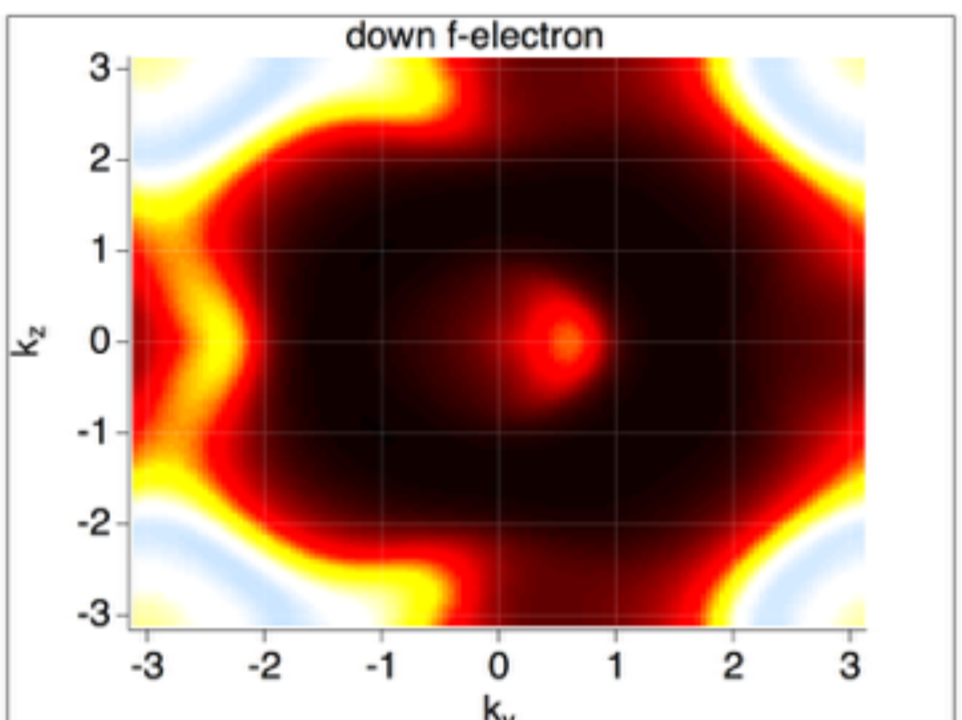
- **For surfaces where the magnetization is in-plane, we find Dirac cones at the surface.**

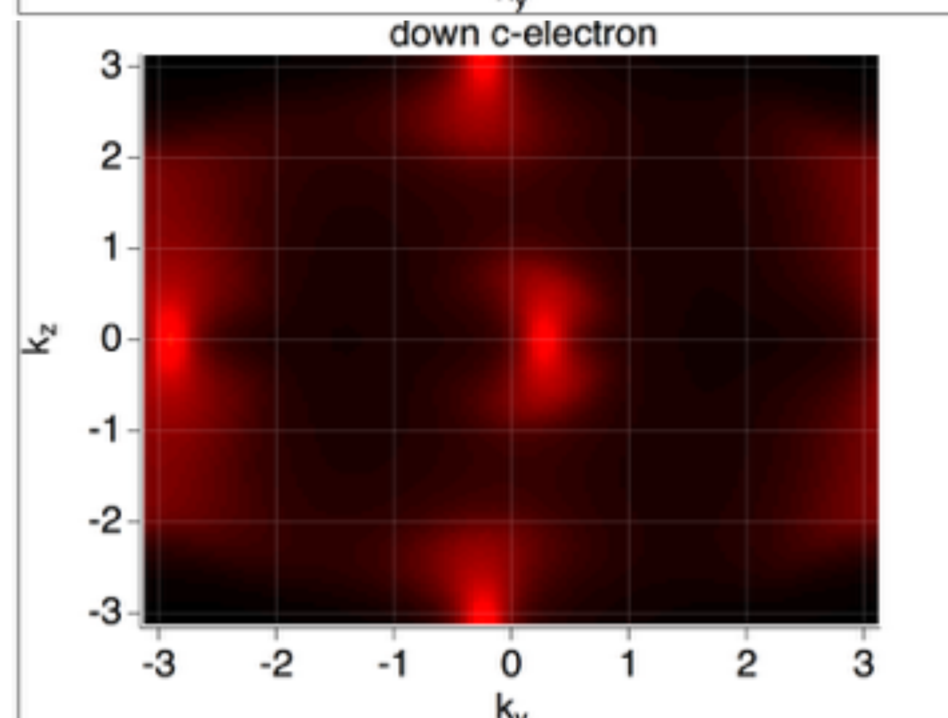
Ferromagnetism by Doping

open surface: x-direction



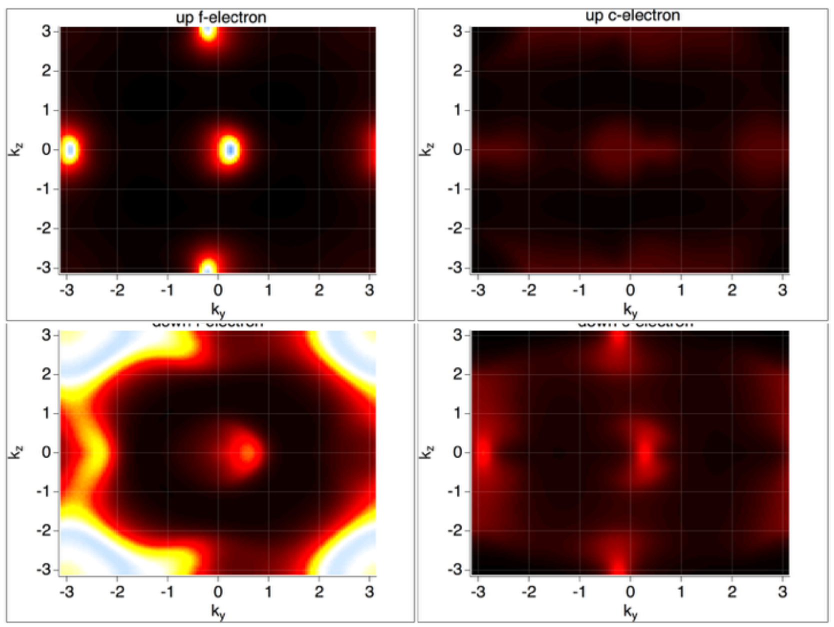






Ferromagnetism by Doping

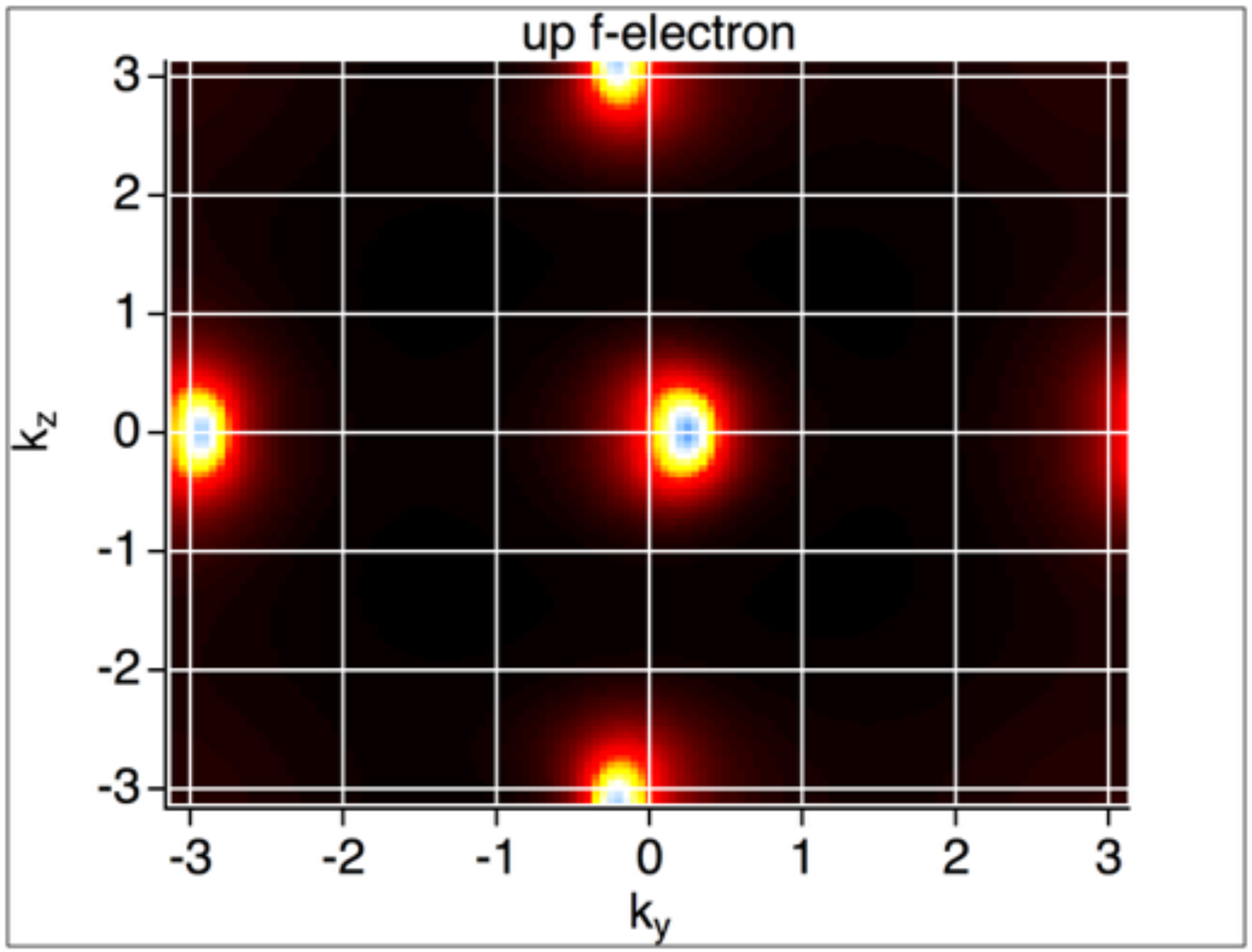
open surface: x-direction



- spin-selective gap and Dirac-cones
  - f-up and c-down electrons are gapped in the bulk and show Dirac cones at the surface
  - f-down electrons are metallic

Ferromagnetism by Doping

open surface: x-direction



- The Dirac cones lie not at $k_y = 0$ and $k_y = \pi$

Topological Protection?

- The ferromagnetic state has a bulk gap in one of these components (here: f-up +c-down)

spin-selective Kondoinsulator

RP et al. Phys. Rev. Lett. **108**, 08640 (2012)

Yoshida et al. Phys. Rev. B **87** 165109 (2013)

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spin-selective Kondoinsulator

RP et al. Phys. Rev. Lett. **108**, 08640 (2012)

Yoshida et al. Phys. Rev. B **87** 165109 (2013)

- The Hamiltonian describes a cubic system.
- We can define **reflection operators** $R_z = i\sigma^z P_z$

reflection for one plane $P_z : k_z \to -k_z$

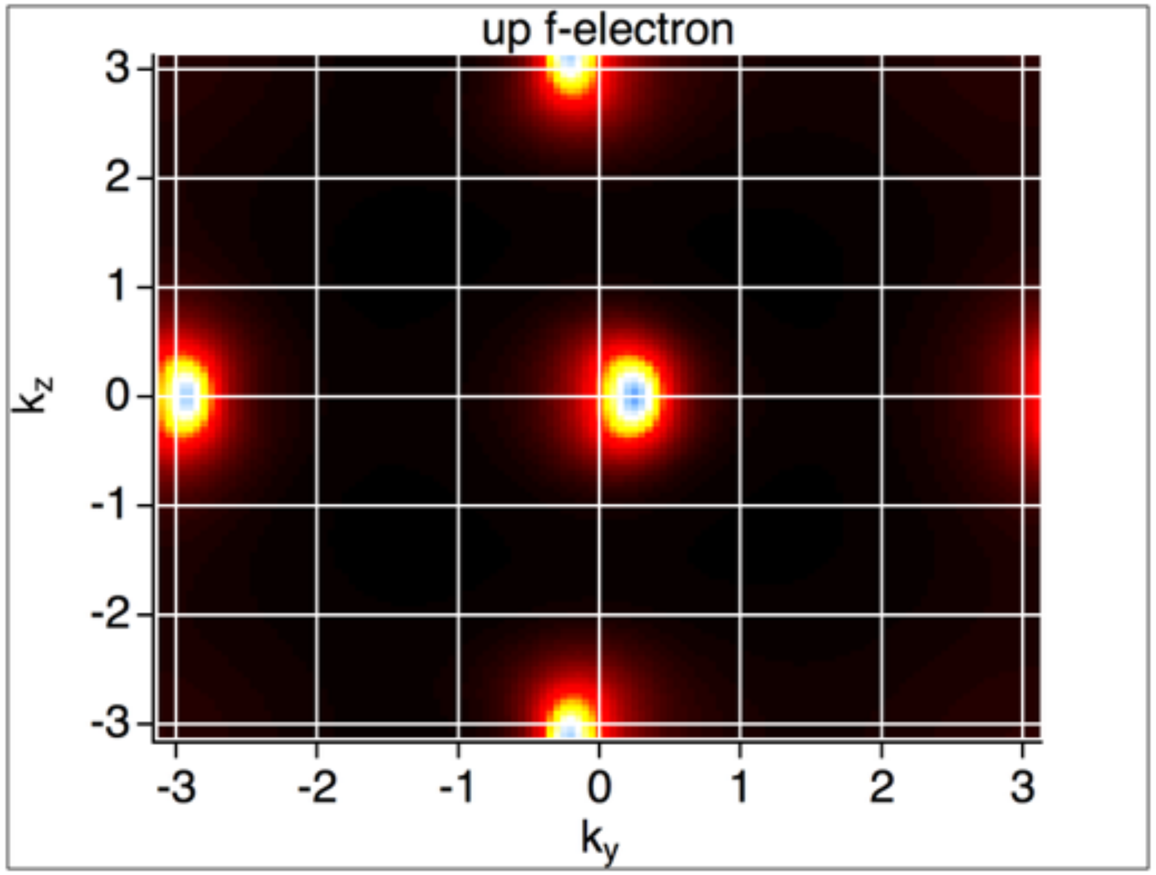
- This operator commutes with the Hamiltonian for certain momenta, $k_z = 0$ and $k_z = \pi$, even in the presence of a magnetic order in z-direction

Topological Protection?

- This reflection operator, $R_{xy} = i\sigma^z P_z$ defines two planes on which topological protection works

$$(k_x, k_y, k_z) = (k_x, k_y, \pm\pi)$$

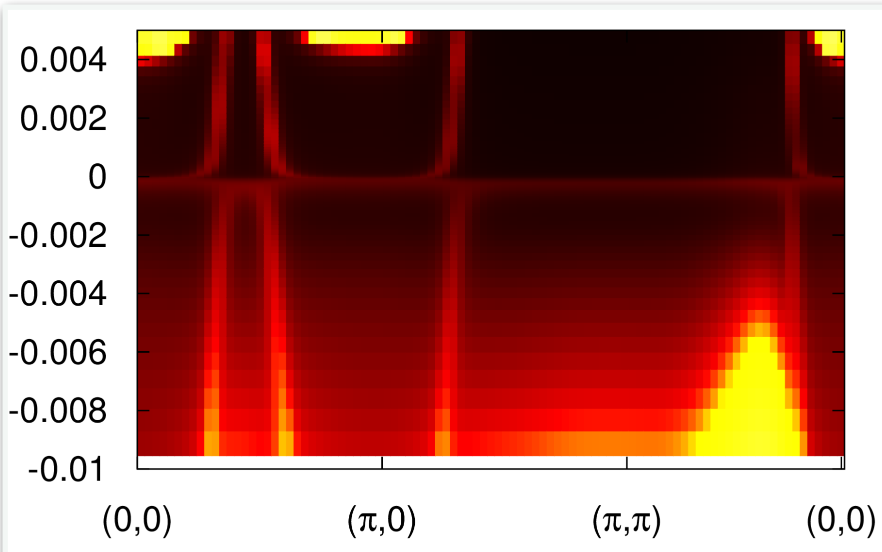
$$(k_x, k_y, k_z) = (k_x, k_y, 0)$$

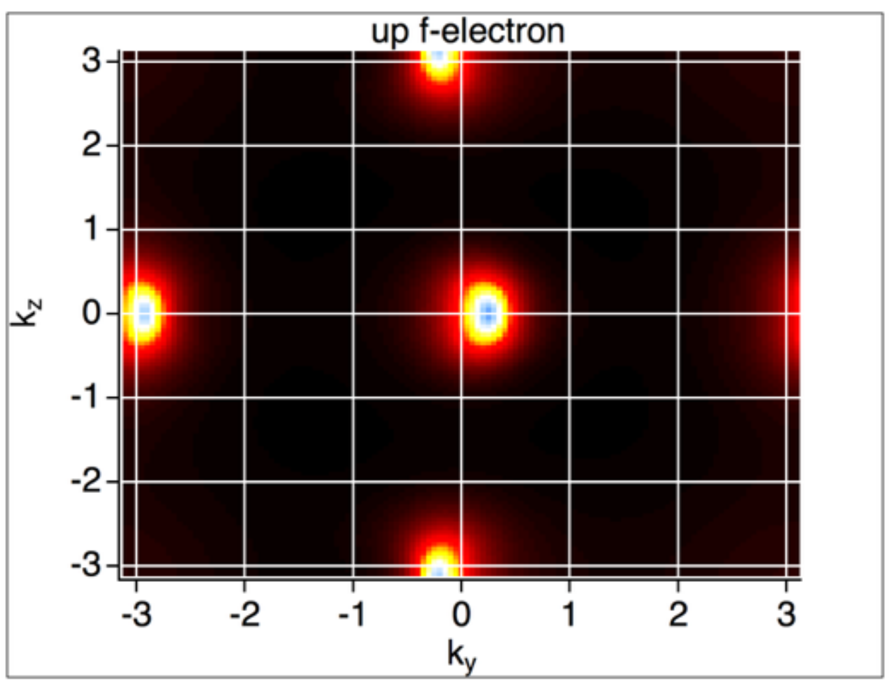


$$k_z = \pi$$

$$k_z = 0$$

Conclusions





- surface is of topological Kondo insulator is much stronger correlated than the bulk

→ (1) combination of light and heavy surface states

→ (2) Kondo breakdown when increasing temperature

- We can realize a ferromagnetic state by doping

(1) We find a spin-selective Kondo insulator, where surface Dirac cones are protected by reflection symmetry