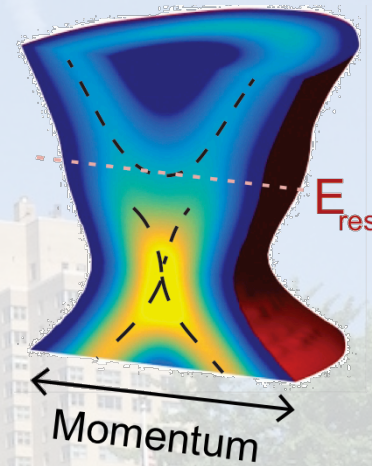
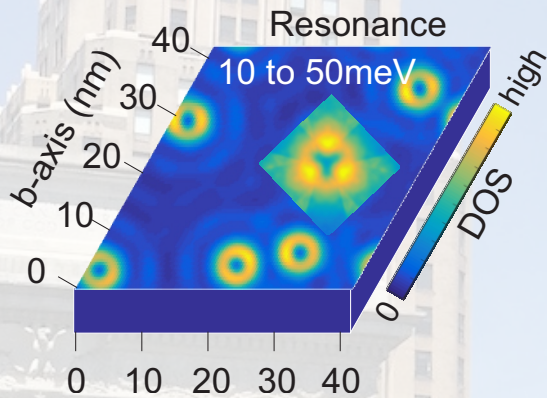


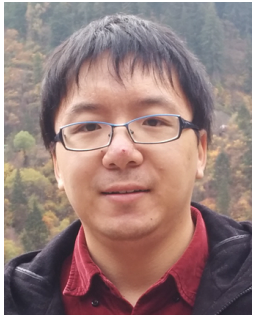
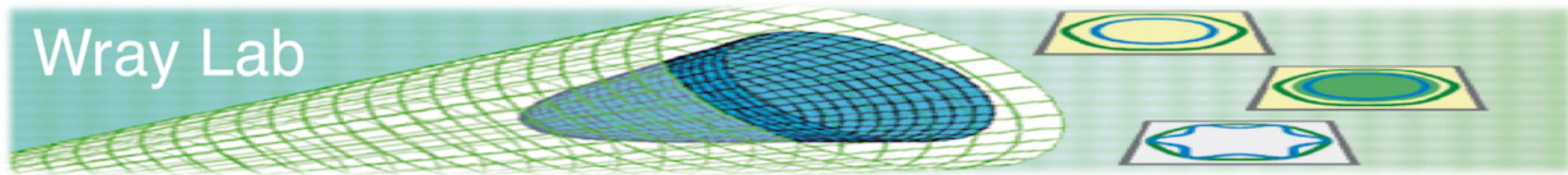


# The birth of new particles from structure and disorder at a topological insulator surface

L. Andrew Wray

*Center for Quantum Phenomena & NYU-ECNU Joint Physics Research Institute,  
Physics Department, New York University*





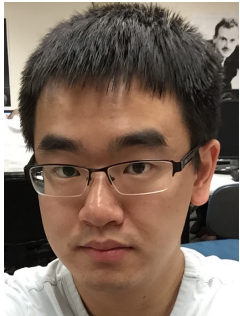
Lin Miao, postdoc



Yishuai Xu



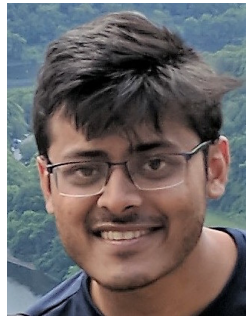
Erica Kotta



Haowei He



Divyanshi Sar



Rourav Basak

RIXS, XAS and ARPES on  
**strongly correlated materials**  
and **topologically ordered**  
**materials**

### ALS

Jonathan Denlinger  
Yi-De Chuang  
Wanli Yang  
MAESTRO collaboration

### UCSD

Sheng Ran  
Brian Maple

### Purdue

Guodon Jiang  
Rudro Biswas

### NIST/UMD

Nick Butch

### Rutgers

Wenhan Zhang  
Weida Wu  
Gabriel Kotliar

### NSLS-II

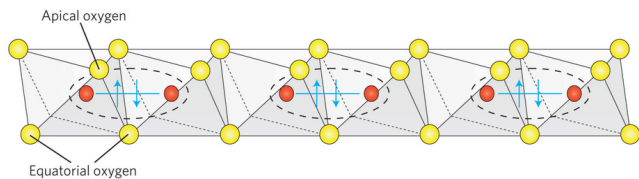
Ignace Jarrige  
Yilin Wang

### MIT

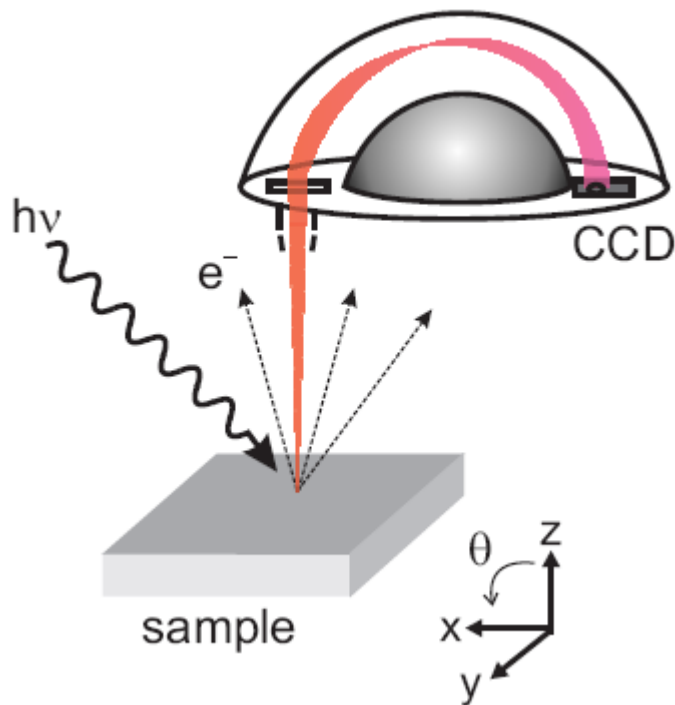
Takehito Suzuki  
Joe Checkelsky

### MS&T

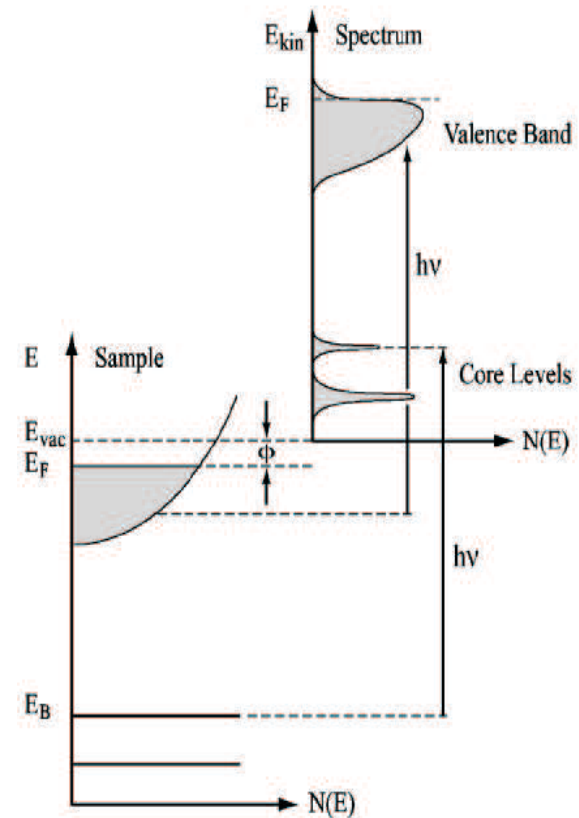
Yew San Hor



# Angle Resolved Photoemission (ARPES)

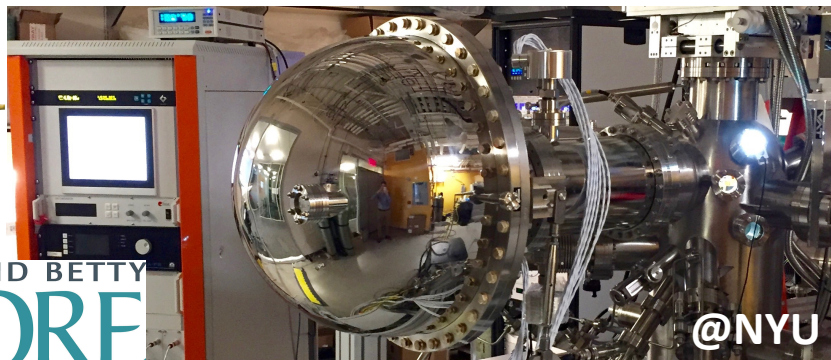


Photoemission: Einstein 1906

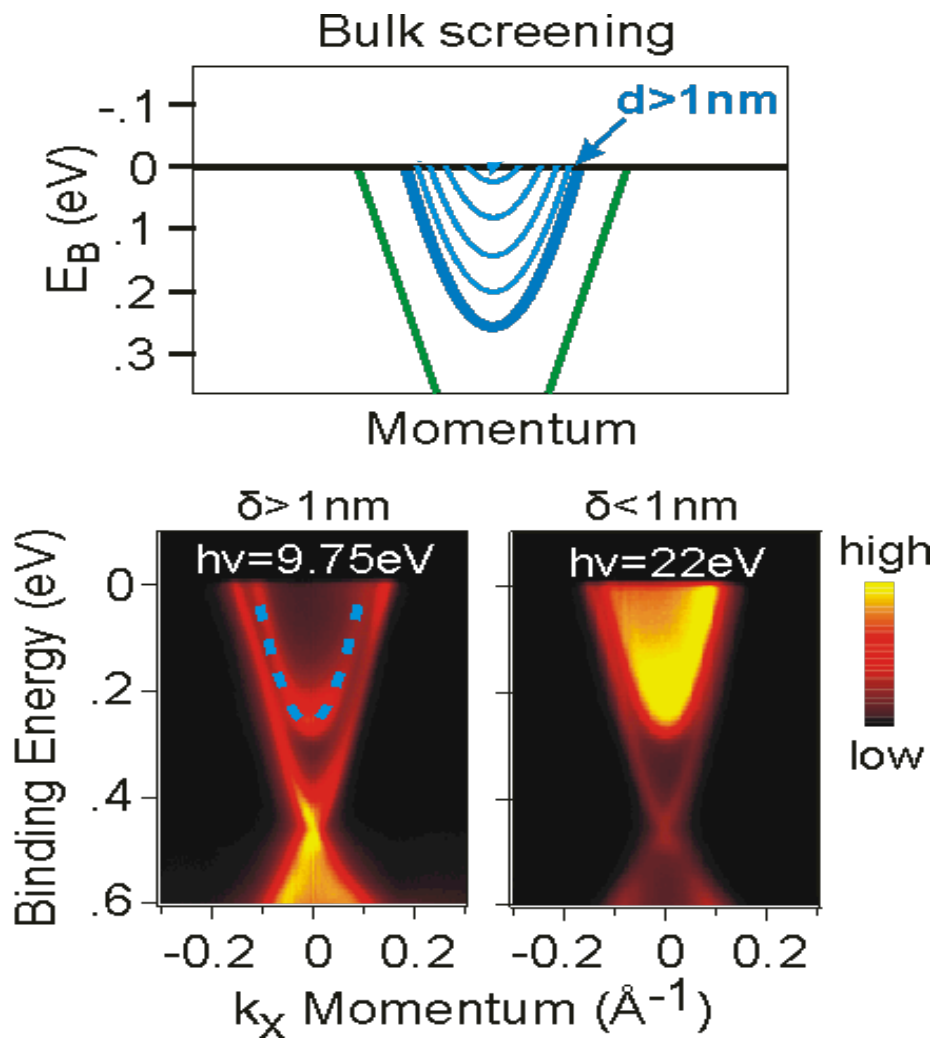
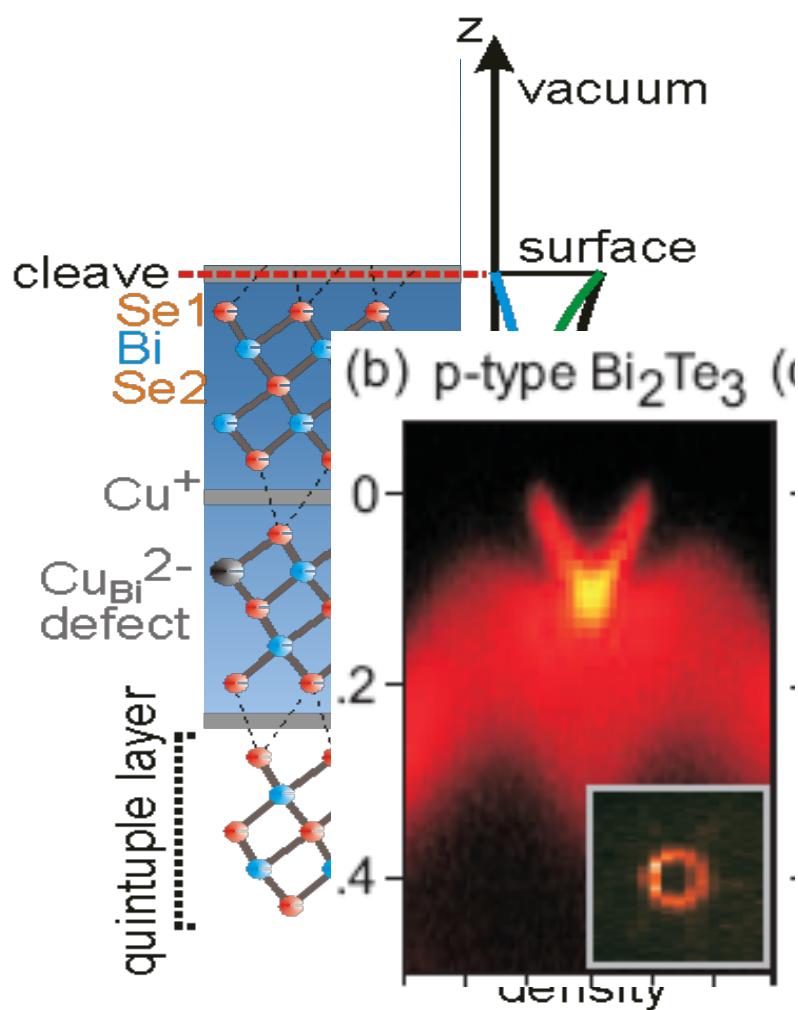


Reveals electron-derived  
'quasiparticles' inside materials:

- Band structure
- Topological surface states
- Majorana Fermions



# Photoemission on a TI (ARPES)



# Phase Transitions and Electronic Topology

## The Nobel Prize in Physics 2016



Photo: A. Mahmoud  
**David J. Thouless**  
Prize share: 1/2

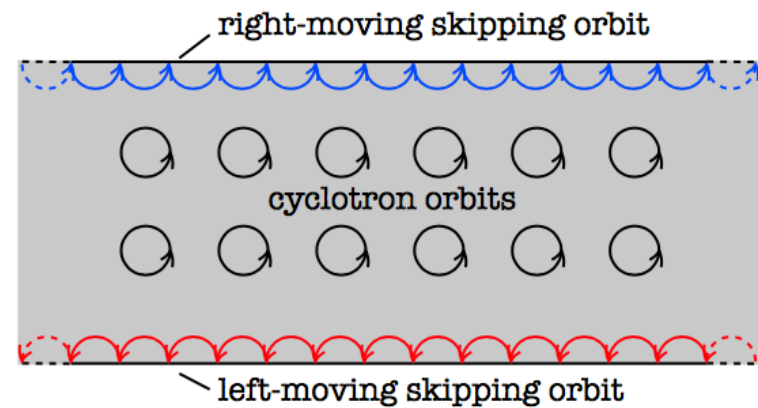


Photo: A. Mahmoud  
**F. Duncan M. Haldane**  
Prize share: 1/4



Photo: A. Mahmoud  
**J. Michael Kosterlitz**  
Prize share: 1/4

### Bulk-Boundary Correspondence Quantum Hall Edge States



The Nobel Prize in Physics 2016 was awarded with one half to David J. Thouless, and the other half to F. Duncan M. Haldane and J. Michael Kosterlitz *"for theoretical discoveries of topological phase transitions and topological phases of matter"*.

# History of 3D Topological Matter

**2005:** Theoretical prediction of the Z2 TI phase (C.L. Kane and E.J. Mele *PRL* 2005)

**2006-2007:** Achievement of a 2D TI phase in HgTe (B.A. Bernevig, T.L. Hughes, S.-C. Zhang, *SCIENCE* 2006, M. König et al. *SCIENCE* 2007)

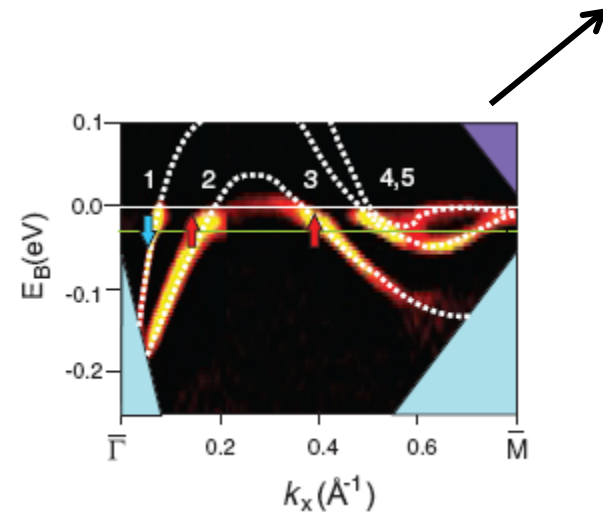
**2007-2009:** First discovery of a 3D TI ( $\text{Bi}_{1-x}\text{Sb}_x$  alloy, L. Fu et al. *PRL* 2007, D. Hsieh, LAW, et al. Zahid Hasan group *NATURE* 2008, *SCIENCE* 2009)

**2008:** Discovery of the  $\text{M}_2\text{X}_3$  TI class (Y. Xia, arXiv 2008, H.-J. Zhang et al. *NATURE* 2009, D. Hsieh et al. *NATURE* 2009)

**2010:** Symmetry breaking: Observation of unconventional superconductivity in  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , magnetism in  $\text{Mn}_x\text{Bi}_{2-x}\text{Te}_3$  (LAW et al. *Nat. Phys.* 2010, Y.-S. Hor et al. *PRB* 2010)

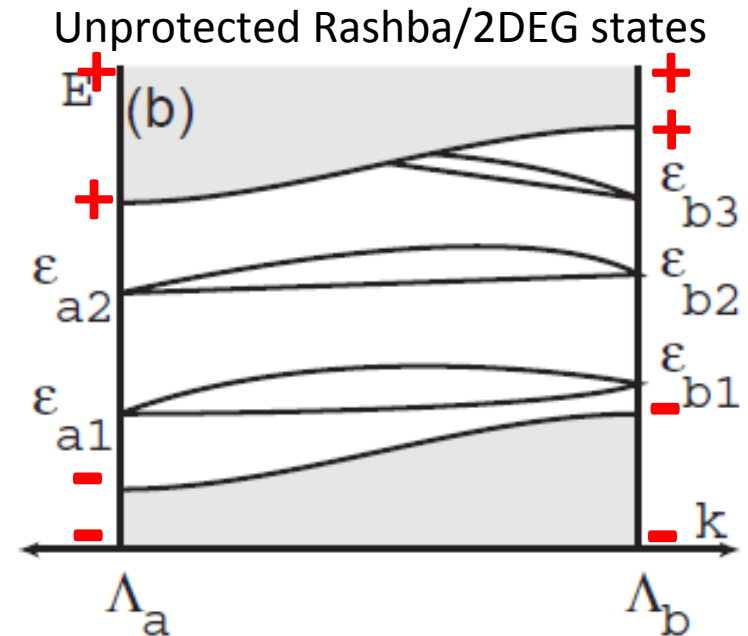
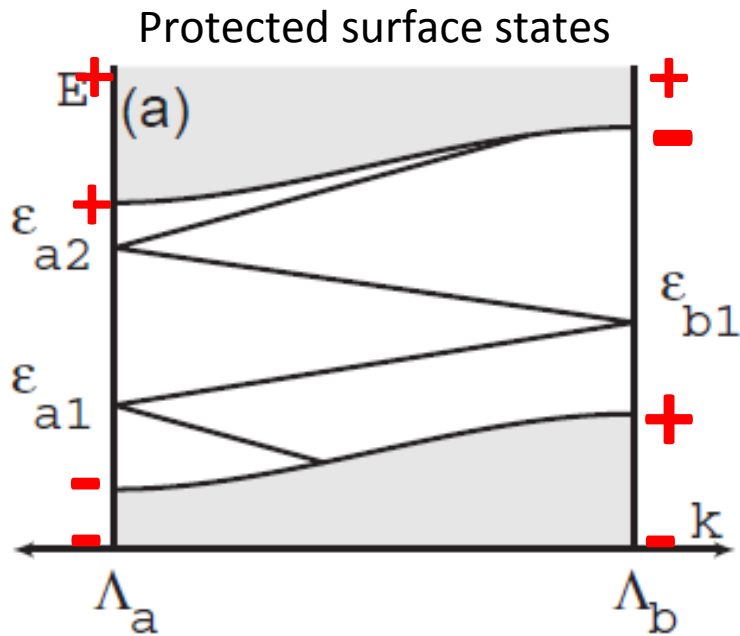
**2011-2012:** Discovery of “Topological Crystalline Insulators” (L. Fu et al., *PRL* 2011; T. Hsieh et al., *Nat. Comm.* 2012, S. Xu, LAW et al., *Nat Comm* 2012)

**2010-present:** Higher order topological insulators, Weyl, Dirac, nodal line topological semimetals, many new materials



# Surface states and Kramers Points

2 scenarios (i.e.  $Z_2$ )

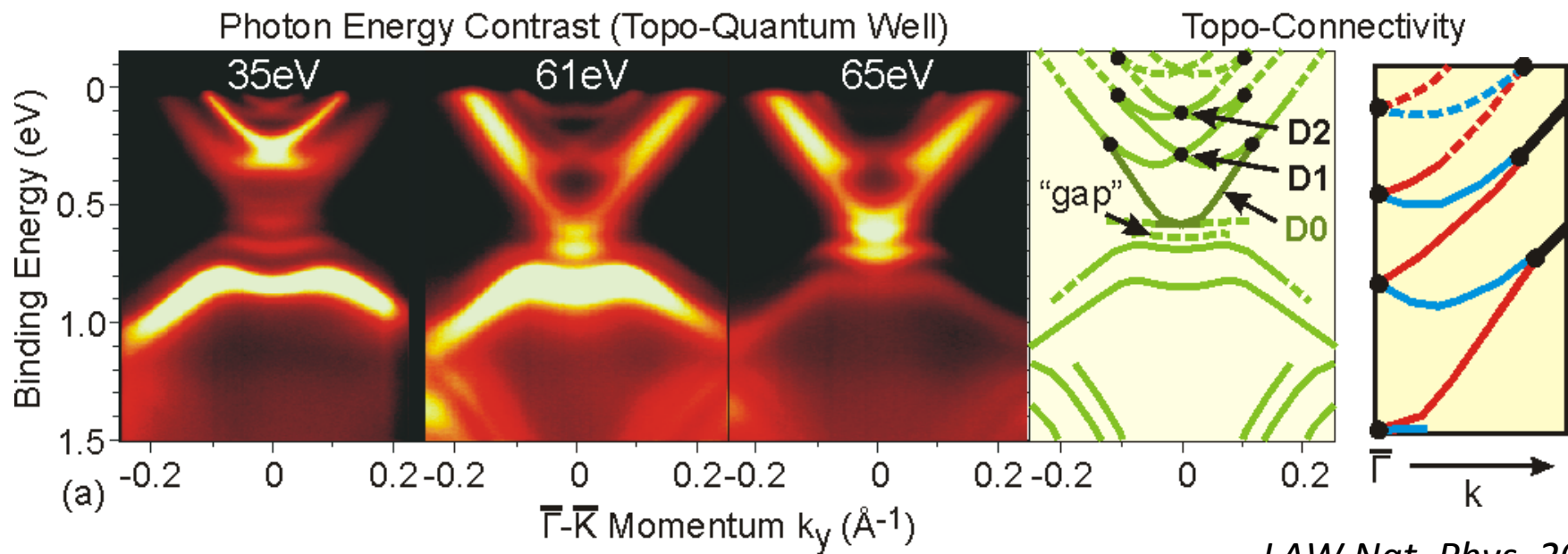
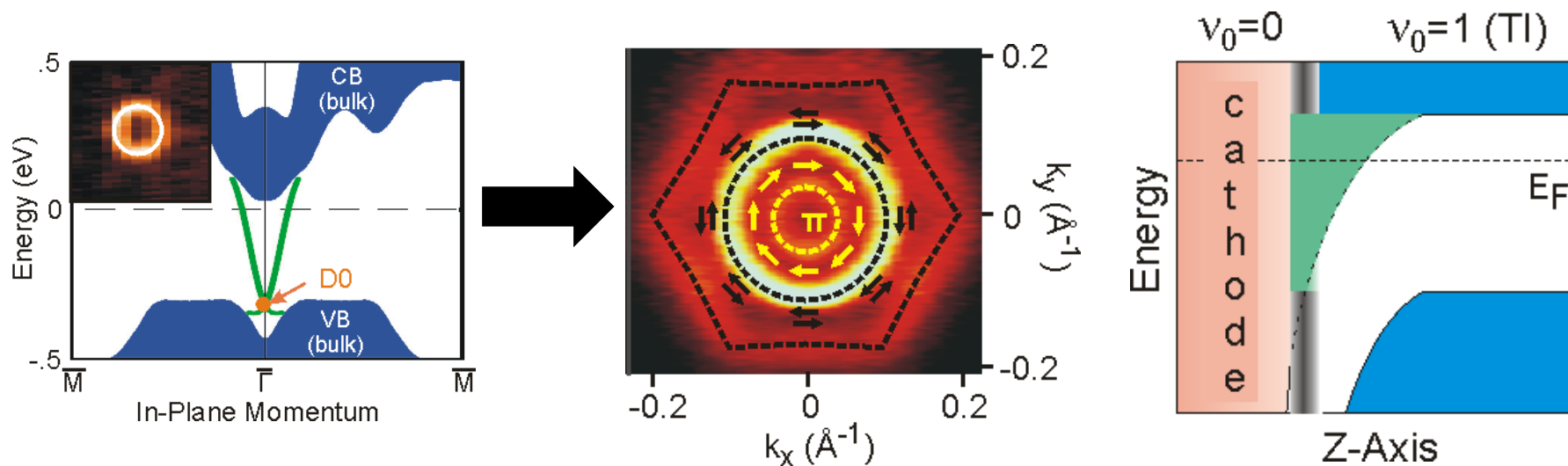


Fu PRL 2007

• Terminology: All 2DEG's and Rashba states are "surface states", with respect to topology.

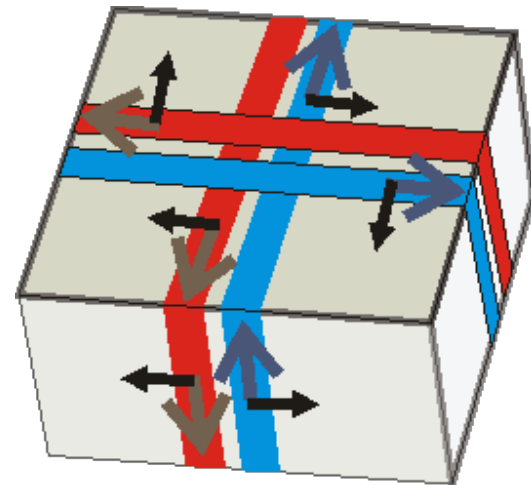
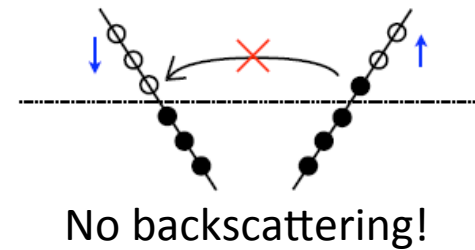
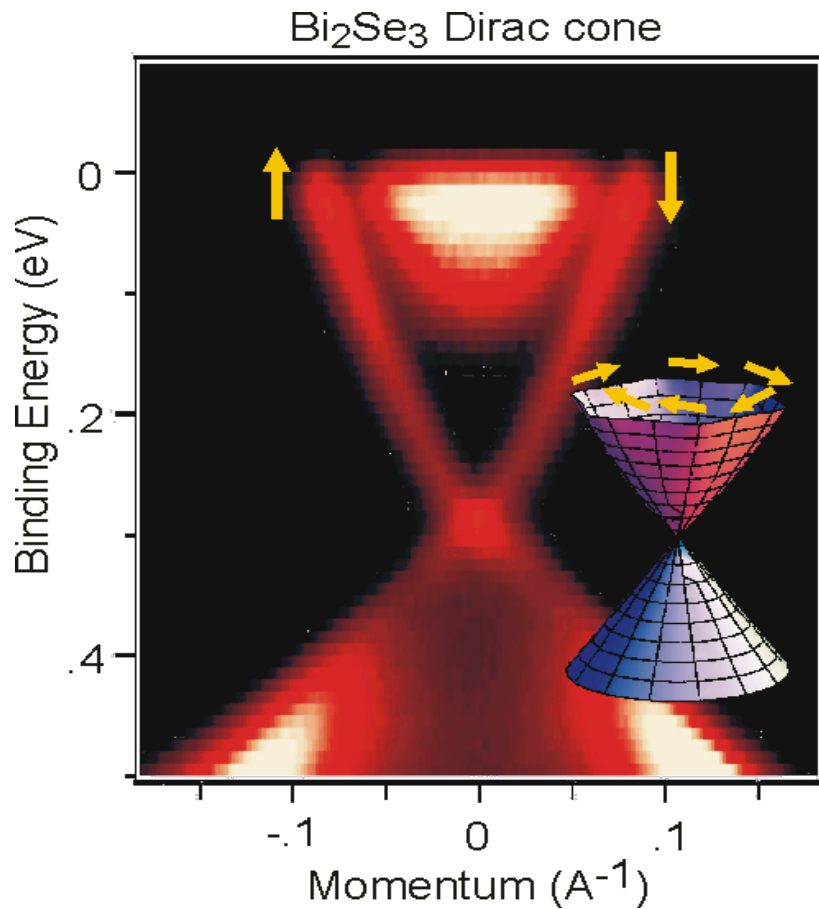
1

# Topological connections





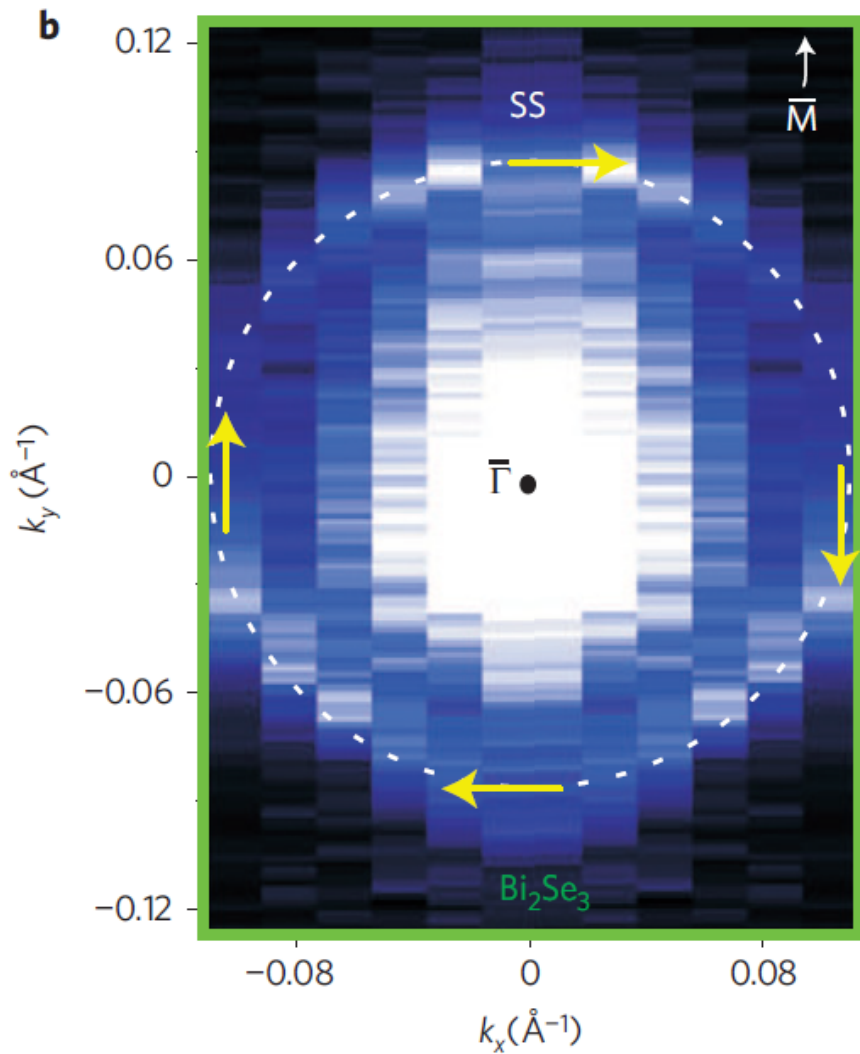
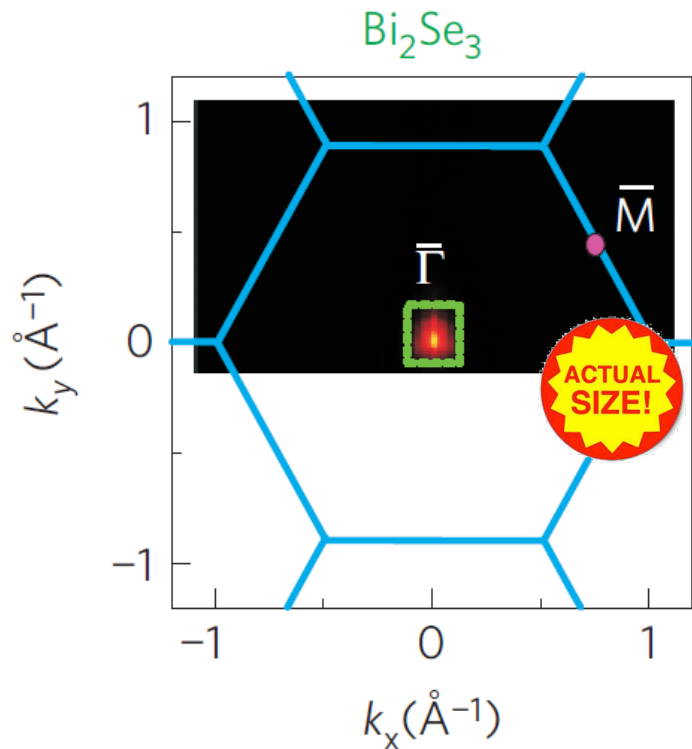
# $\text{Bi}_2\text{Se}_3$ : a single Dirac cone TI



A 3D insulator, wrapped in a 2D metal

*TI surface electrons are also protected from Anderson localization (See papers by Konig, Fu, Ostrovsky, Ryu)*

# Not many electrons are involved (usually)



# More Is Different

Broken symmetry and the nature of  
the hierarchical structure of science.

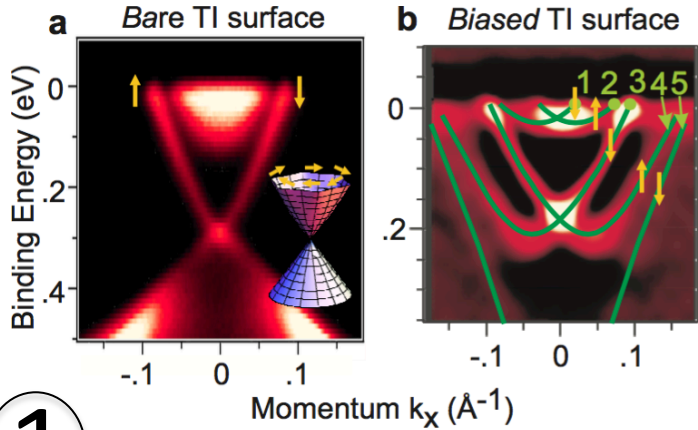
P. W. Anderson

*Science* **177**, 393 (1972)

**A big question:** What do we get from adding topological bulk-boundary correspondence to the many-body principles and states that we already know?

# Disrupting the system brings in-gap surprises

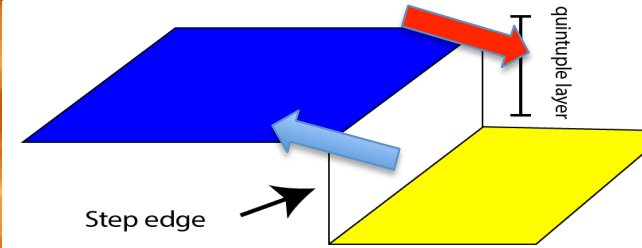
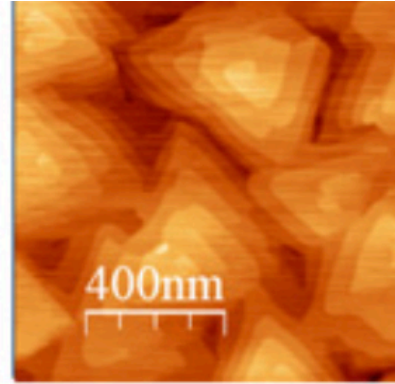
## Gating creates new Dirac points



1

LAW Nat. Phys. 2011

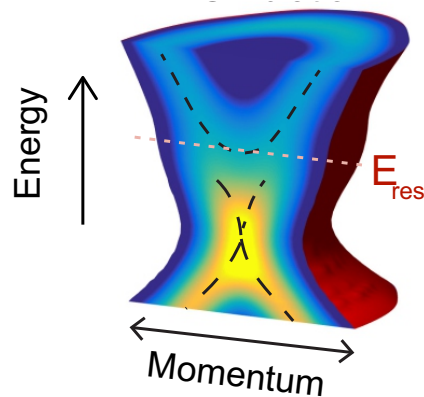
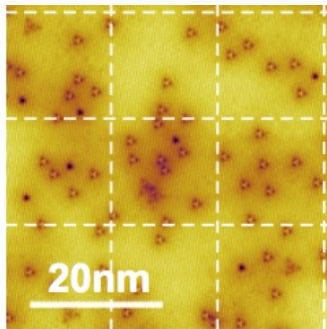
## Complex structure changes the game



Miao, PNAS 2013; Xu, Miao, LAW in prep (2018)

3

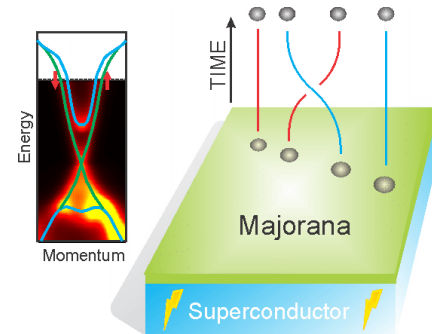
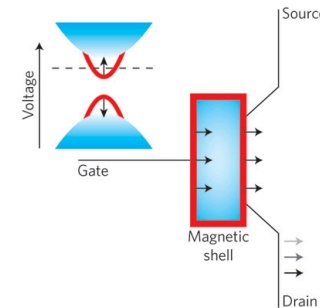
## Defects create new band structure



2

Xu, Biswas, LAW Nat. Comm. 2017

## Superconductivity and Magnetism



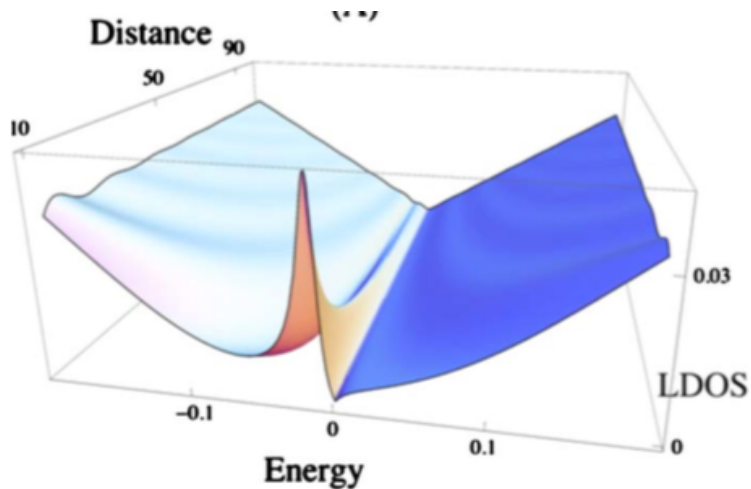
Fu PRL 2008, LAW Nat. Phys. 2010

J. Checkelsky, Nat. Phys. 2012; News and Views by LAW

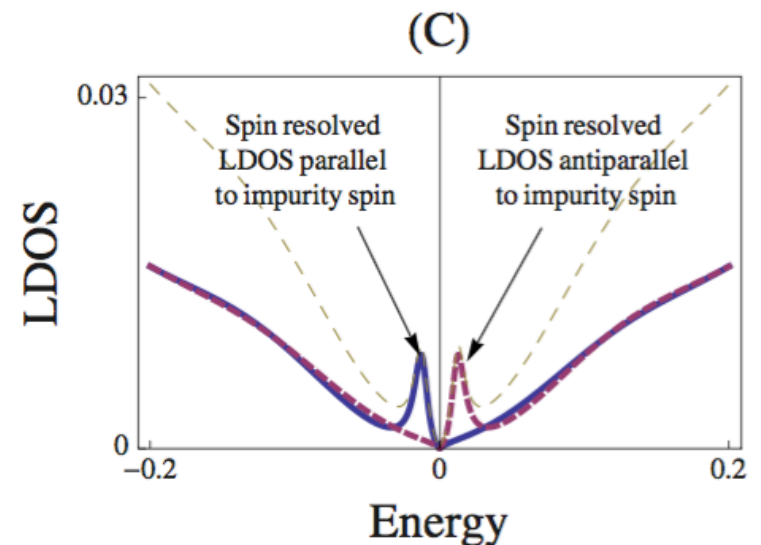
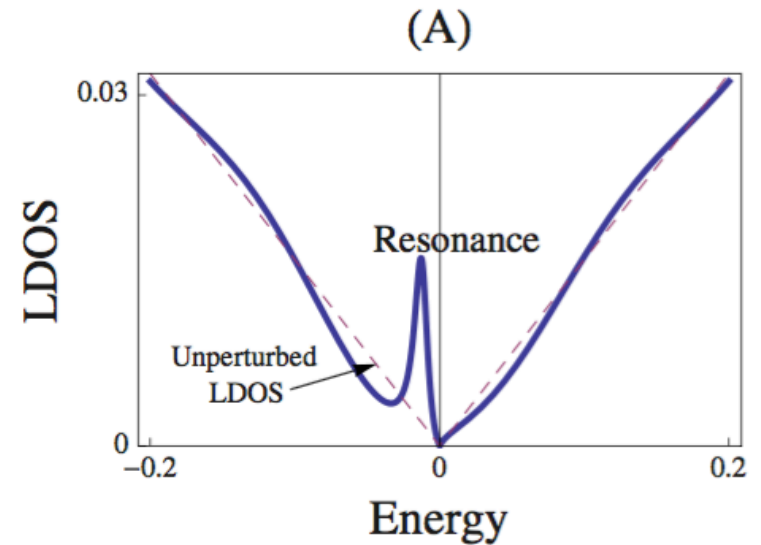
# The theory of in-gap states

$$\mathcal{H}_0 = \boldsymbol{\sigma} \cdot \mathbf{p}$$

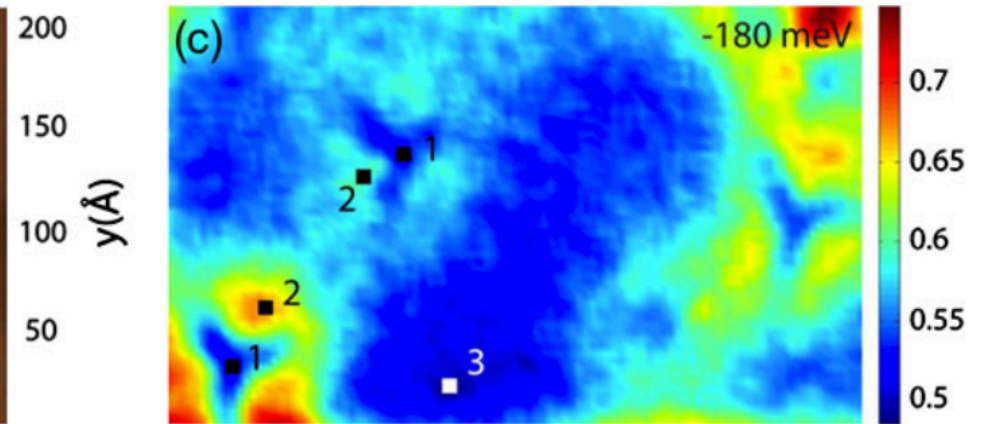
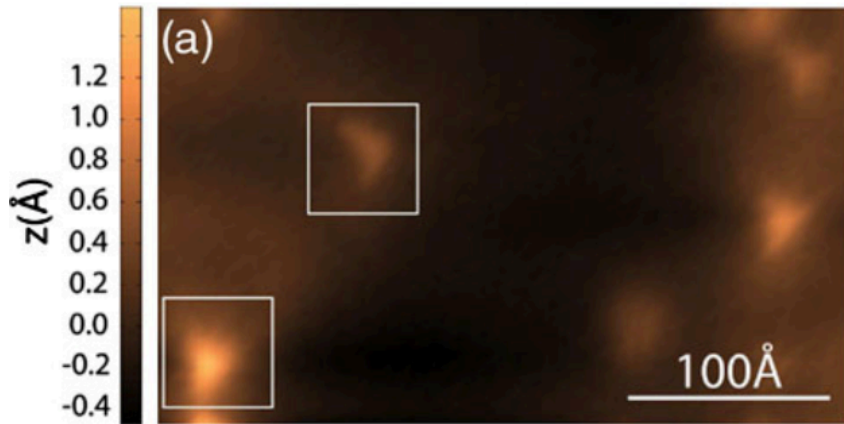
$$\hat{V}_{\text{pot}} = U \mathbb{1} \delta(\hat{\mathbf{r}}), \quad \hat{V}_{\text{mag}} = U \mathbf{S} \cdot \boldsymbol{\sigma} \delta(\hat{\mathbf{r}})$$



*Biswas and Balatsky PRB 81, 233405 (2010)*  
 See also work by A. Black-Schaffer and D. Yudin

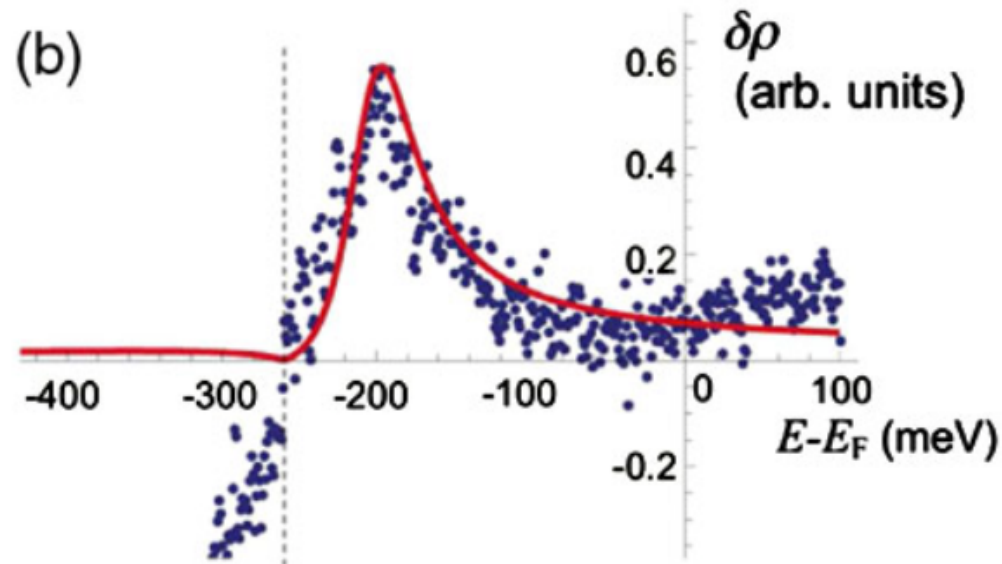


# In-gap states “in practice”



*Alpichshev, Biswas, Kaptiulnik PRL 2012*

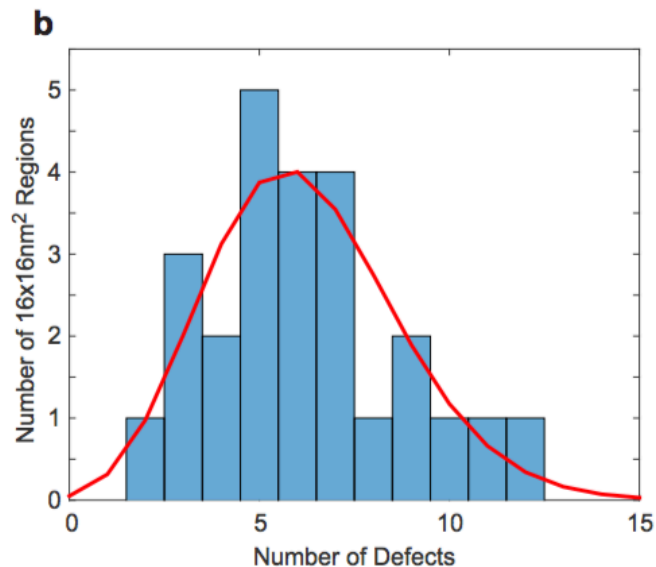
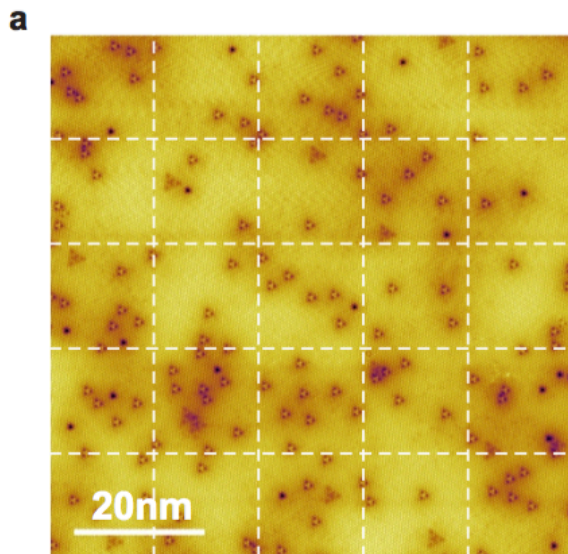
Local density  
of states:



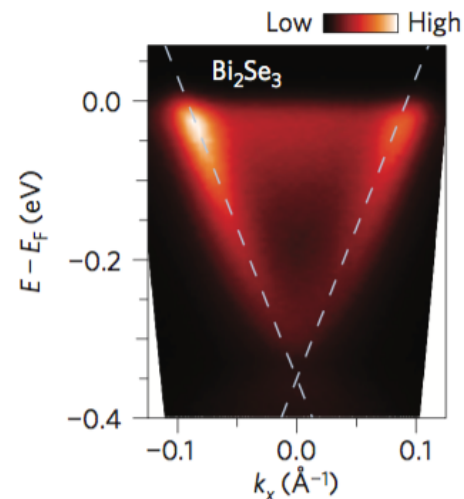
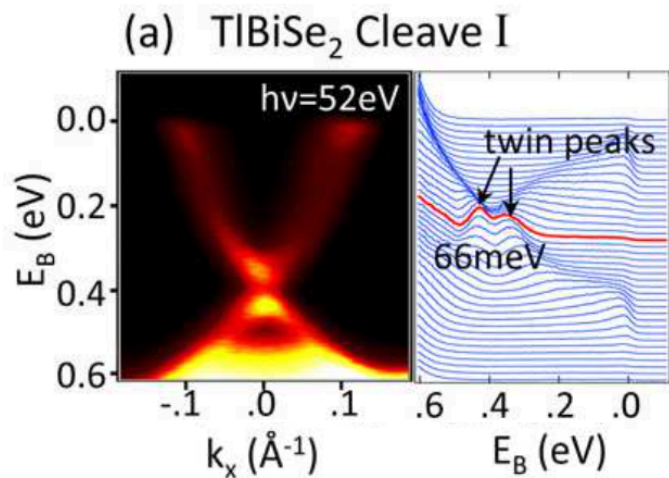
# Is more different? (past experiments)

Selenium vacancies:  
( $\text{Bi}_2\text{Se}_{3-\delta}$ )

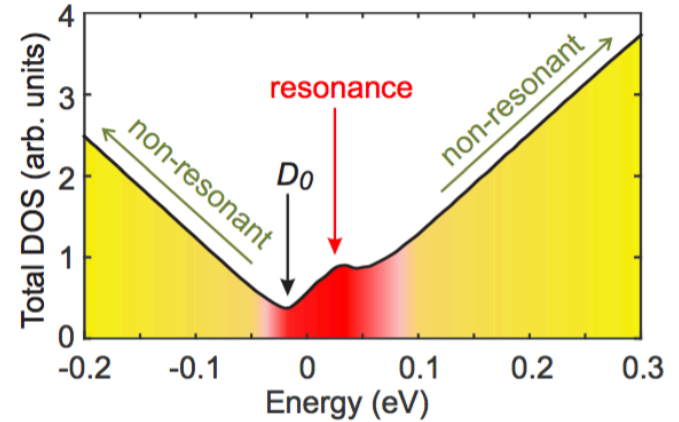
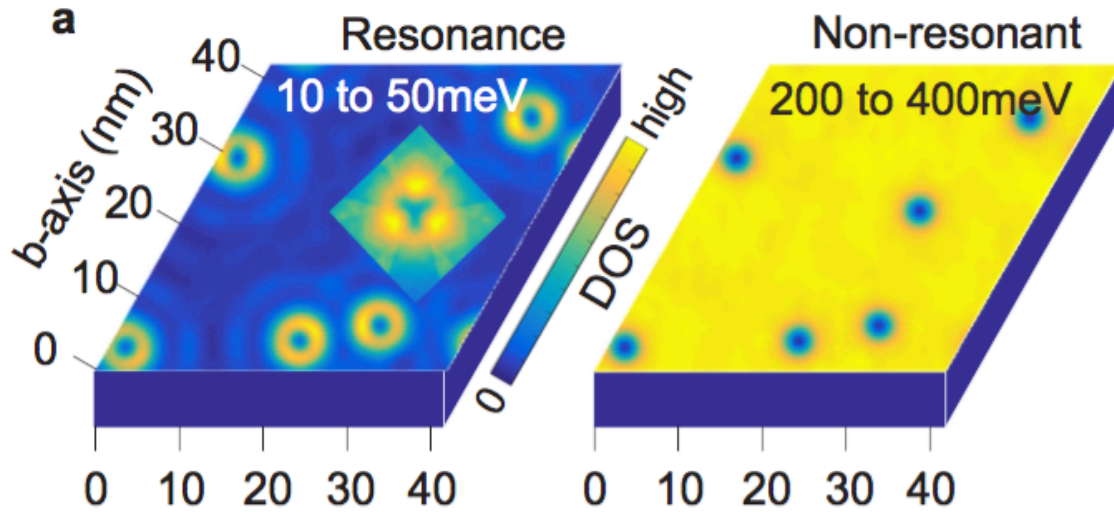
But real defect  
densities rarely  
exceed  
 $N_d/N=0.001$  !!!!!



ARPES oddities:



# Is more different? (theory)



*Xu, Chiu, Miao, Alpichshev,  
Kapitulnik, Biswas, LAW, Nat.  
Comm. 2017*

*These look like semiconductor impurity states, but...*

*(1) Why do they show up in total DOS,  
with  $N_d/N=0.0006$  ?!*

*(2) Theoretically, they can't be localized?!*

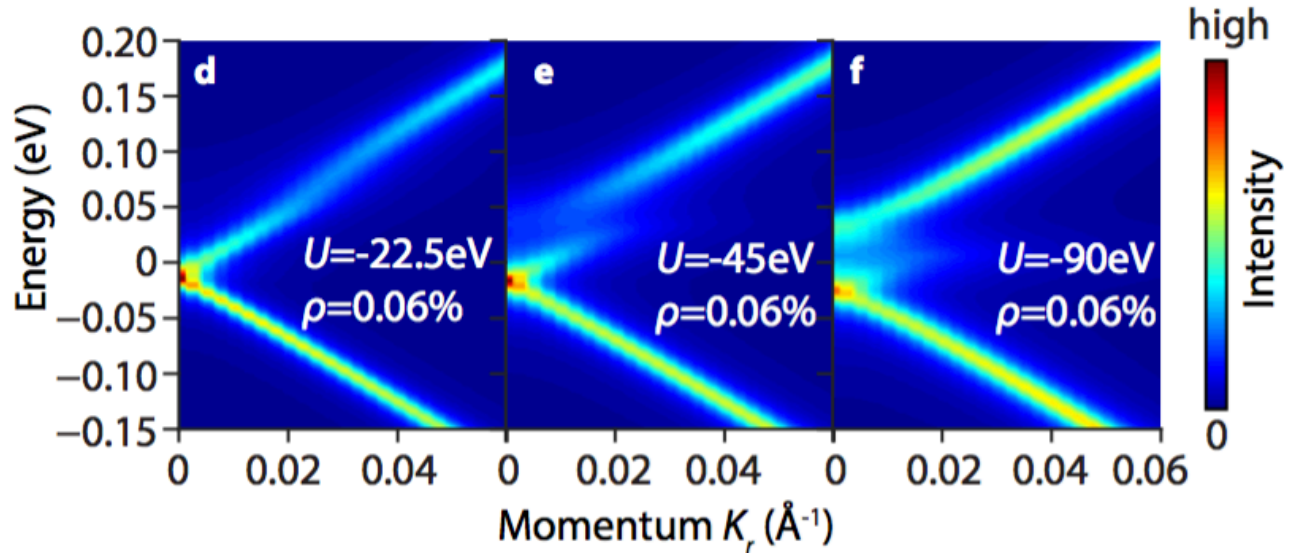
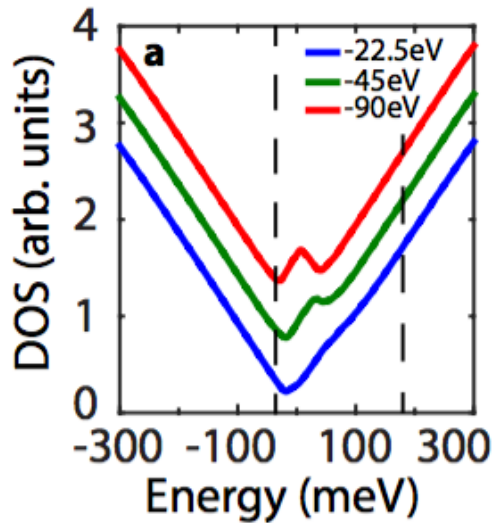


Yishuai Xu

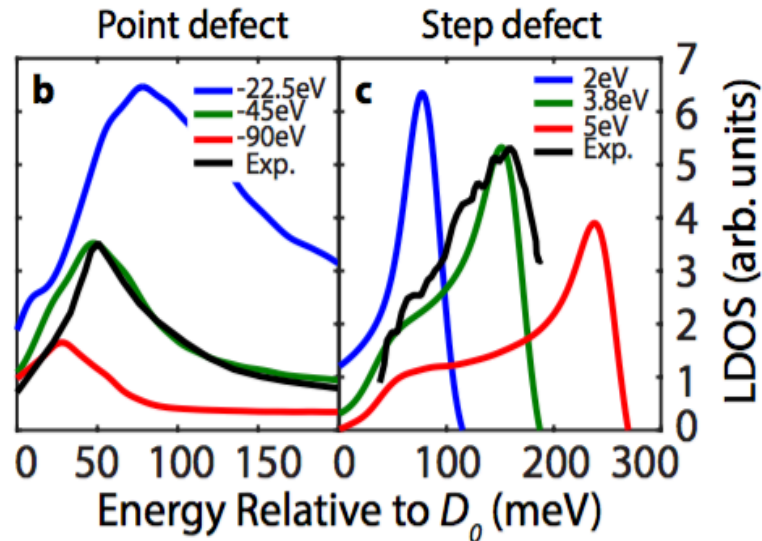
Janet Chiu



# What are the k-space implications?

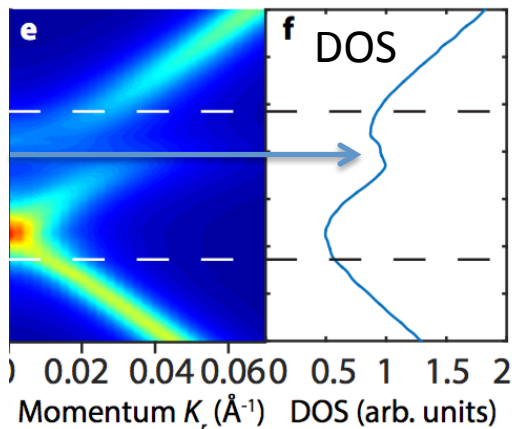
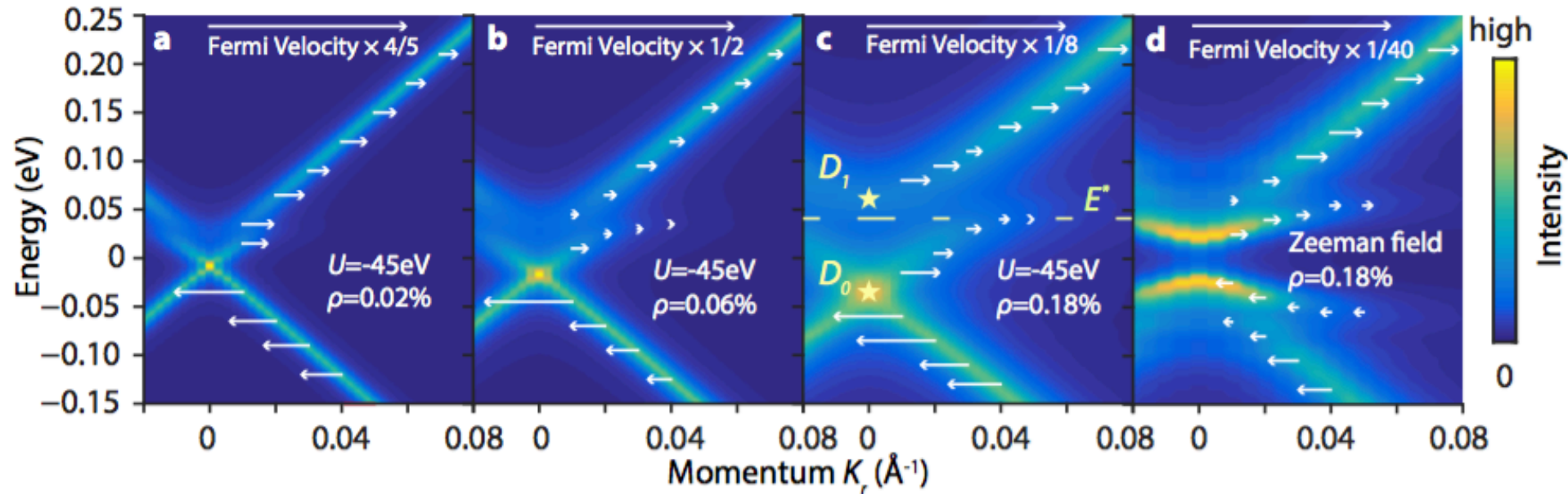


Does the theory still work?



# A “Non-Topological” Quasiparticle?

To see this, you want 100nm + ~20meV resolution



A) *Not a real gap (and no Luttinger theorem).*

B) *The constraints from band topology are also an open question.*

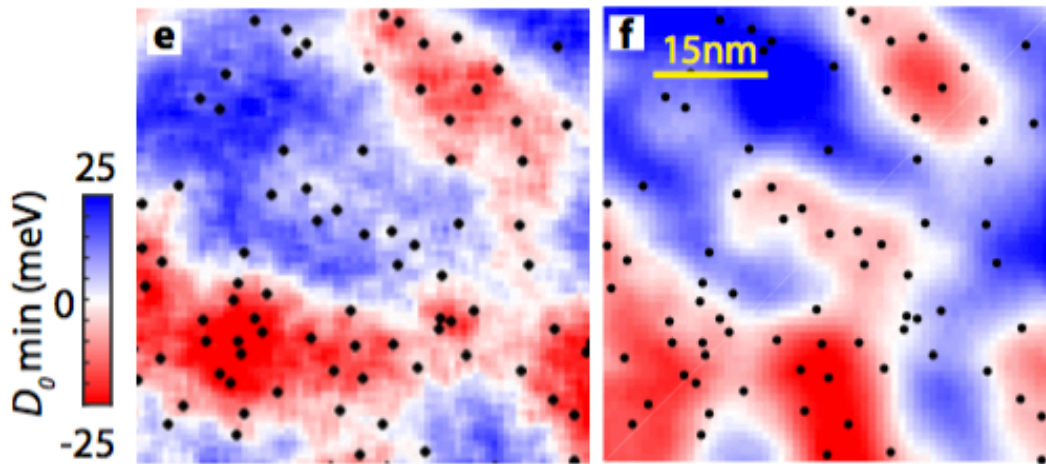
Twist velocity:

$$\mathbf{v}_\theta(\alpha) = \nabla_{\mathbf{K}_\theta} E_\alpha$$

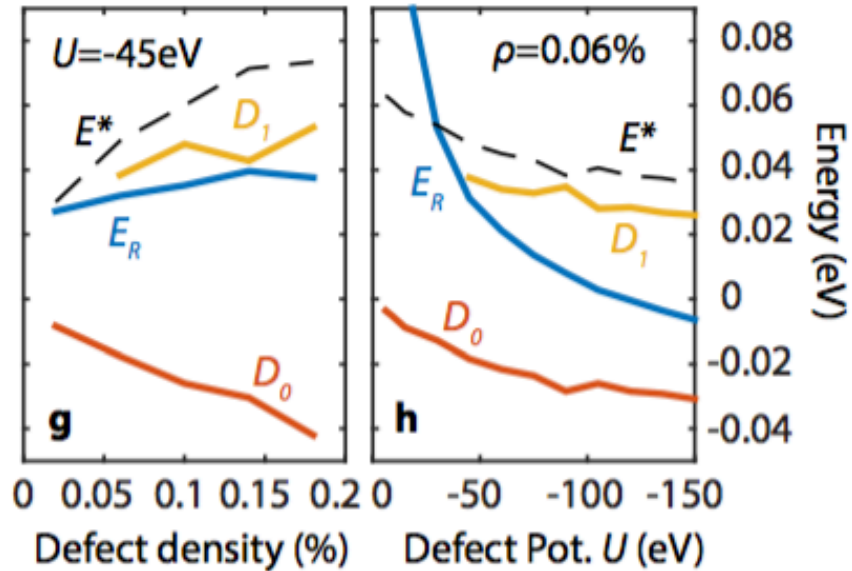
$$\mathbf{K}_\theta = \theta_x/L_x \hat{\mathbf{k}}_x + \theta_y/L_y \hat{\mathbf{k}}_y$$

# What new principles does this bring into play?

To see *this*, you want 20nm resolution



STM from **Weida Wu** group (see Dai PRL 117, 106401 [2016])



**But!** this defect density ( $\sim 0.19\%$ ) has not been achieved in large single crystals!

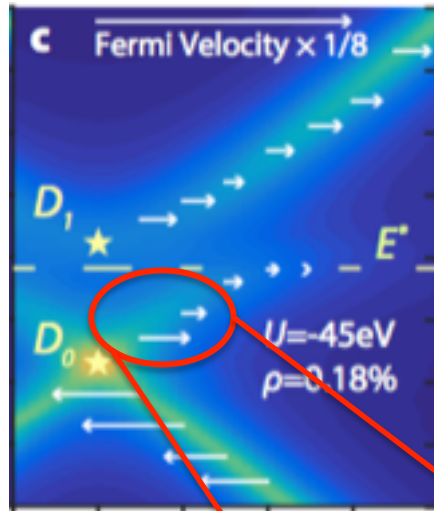
$$N_E = \frac{\sqrt{3}a^2 N E^2}{4\pi v_0^2}$$

$$N_E = N_R \equiv 2\rho N$$

Density  
Threshold:

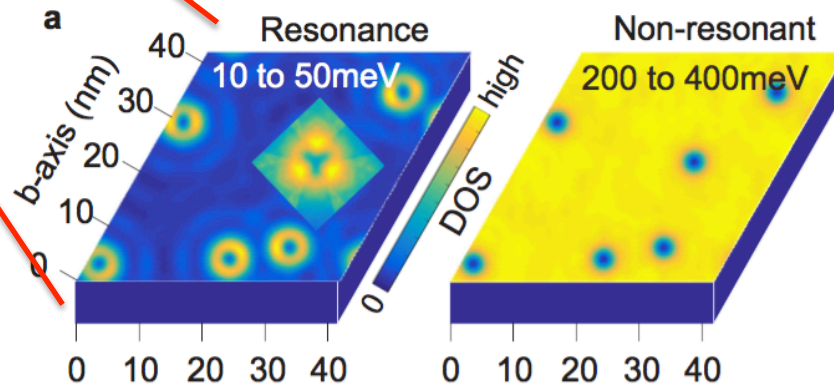
$$E^* = \sqrt{\frac{8\pi v_0^2 \rho}{\sqrt{3}a^2}}$$

# A Quasiparticle Without Translational Symmetry?

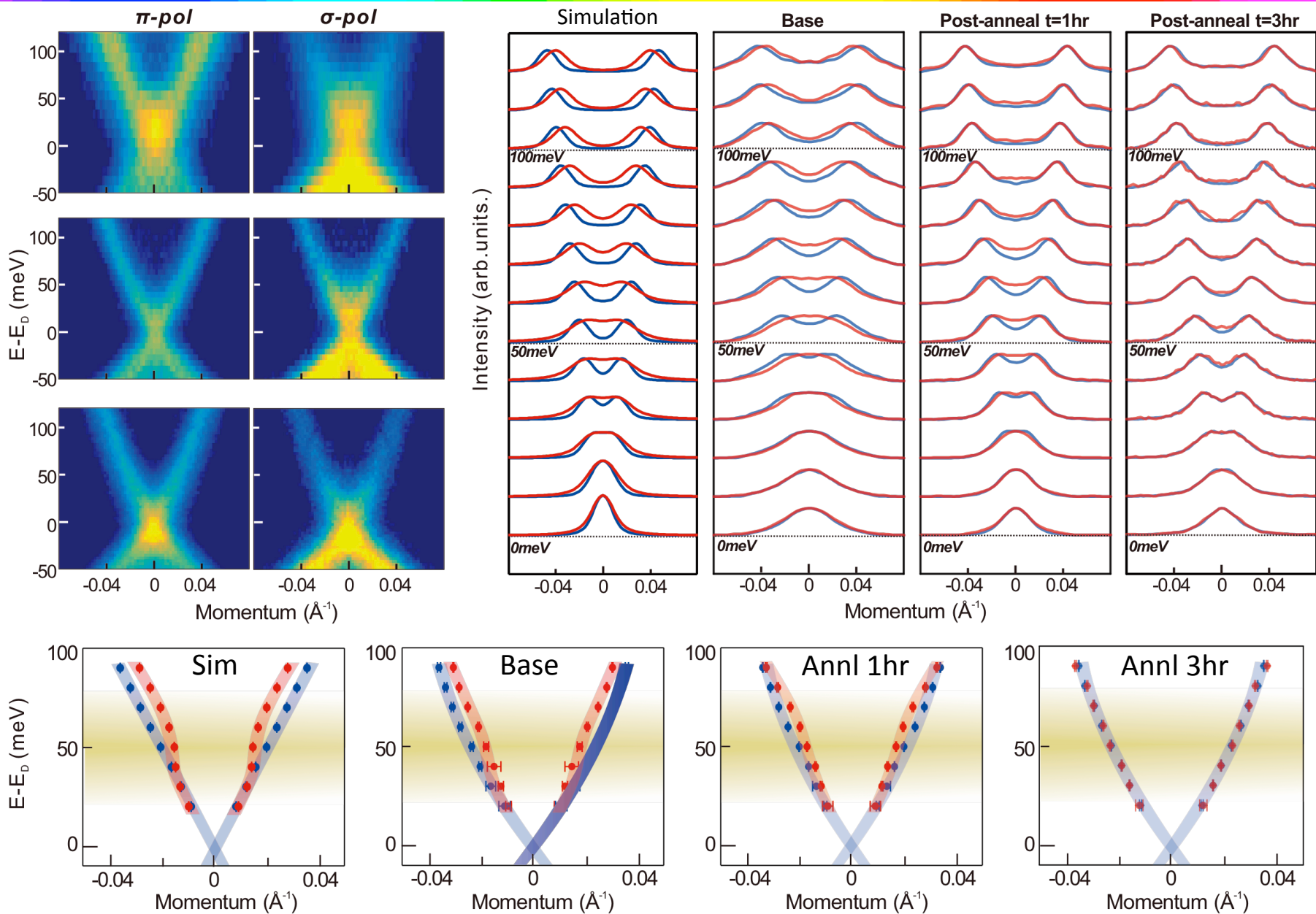


$$T(x) = \exp(-ixP/\hbar)$$

Normal states are either (near-) eigenstates of *both* translation (**T**) and momentum (**B**) symmetry, or *neither*.

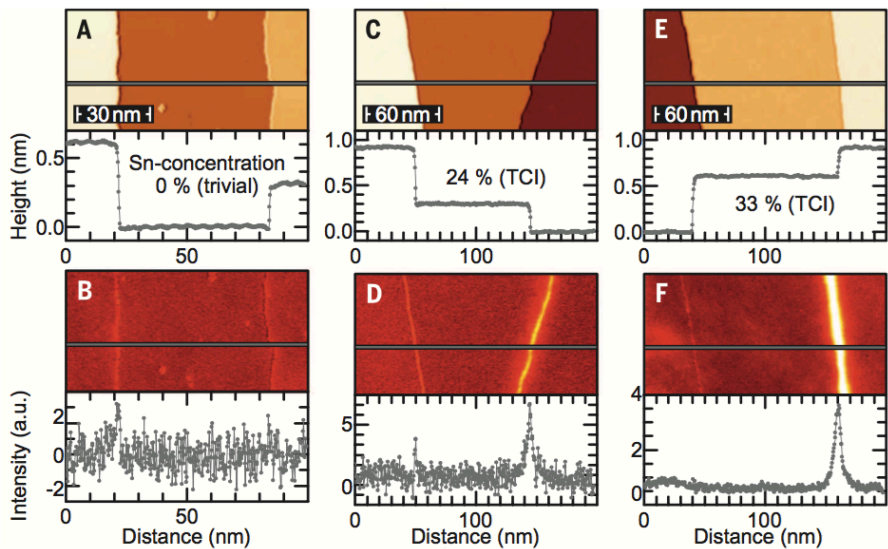


# Post-Growth Sample Tuning

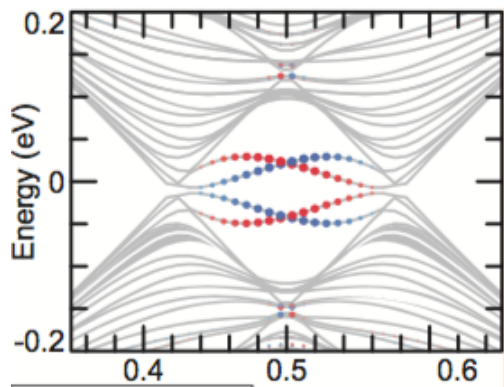


# Surface steps: on the edge of 'topological'

(semi-)topological TCI edge states

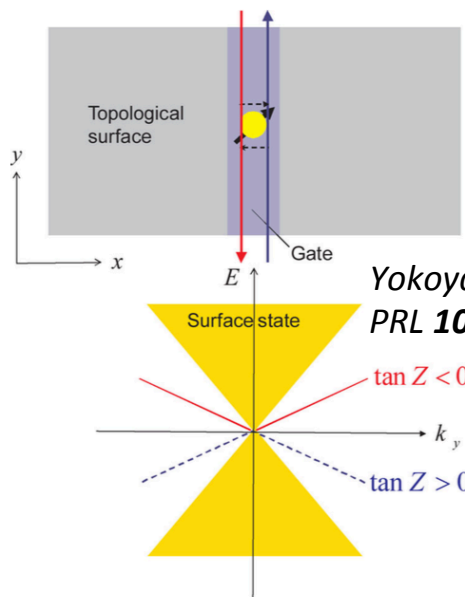


An even-odd 1D topological distinction unique to TCI

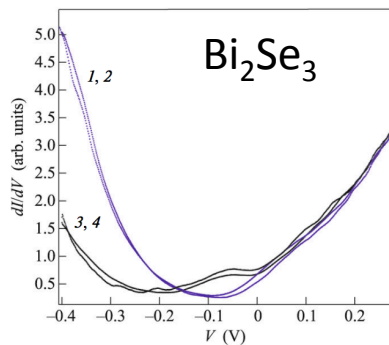


Sessi et al, Science **354**, 1269 (2016)

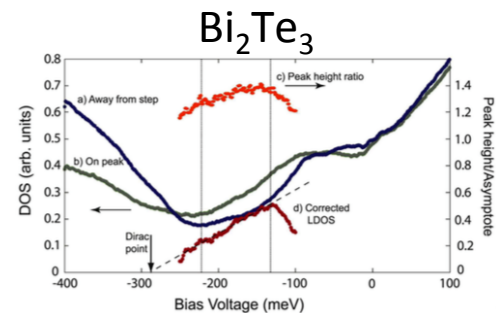
Dirac-connected states beneath a delta function potential



Yokoyama, Balatsky, Nagaosa, PRL **104**, 246806 (2010)

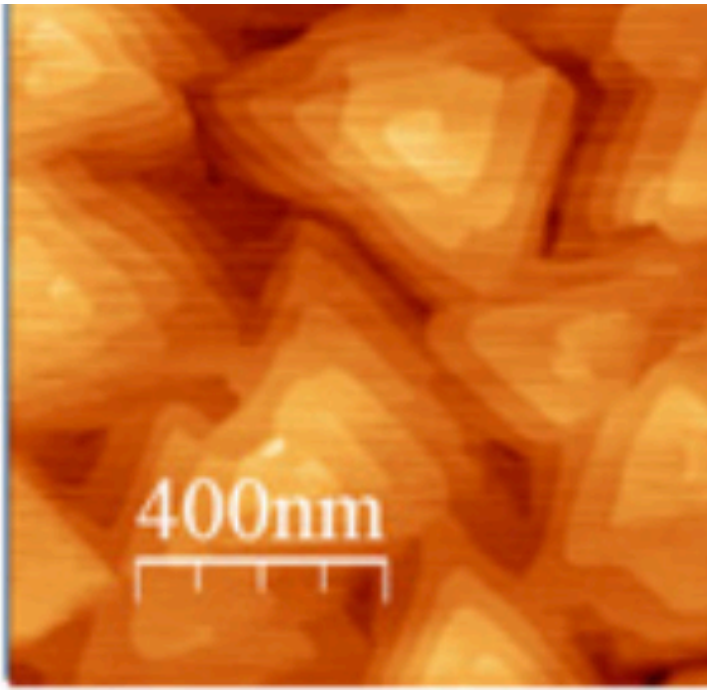


Dmitriev, JETP Letters, **100**, 398 (2014)

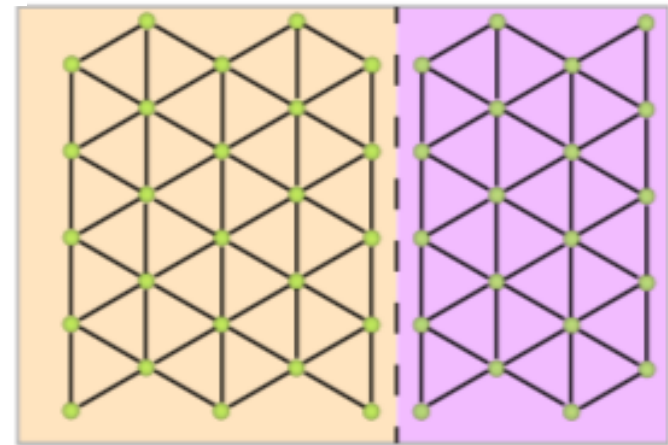
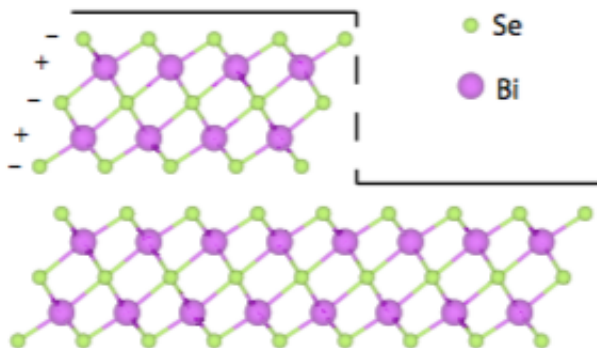


Alpischev, Kapitulnik PRB **84**, 041104 (2011)

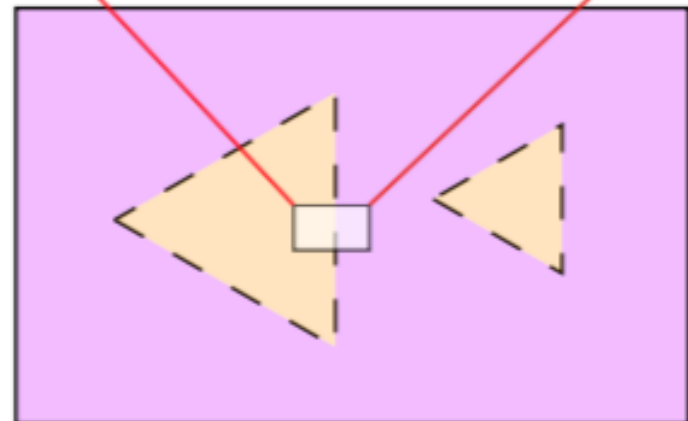
# Step edges on $\text{Bi}_2\text{Se}_3$



Teague et al., *Solid State Comm.* 152, 747 (2012)



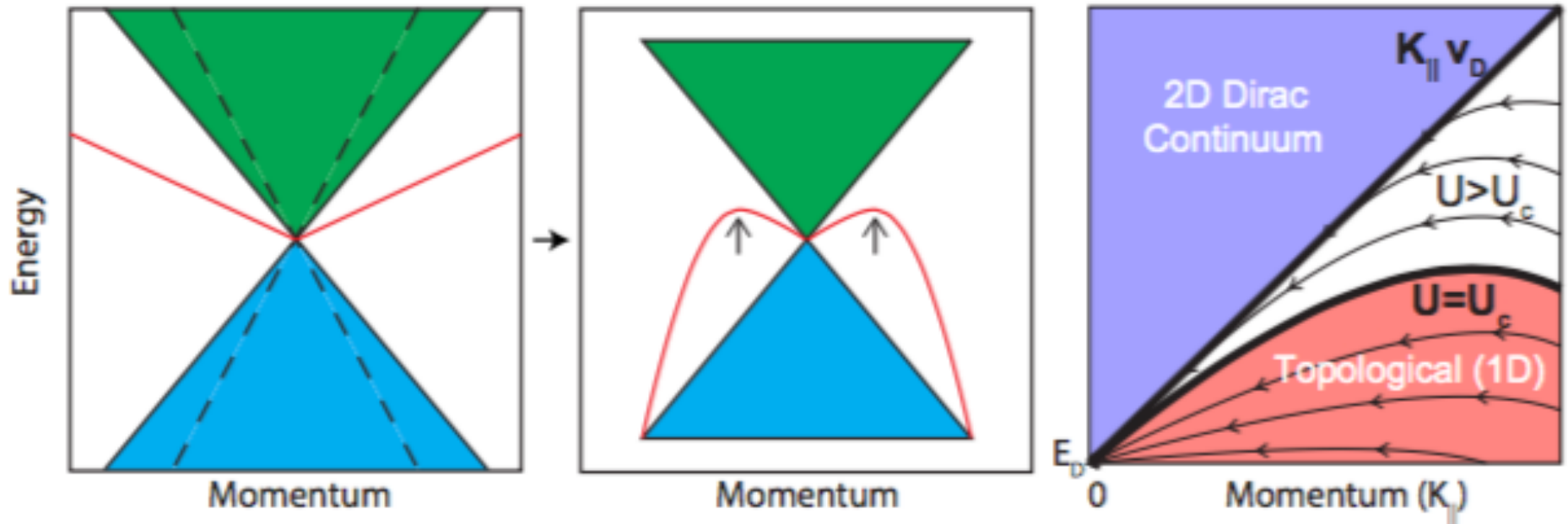
Surface view



# (anti-)Bound states of a 2D Weyl cone

Infinite Dirac cone

Finite Dirac cone

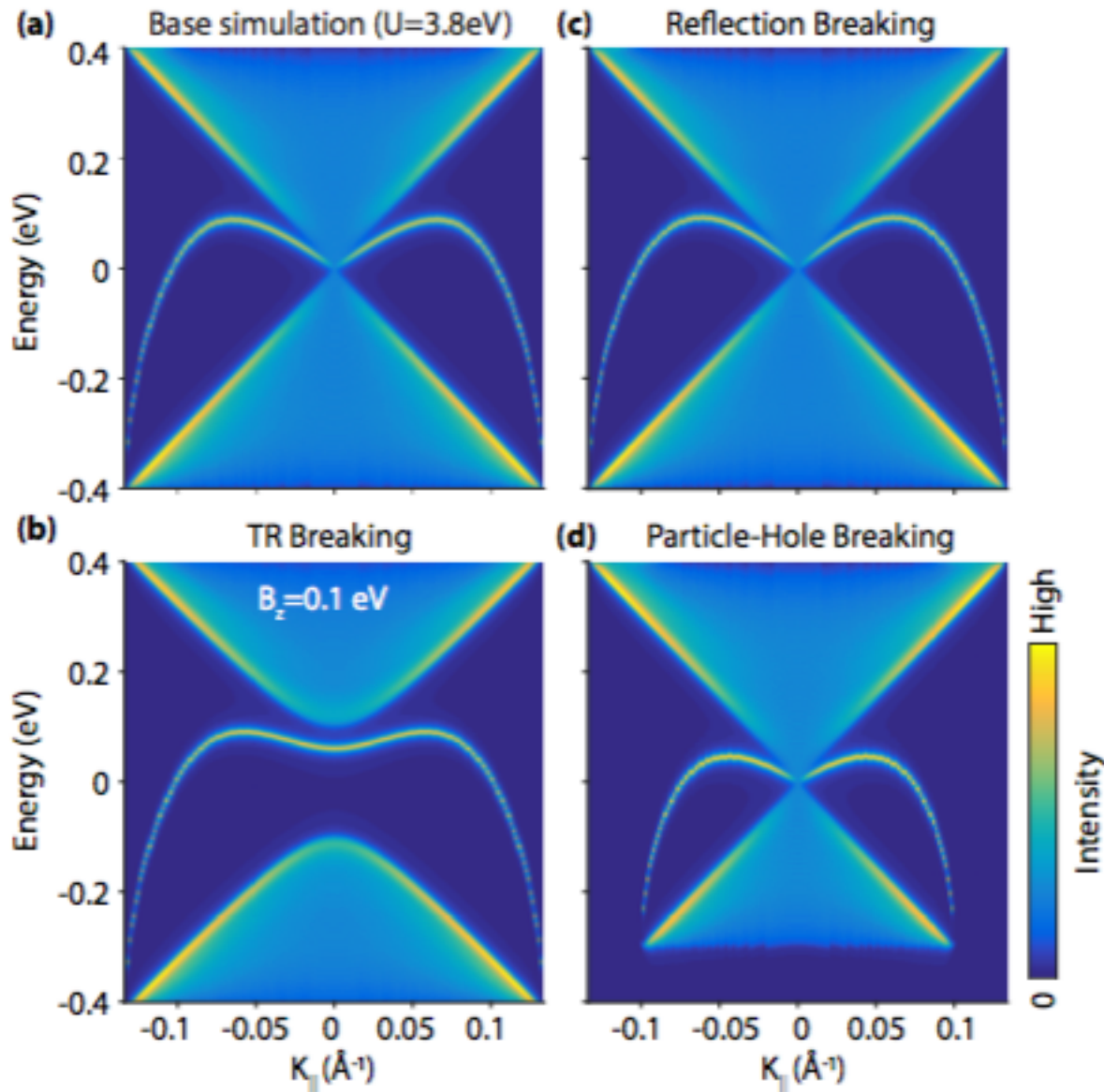


$$H_T = v_D(\mathbf{k} \times \boldsymbol{\sigma})$$

Y. Xu, R. Biswas, LAW,  
submitted to N. J. Phys. 2018



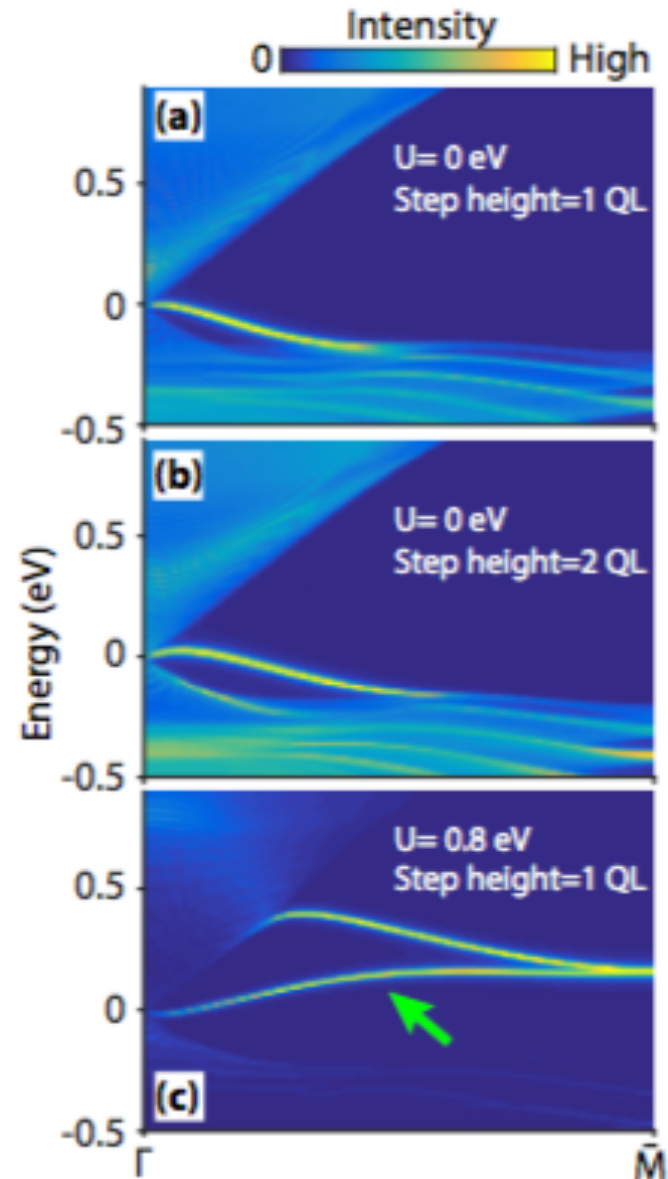
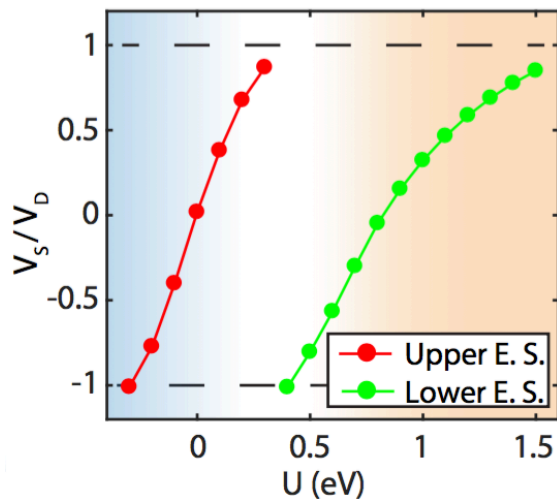
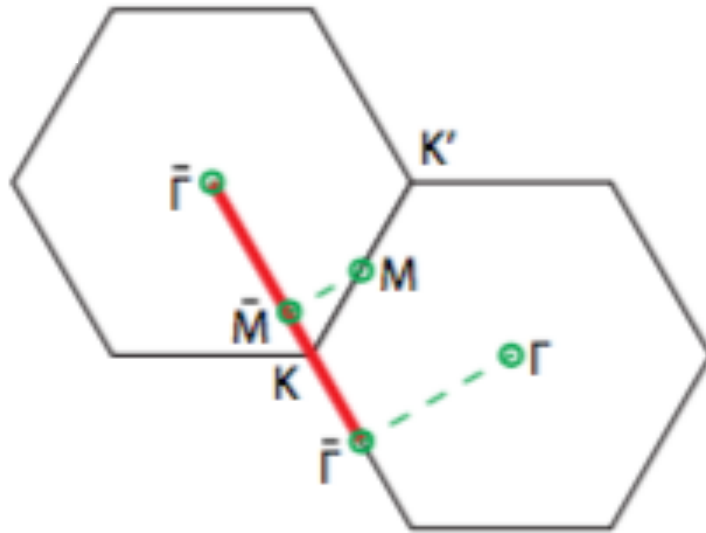
# Symmetry protection



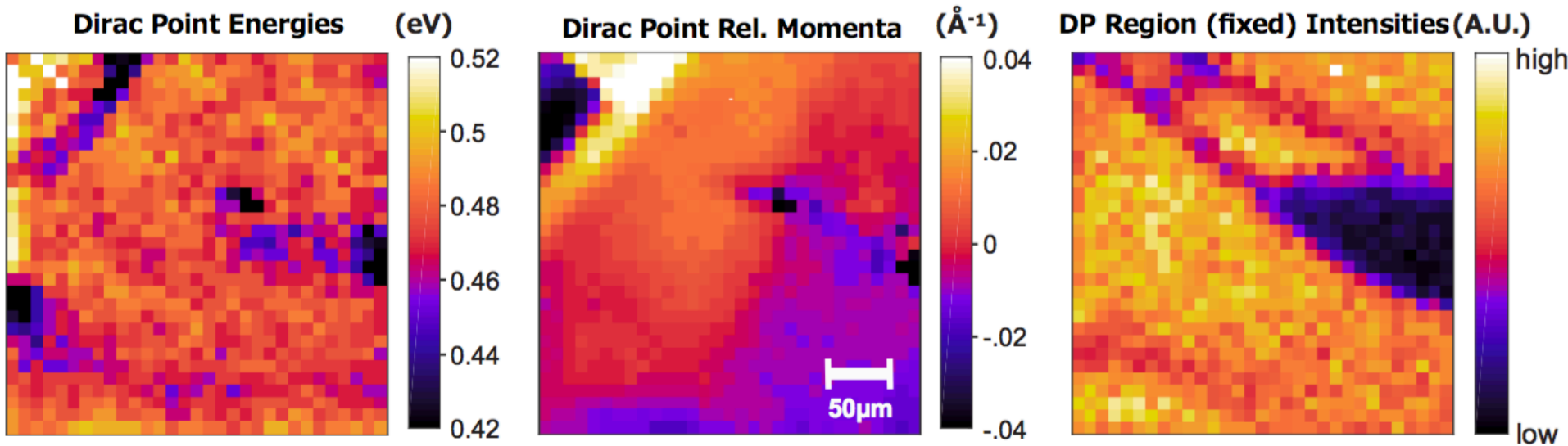
$$H_T = v_D(\mathbf{k} \times \boldsymbol{\sigma})$$

$$H_U = U \sum_{\alpha} n_{\alpha}$$

# A universal phenomenon?



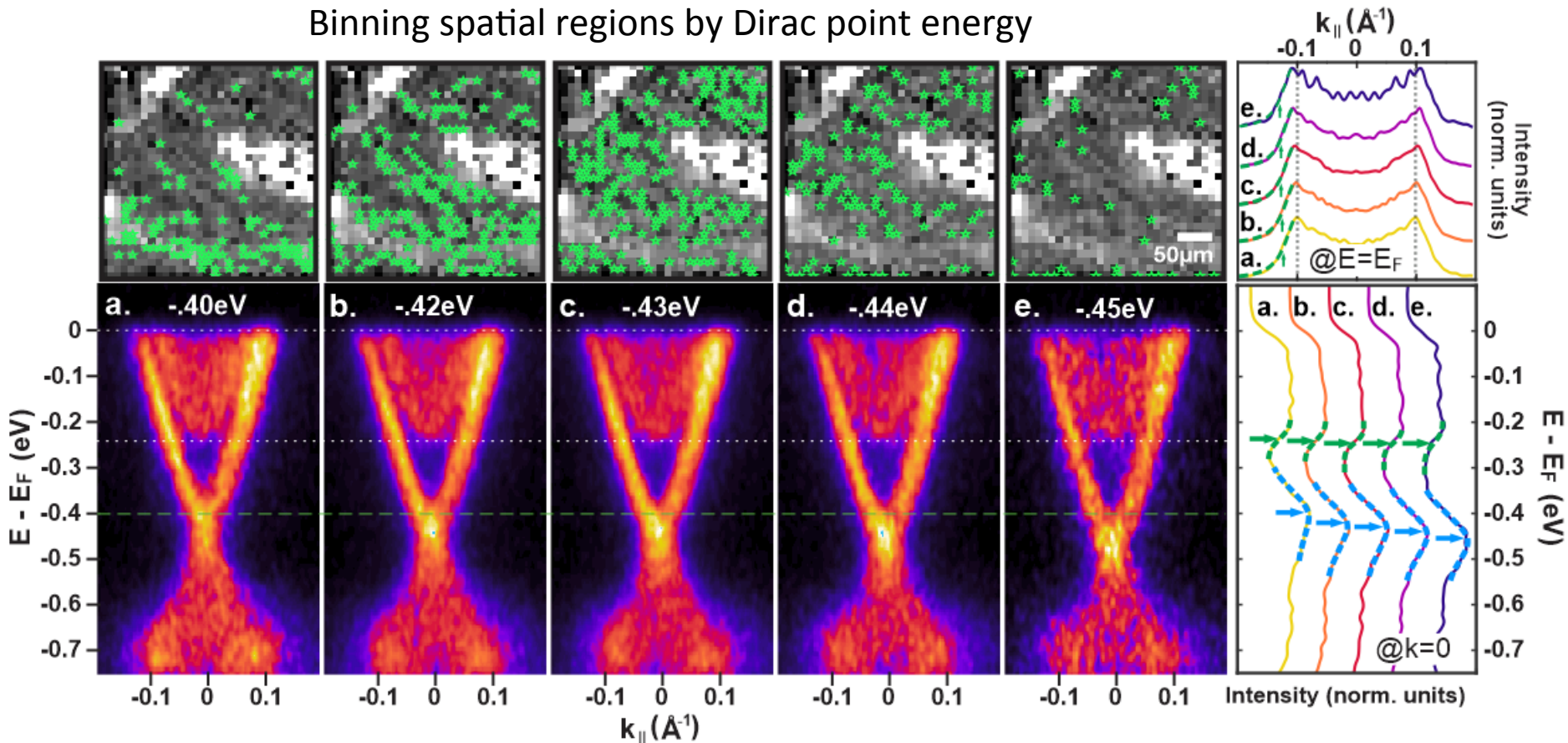
# *micro-ARPES: a step into the future*



*30 minute ALS MAESTRO image, April 2017*

# Anisotropy $\sim$ structural control

Binning spatial regions by Dirac point energy



- What are the causal relationships between different elements of crystallographic and electronic structure?
- Nano-ARPES is also possible! (100 nm beam spot at ALS MAESTRO)

# The Quasiparticle is the Device?

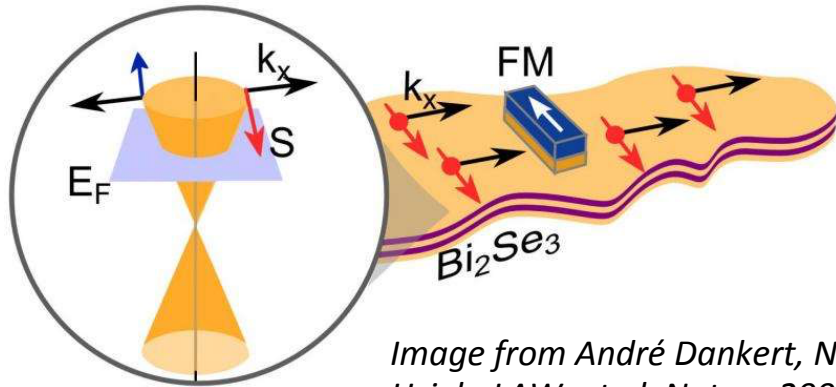
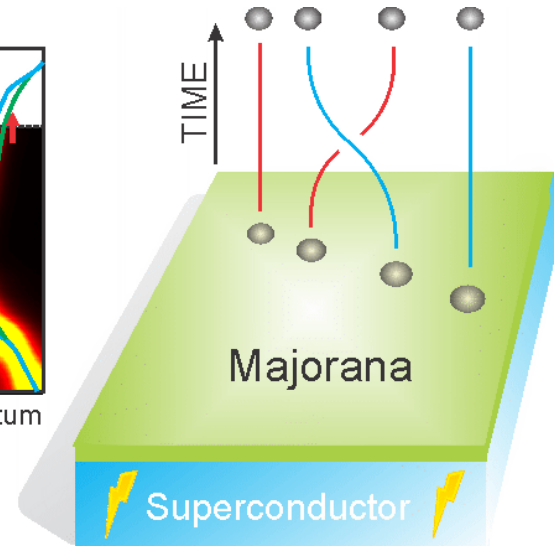
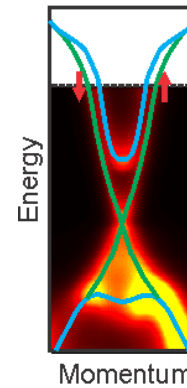
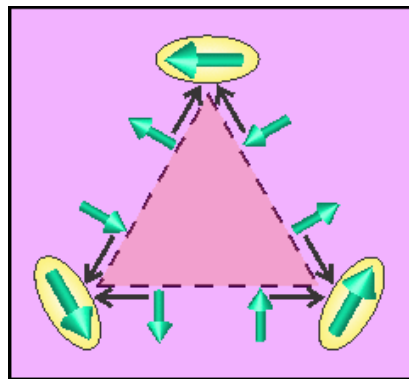


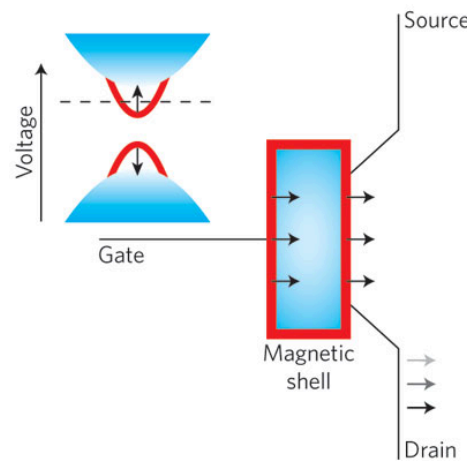
Image from André Dankert, *Nano Letters*  
 Hsieh, LAW, et al, *Nature* 2009 X2  
 A. R. Mellnik et al, *Science* 2014  
 Y. Fan et al, *Nature Materials* 2014



Fu PRL 2008,  
 LAW et al, *Nat. Phys.* 2010



Terrace corner spin moments  
 Y. Xu, R. Biswas, LAW,  
 submitted to *N. J. Phys.* 2018



"Topological Transistor,"  
 LAW *Nat. Phys.* 2012

# Overview

## Topological order opens up new realms of possibility, such as

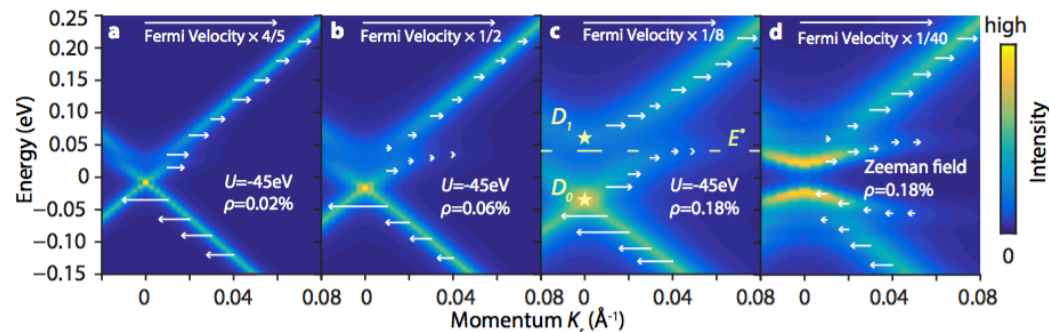
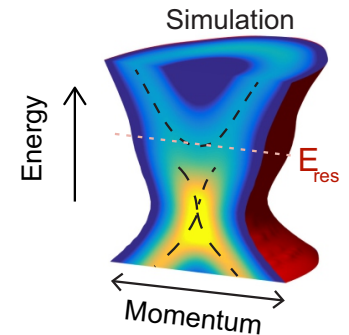
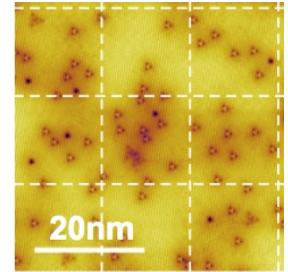
- TO+Gating: “Giant” zig-zag Rashba splitting
- TO+Disorder or Structure: New transport channels!
- TO+superconductivity: Quantum computing
- TO+magnetism: new transistors, 1-way nanowires, and quasiparticles

## Disorder brings about changes to real space and momentum space

- Particle-like states that profoundly lack translational symmetry
- An emergent band-like feature that supports diffusive transport
- A gap-like feature (without a density of states dip)

## Line-like defects act as spin-polarized wires

- 1D ‘wire’ states connect to the 2D Dirac point
- Surface step edges are sufficient to bind these states
- Transport is protected from scattering, similar to spin-Hall edge states



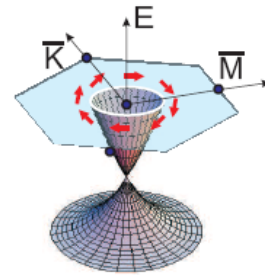
# Towards the Next Generation of Quantum Materials

## Unique heterostructure synthesis capabilities

- MBE, PLD and PVD *in situ* growth systems
- Single atom Se<sub>1</sub> and O<sub>1</sub> sources
- Low temperature MBE
- PVD/PLD high pressure RHEED

## Powerful single-electron analysis

- Small-spot ARPES (<2meV resolution!)
- STM/AFM imaging
- XPS and real-time Auger



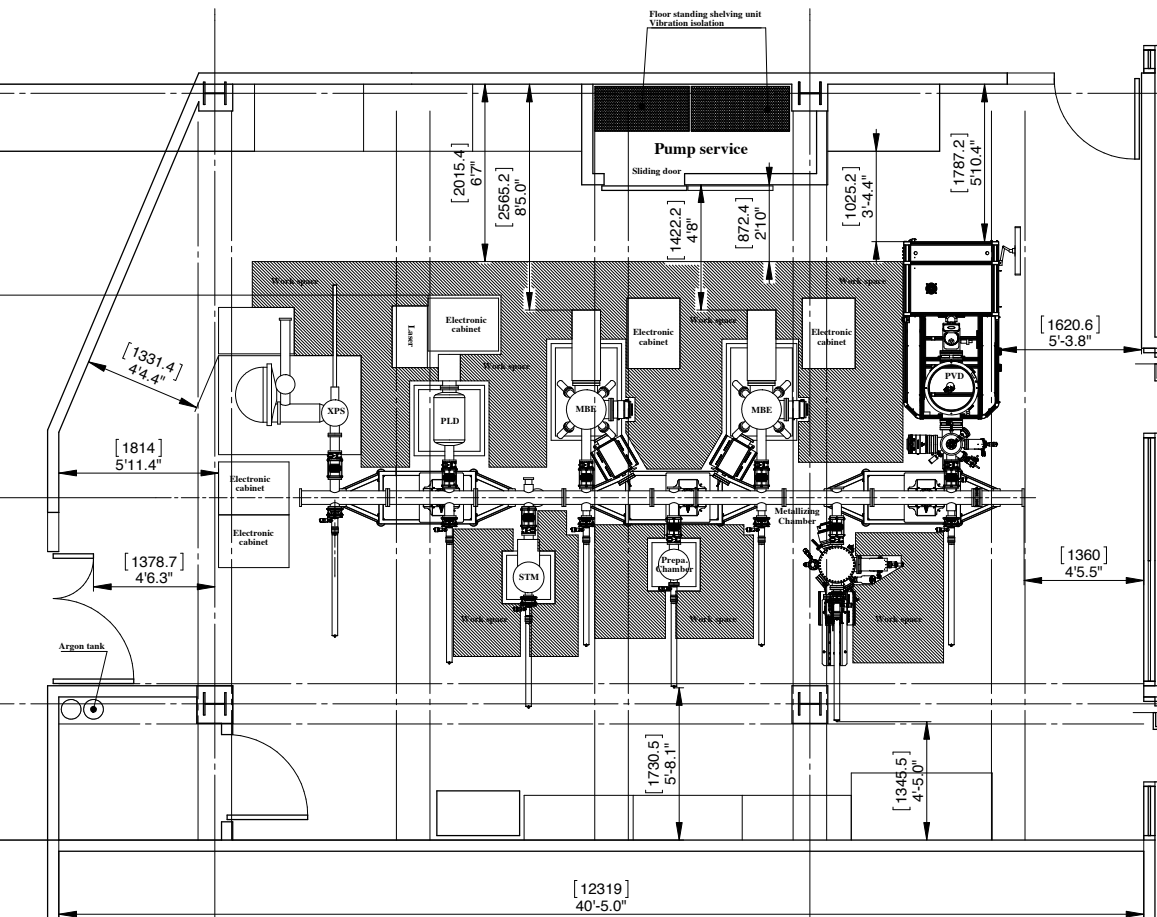
PIs:

Andy Kent

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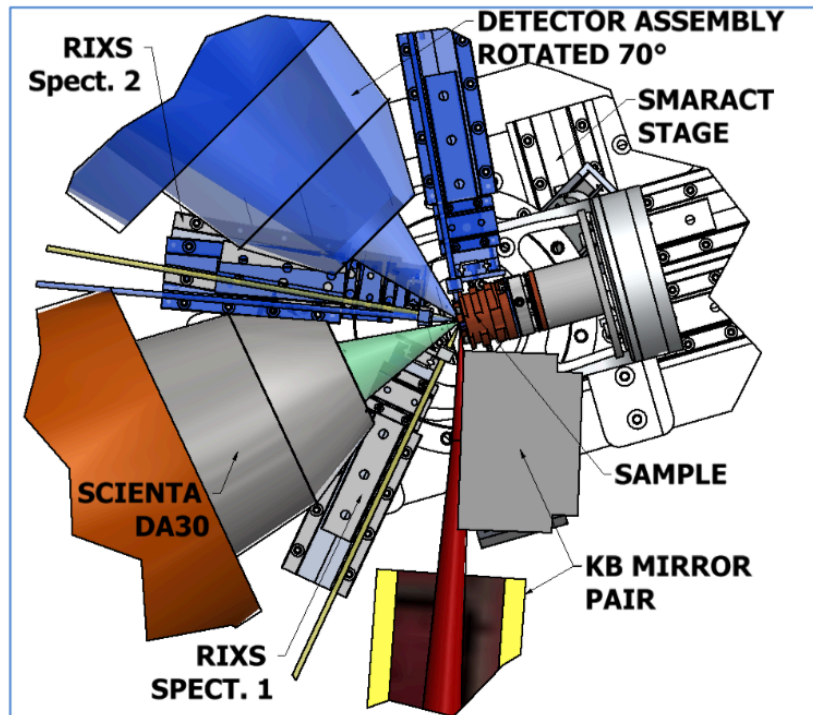


CQP Center for Quantum Phenomena

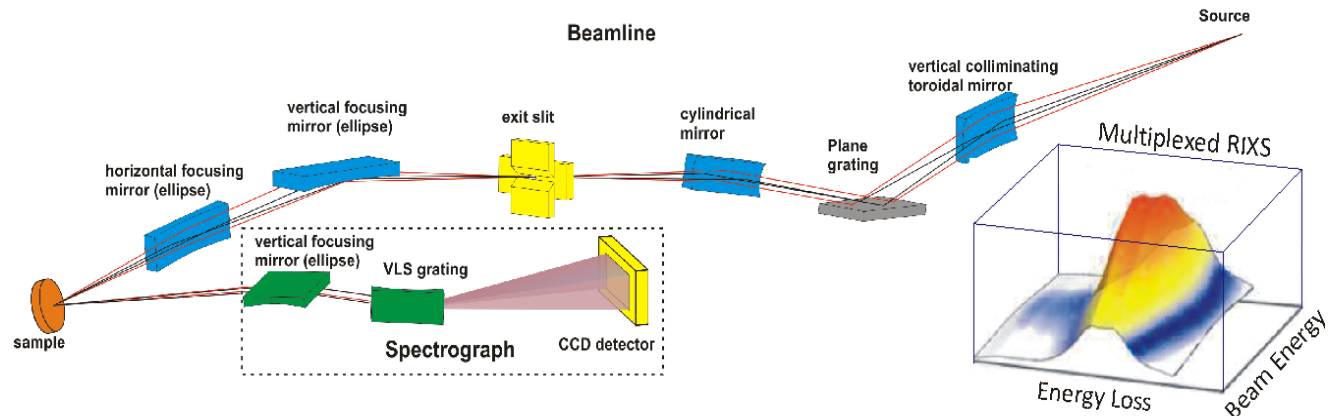


# ...and New Dimensions of Spectroscopic Study

The **ARI beamline** design proposed for NSLS-II offers 100nm resolution from mirror optics for **ARPES** and **RIXS**

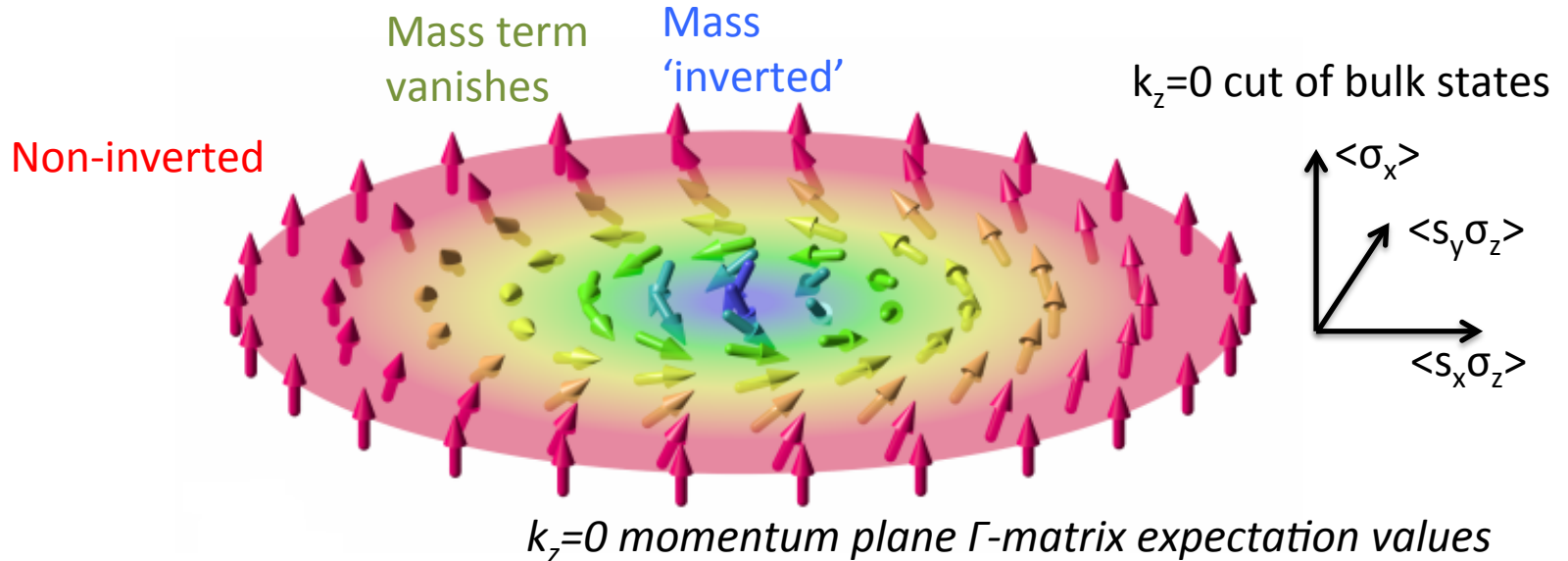


The ALS QERLIN RIXS beamline will map an extra dimension of energy





# The simplest TI bulk picture:



Near the BZ center:

$$H_0(\mathbf{k}) = m\sigma_x + v(k_x\sigma_zs_y - k_y\sigma_zs_x) + v_zk_z\sigma_y$$

orbital x (mass)
spinful orbital z
orbital y (this term is debated)

At larger momenta, the **mass** (parity) term flips sign. The **spinful orbital** term turns spin chirality into a good quantum number.

Alternatively:  $H_0 = m\Gamma_0 + v(k_x\Gamma_1 + k_y\Gamma_2) + v_zk_z\Gamma_3$

Where could you find this kind of basis/model?  
 Leading answers come from **Haldane, Kane & Mele**,  
**S-C Zhang, R. Cava and M. Z. Hasan/H. Lin**)

