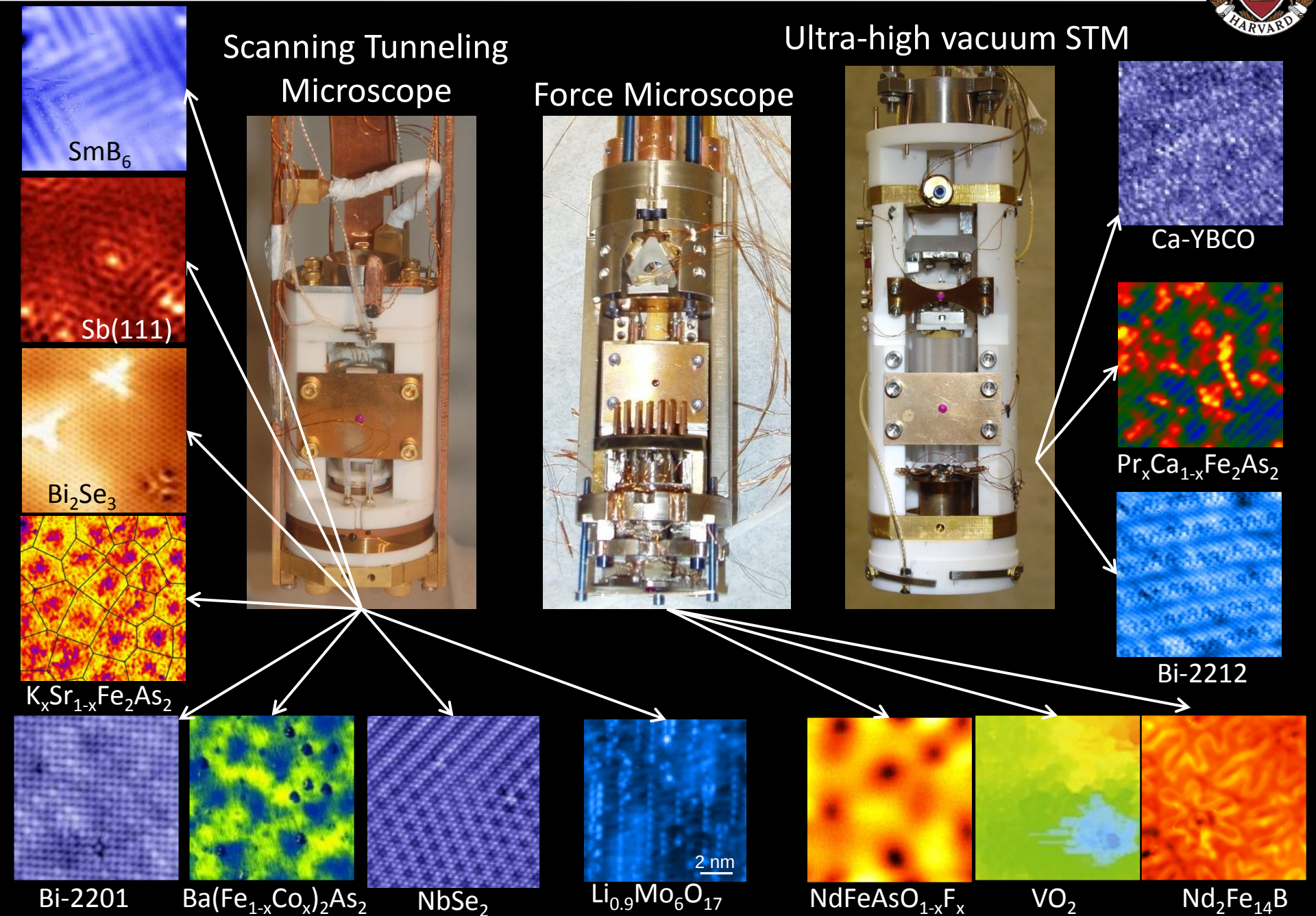
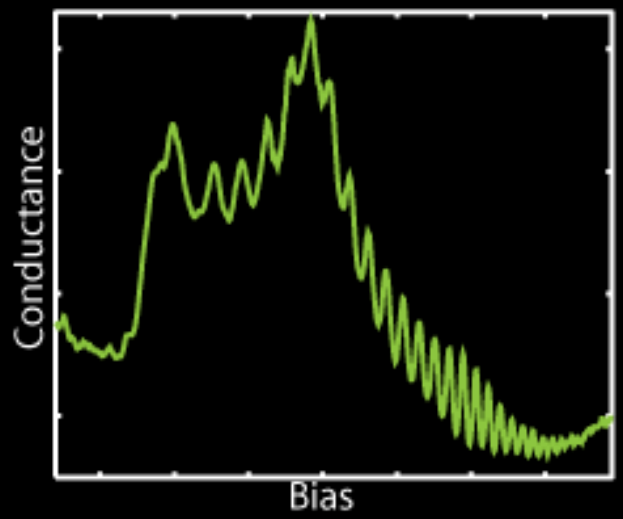
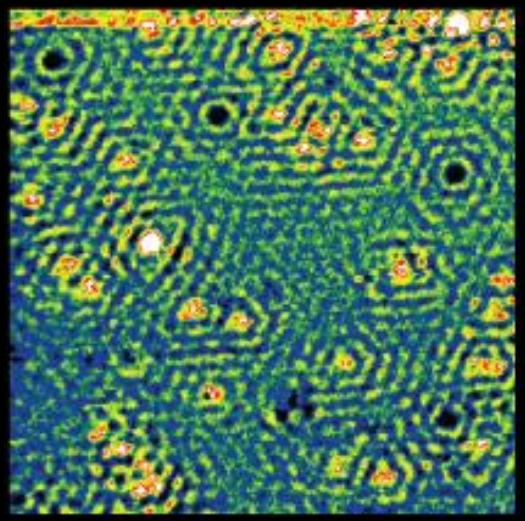
Hoffman Lab Microscopes



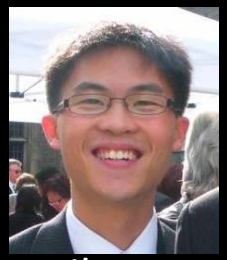
Nanoscale Imaging of Topological Materials: Sb and SmB_6

Jenny Hoffman





Experiments:


Mike Yee


Anjan Soumyanarayanan


Yang He


Jason Zhu

(Harvard)

Samples:

Sb: Dillon Gardner, Young Lee

SmB_6: Dae-Jeong Kim, Zach Fisk

Theory:

Hsin Lin, Arun Bansil

Jay Sau, Anton Akhmerov, Bert Halperin

Funding:

Agency for Science, Technology and Research SINGAPORE

NSERC CRSNG

NSF

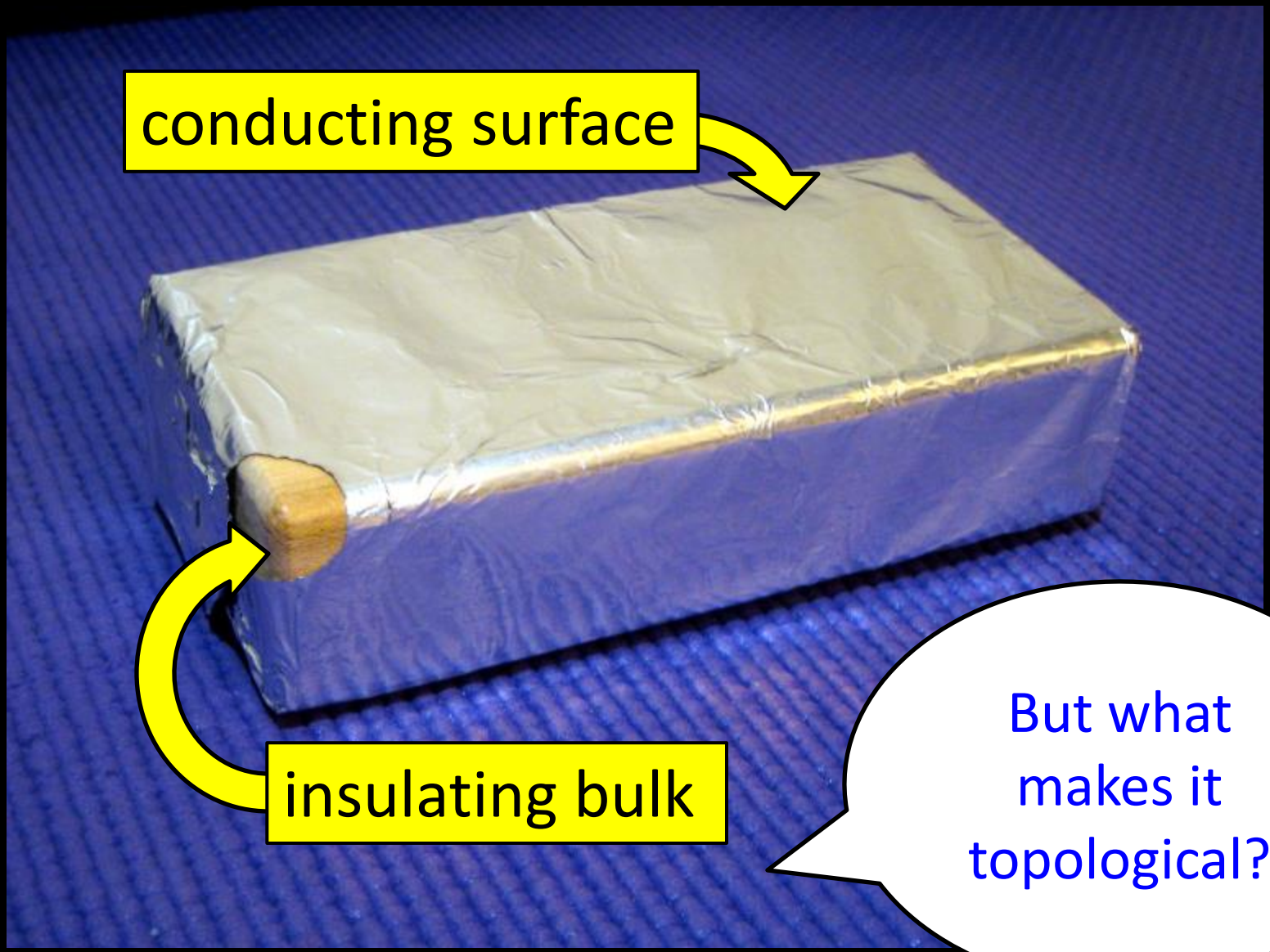
VE RI TAS HARVARD

Outline

- Topological Insulators
- Scanning Tunneling Microscopy
- Nanoscale Band Structure
- Topological: Sb
- Insulator: SmB_6

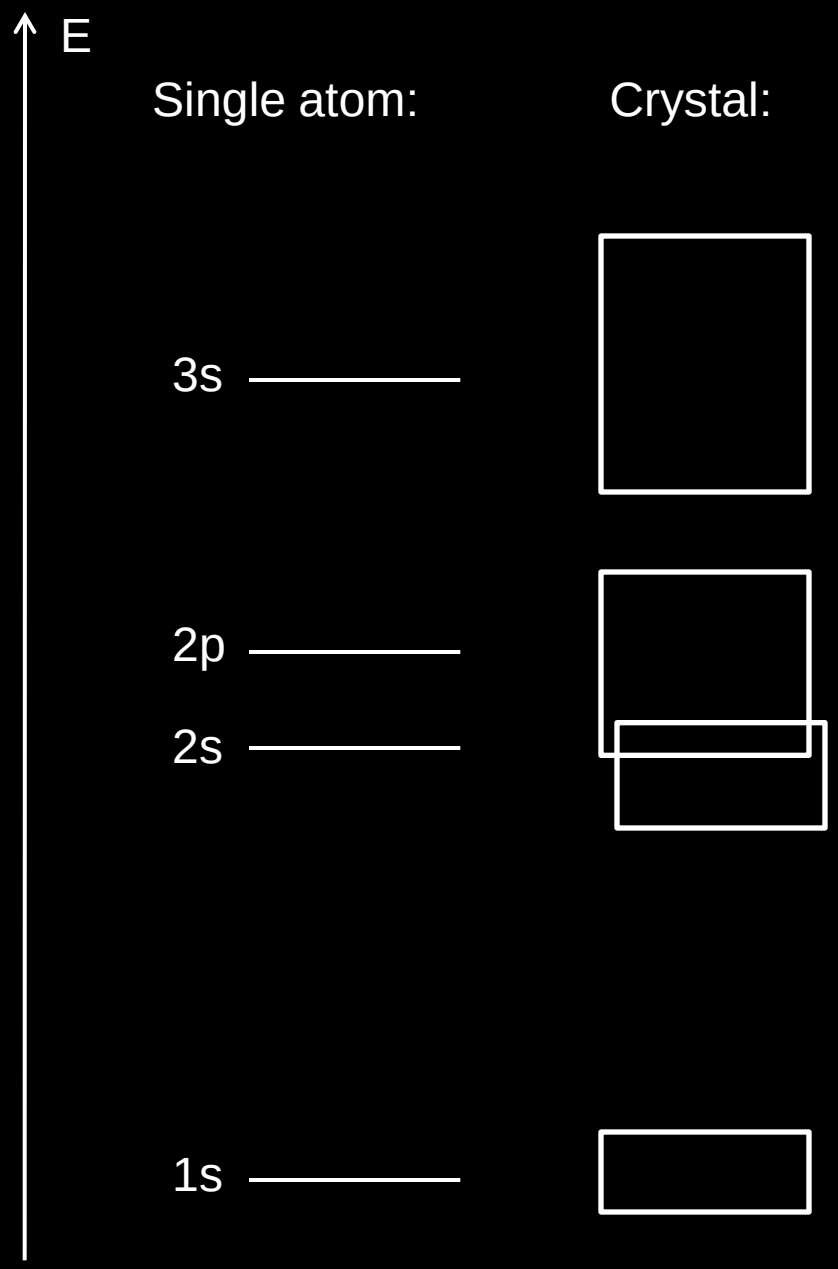
My kids asked me…

A topological insulator is a material with…

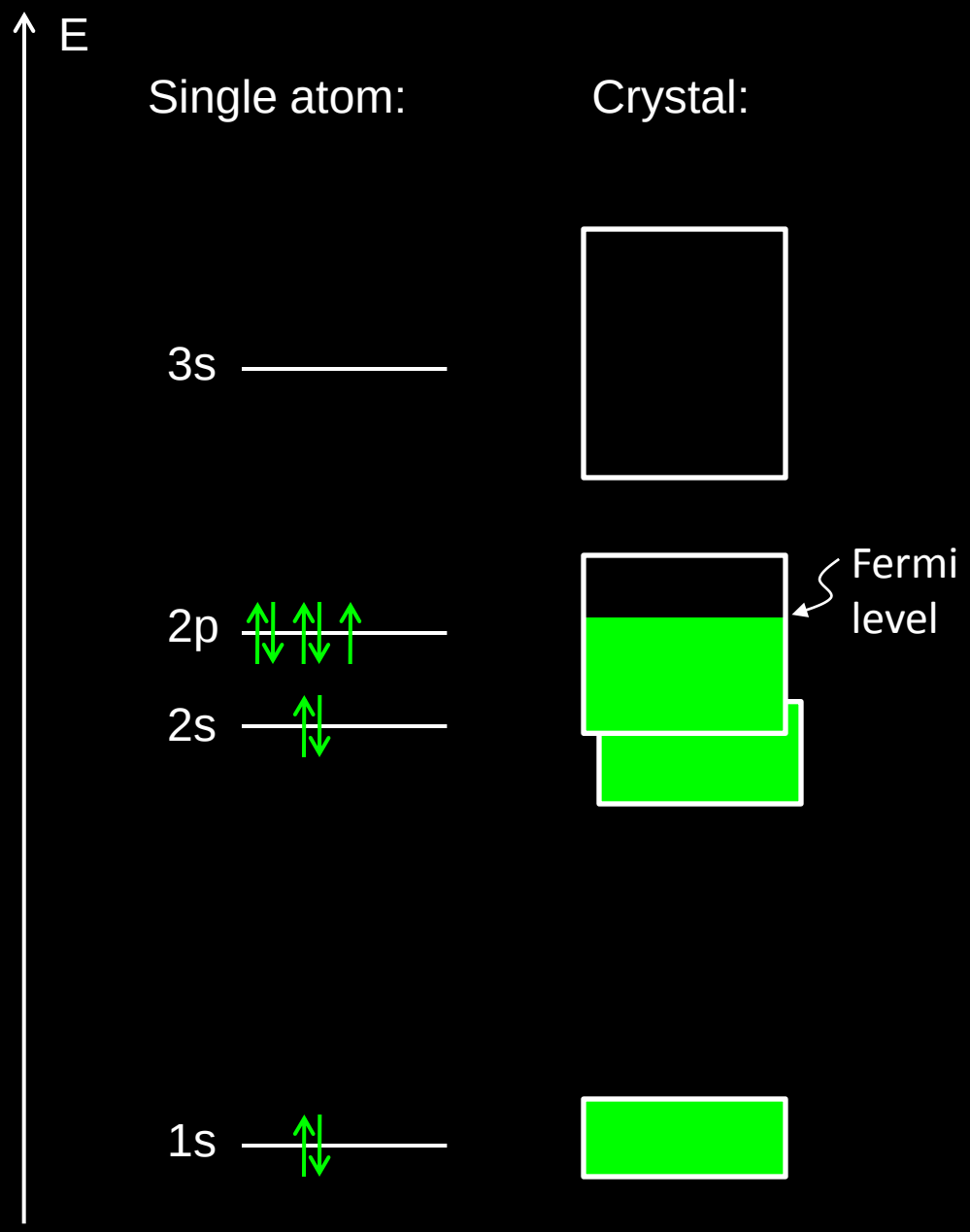


But what makes it topological?

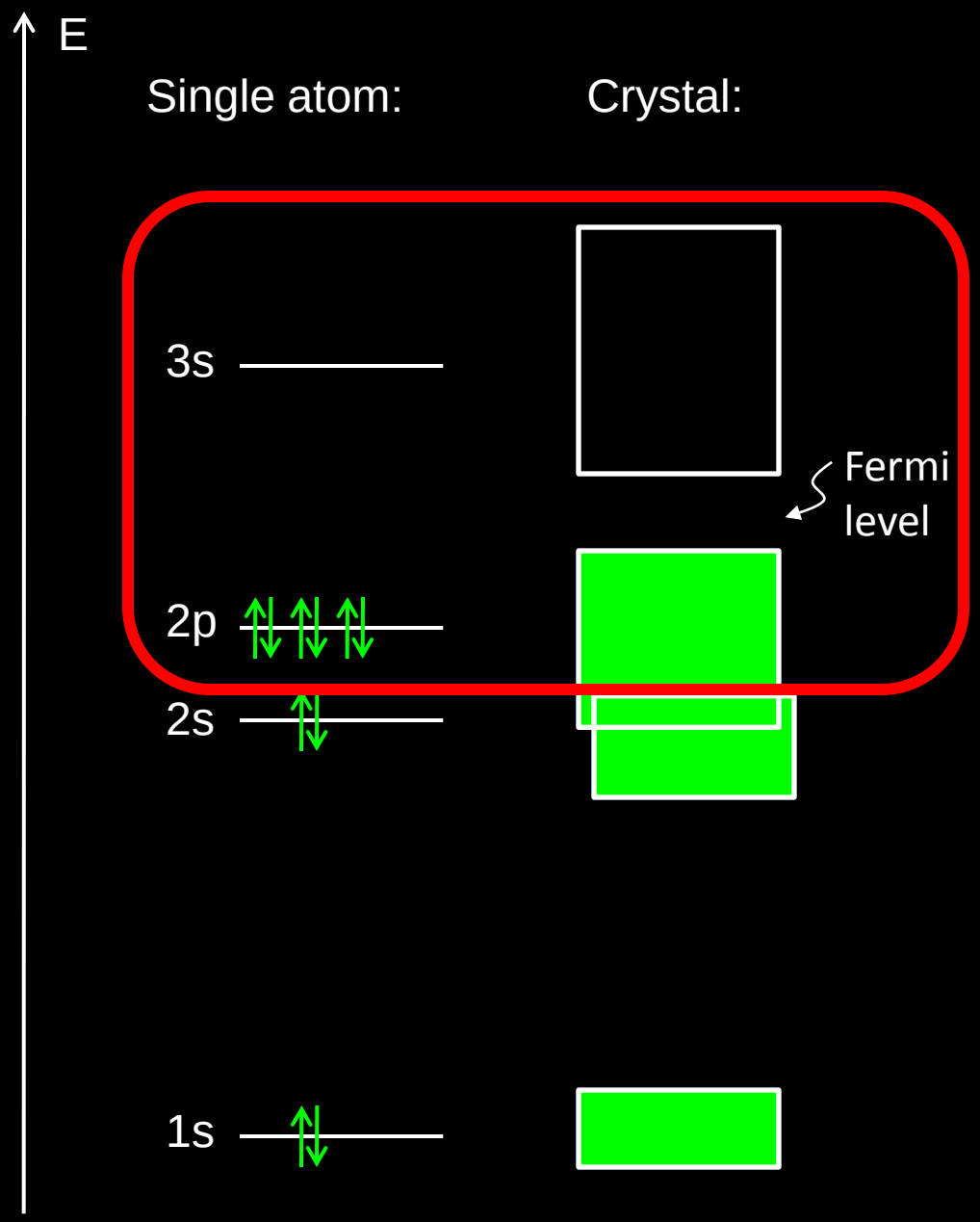
Band Theory



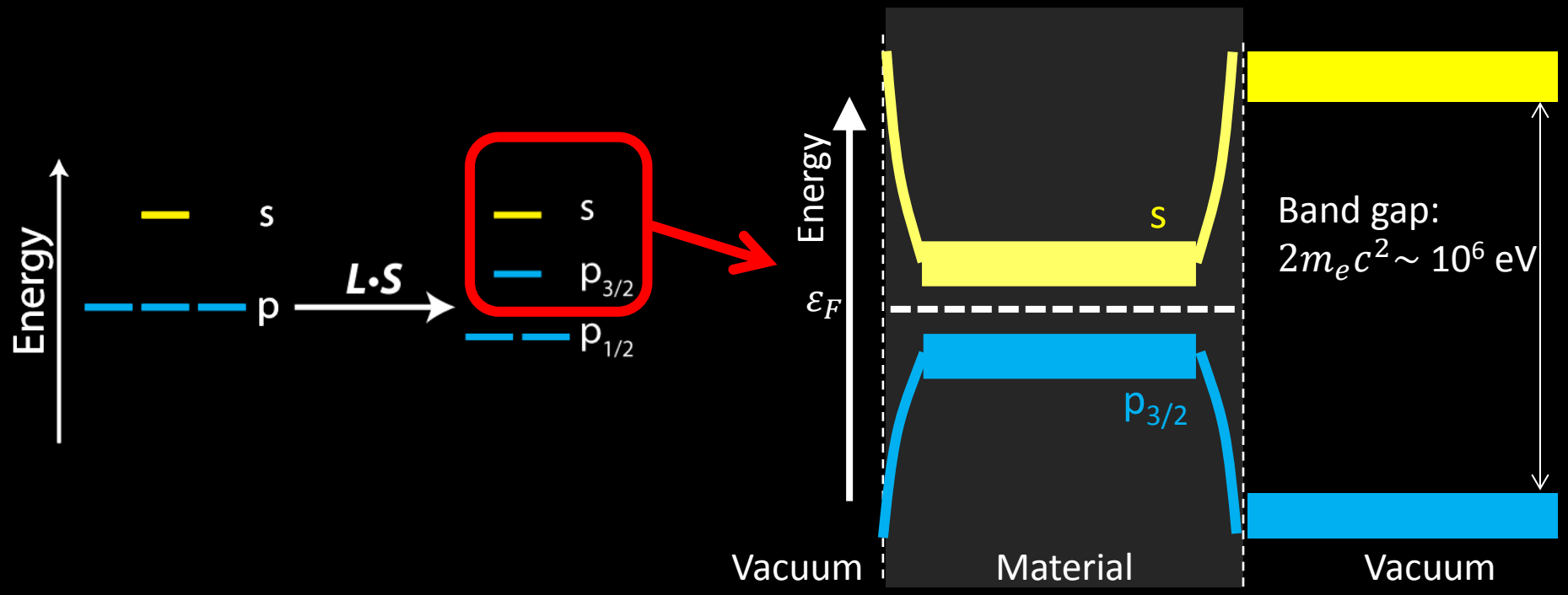
Band Theory: Metal



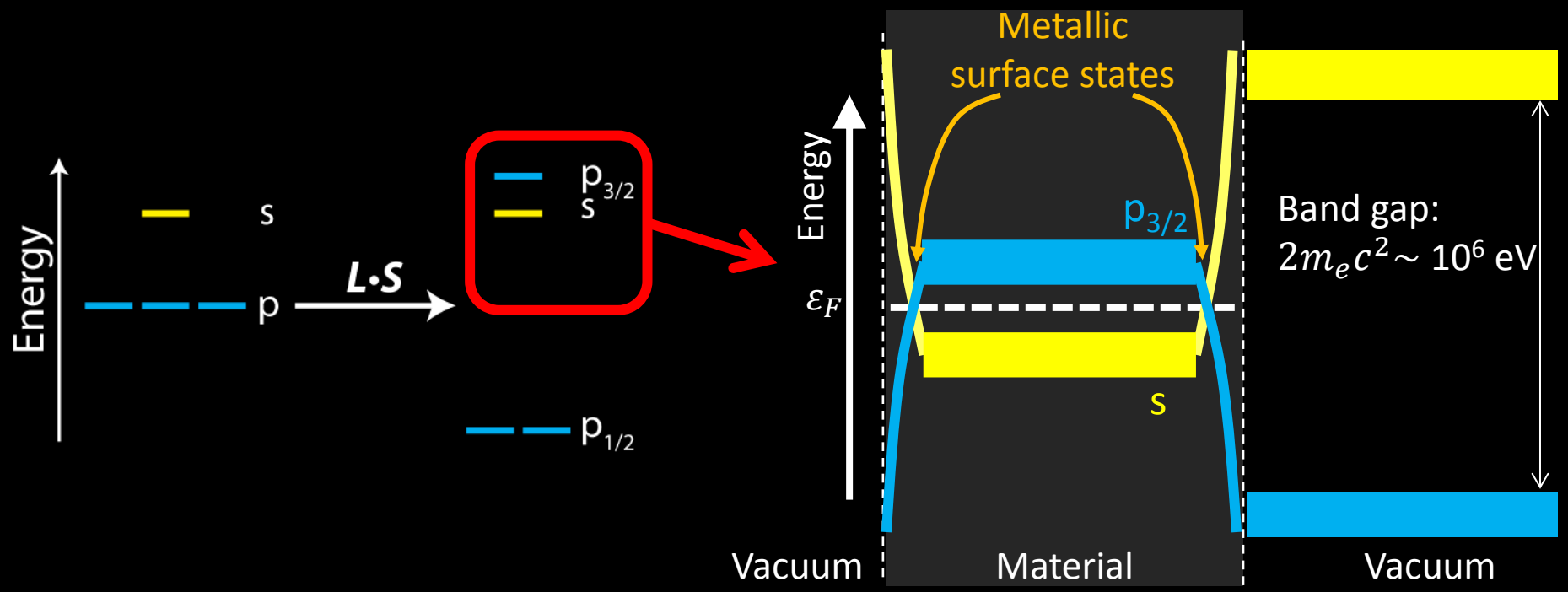
Band Theory: Insulator



Spin-Orbit Coupling → Band Inversion



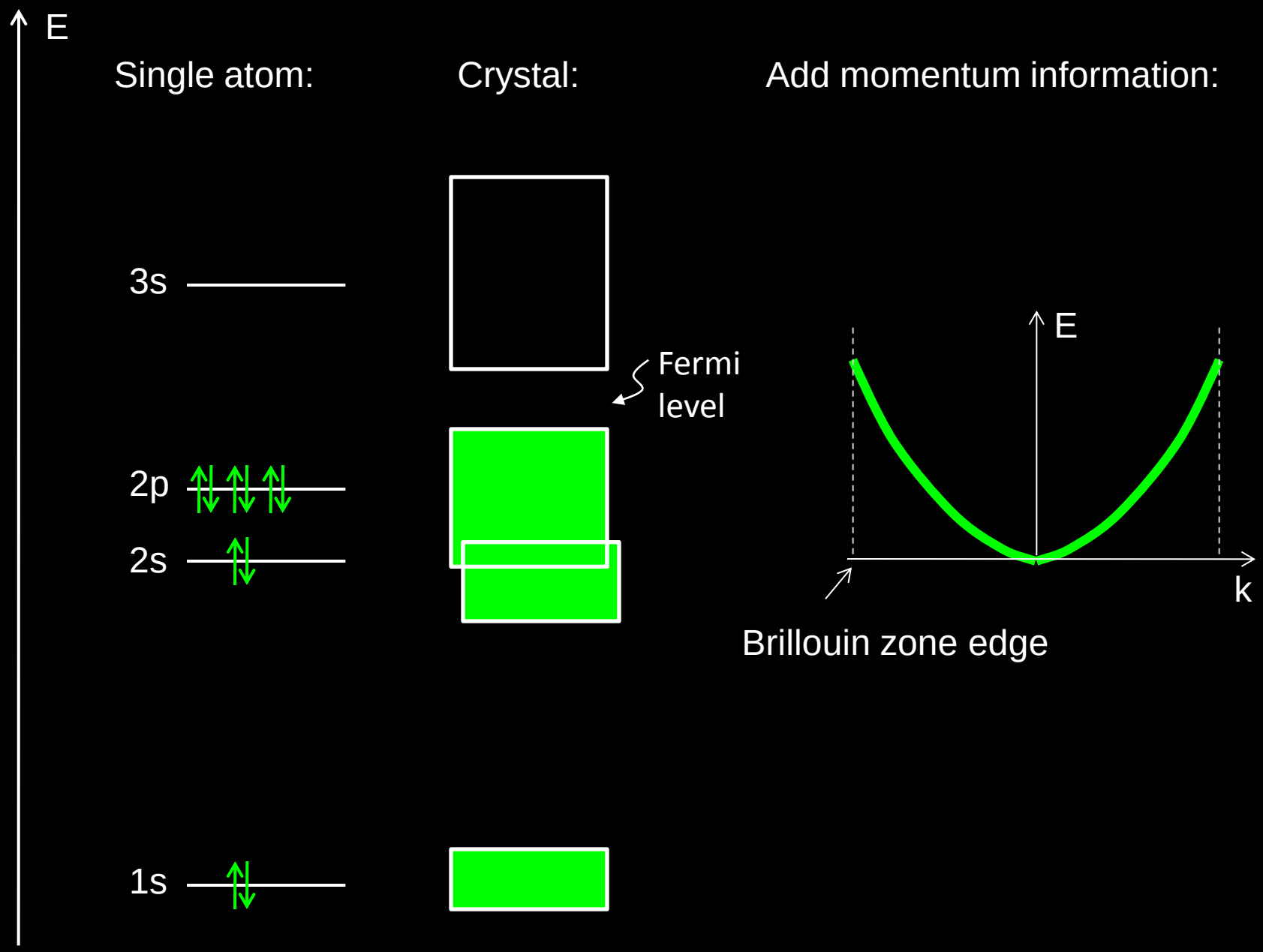
Spin-Orbit Coupling → Band Inversion



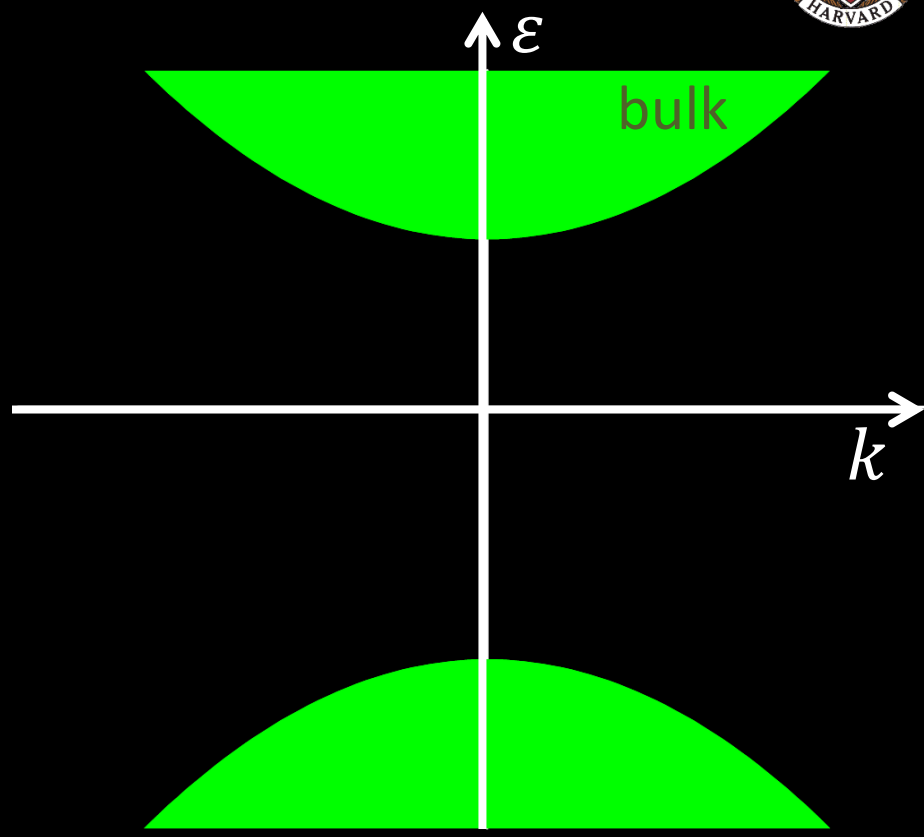
→ topologically protected spin-polarized surface states

Why spin-polarized?

Band Theory: Insulator



Spin-Polarized Surface State Hamiltonian



Spin-Polarized Surface State Hamiltonian

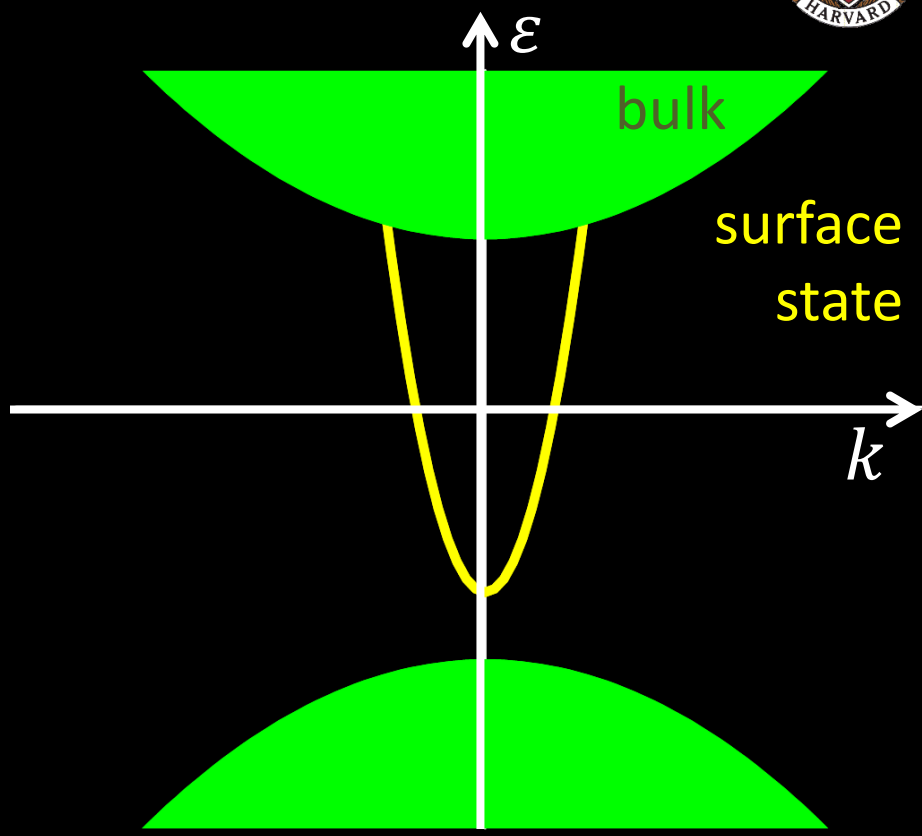
0. Free electrons in 2 dimensions:

$$H = E_0 + \frac{k^2}{2m^*}$$

1. Rashba: Surface breaks symmetry

$$H_R = Ez$$

2. Moving electron with velocity v sees E-field as $B \propto v \times E$



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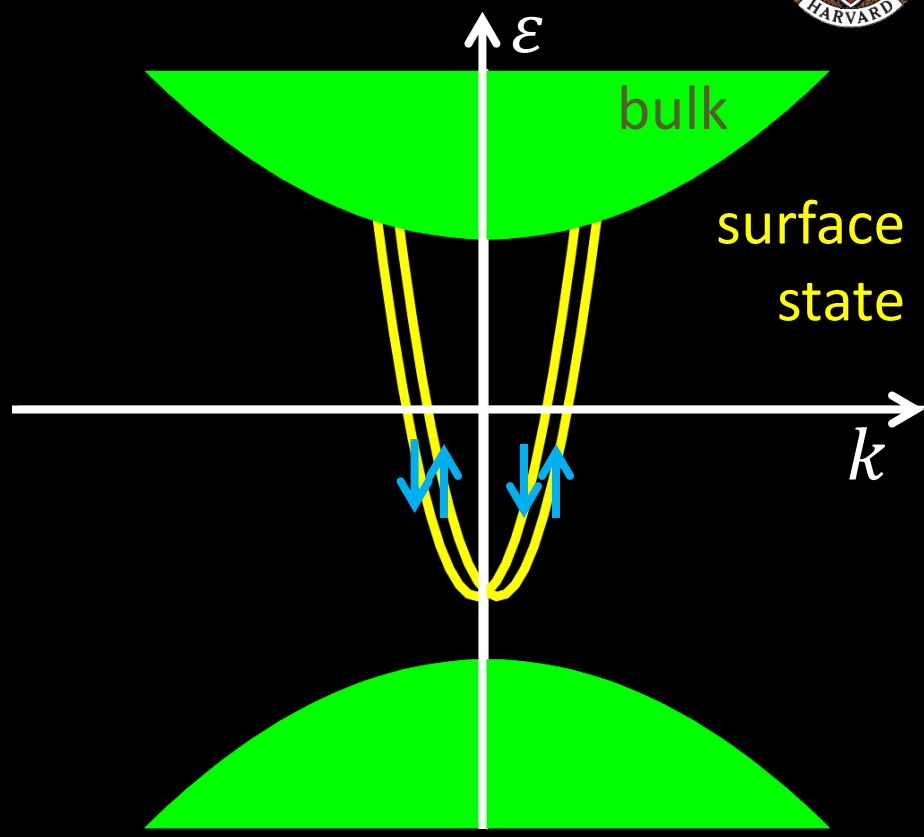
3. Spin-orbit coupling splits bands:

$$H_{SO} \propto (v \times E) \cdot \sigma$$

momentum

spin



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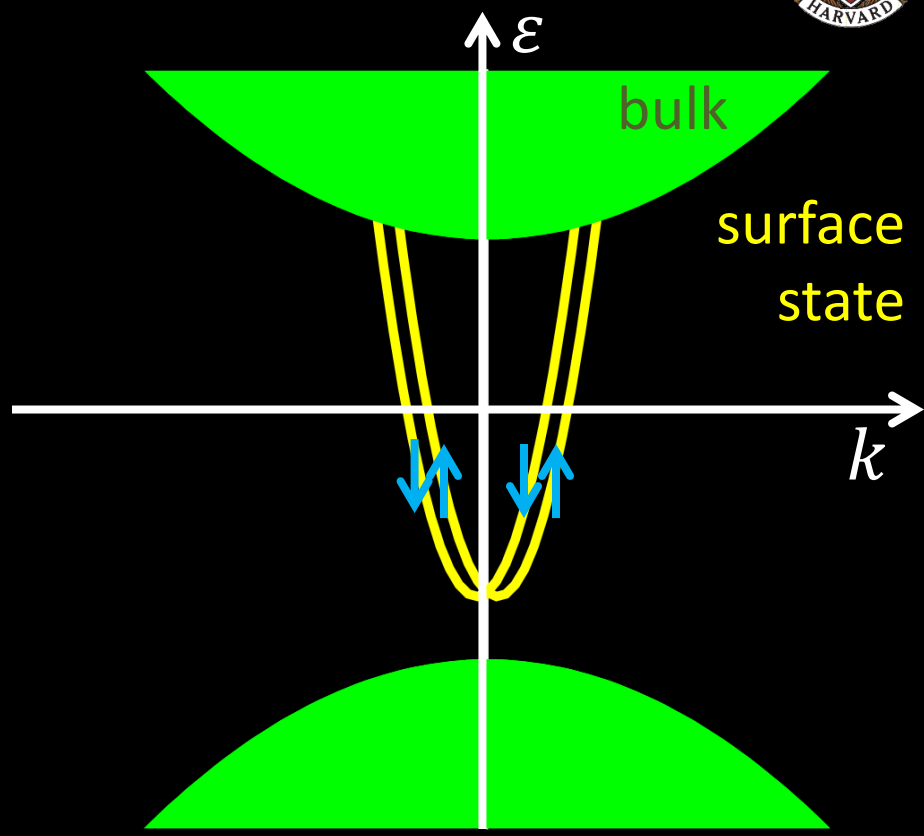
4. $k \cdot p$ theory: expand in small k around Γ point

$$H = E_0 + \frac{k^2}{2m^*} + v(k_x\sigma_y - k_y\sigma_x)$$



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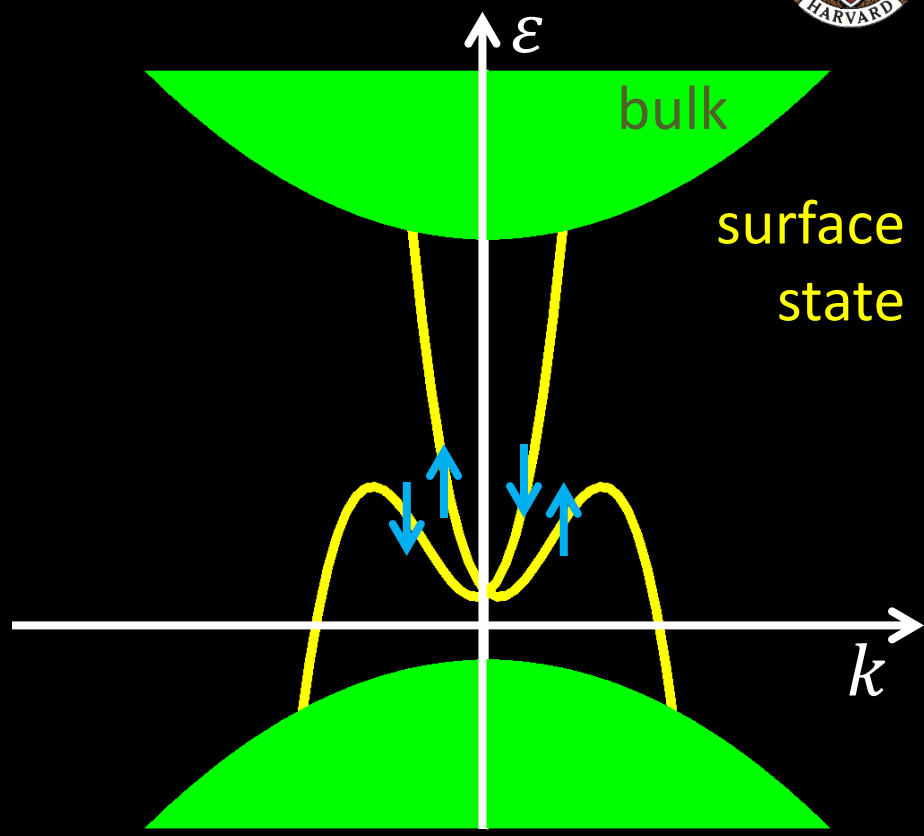
$$H = E_0 + \frac{k^2}{2m^*} + (v_0 + \alpha k^2)(k_x \sigma_y - k_y \sigma_x)$$

new term to bend band down



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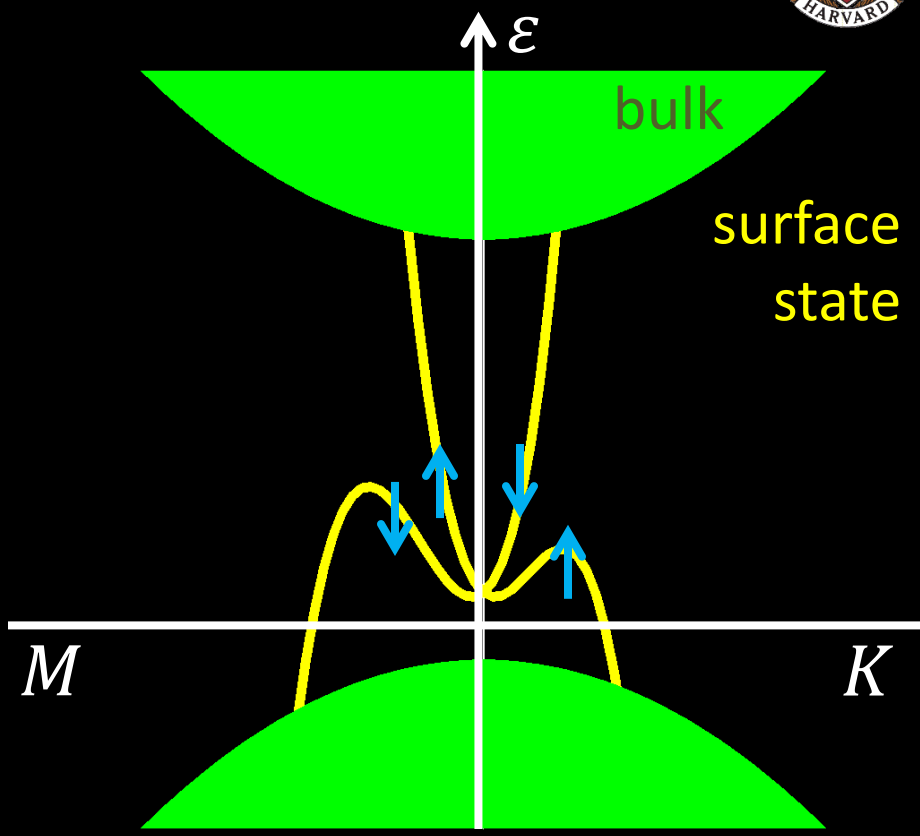
momentum spin



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crystal symmetry

Spin-Polarized Surface State Hamiltonian

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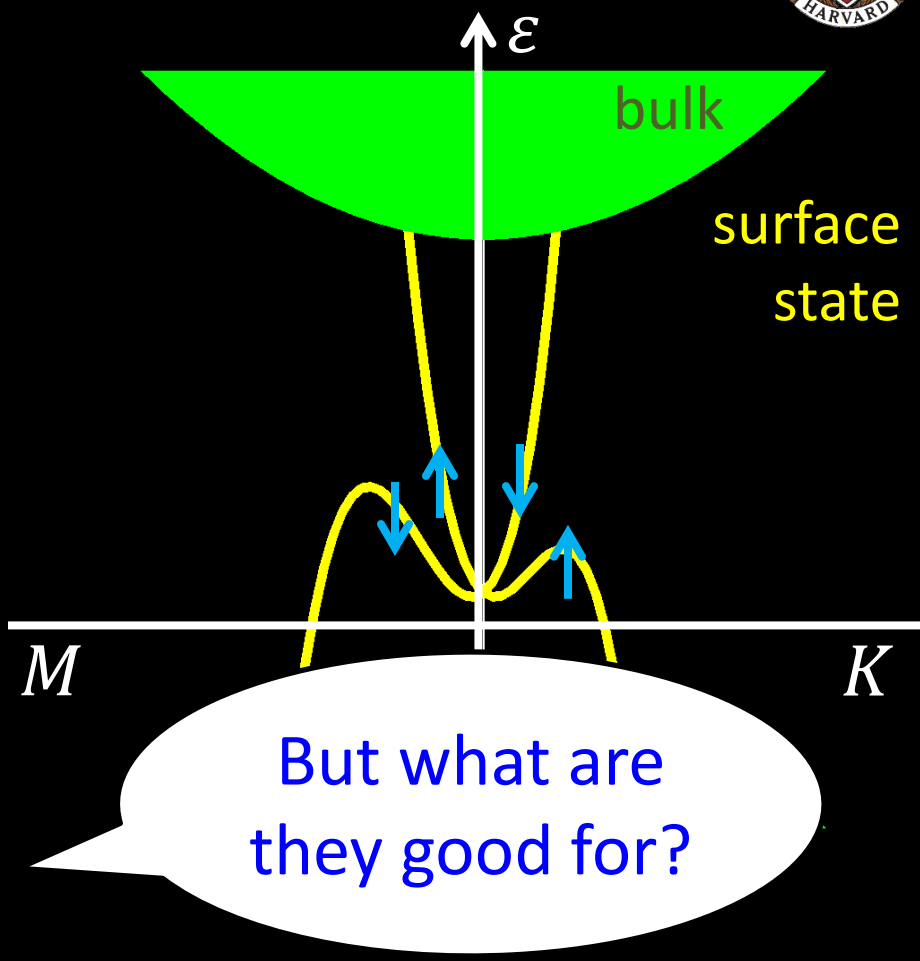
momentum spin



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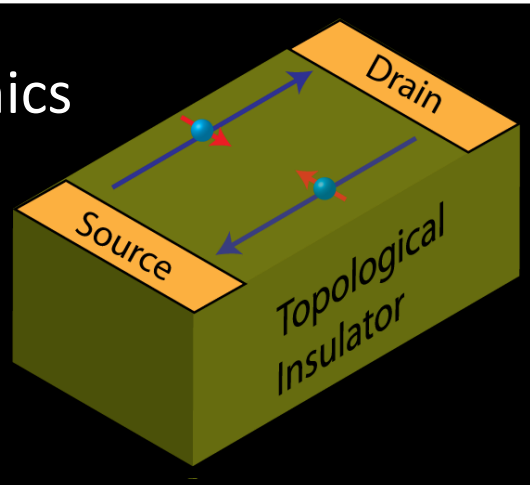
Liang Fu's 5-parameter Hamiltonian [PRL 101, 266801 (2009)]

Applications of Topological Insulators

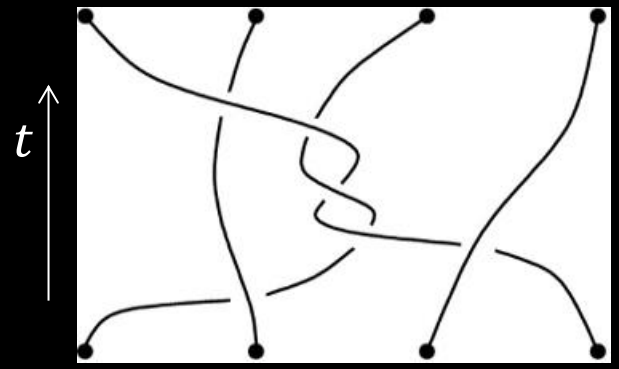
1. Spintronics



How can we realize these applications?

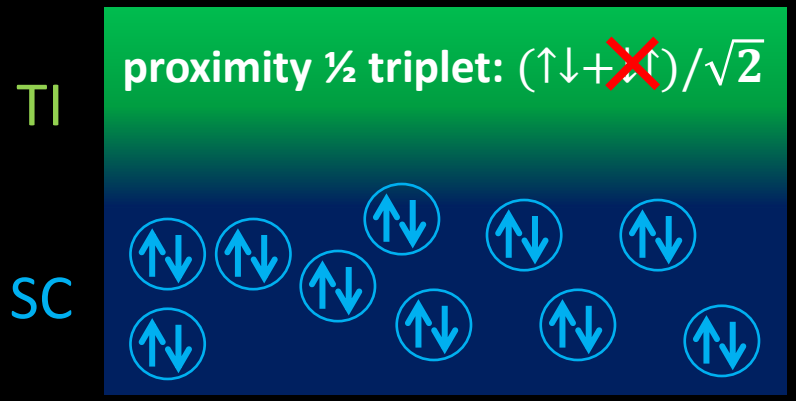
2. Topological quantum computing

Majorana fermion = self-antiparticle
(non-Abelian anyon)



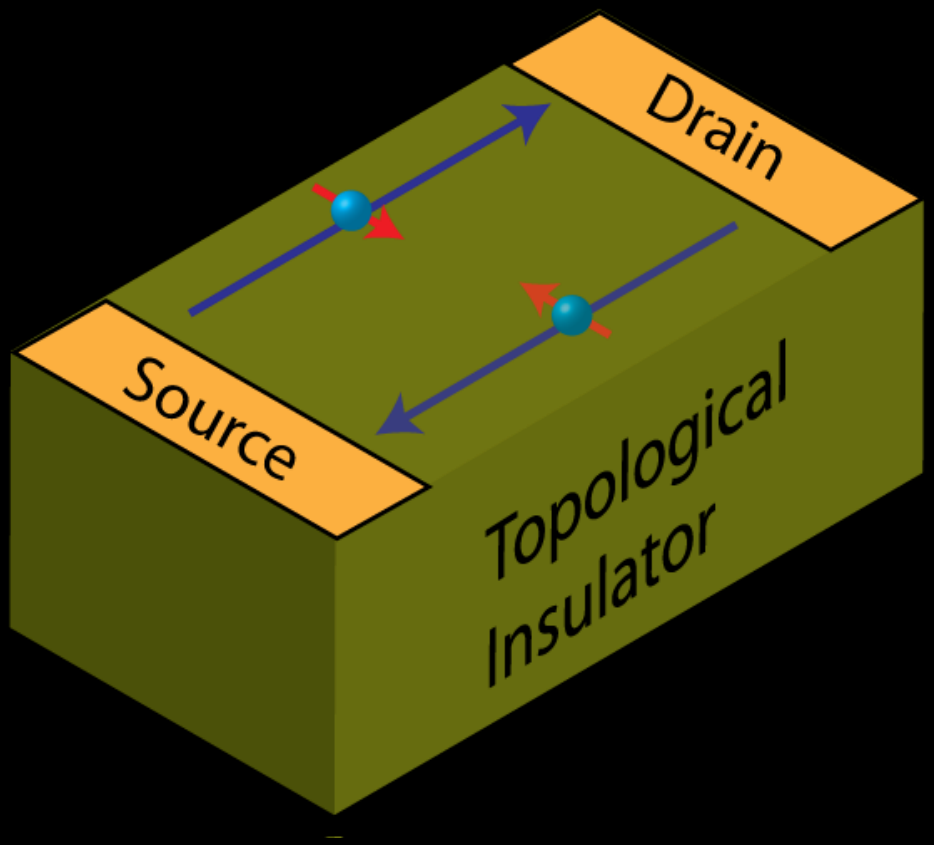
"braid" the world-lines
→ information is encoded topologically

Topological-superconductor interface



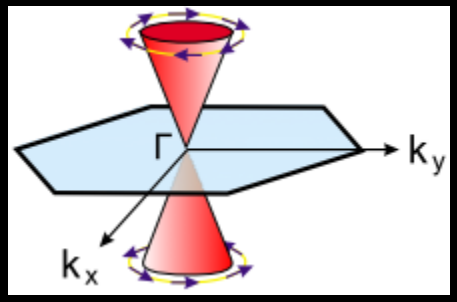
Fu & Kane, PRL 100, 096407 (2008)

Metrics for topological spintronics devices



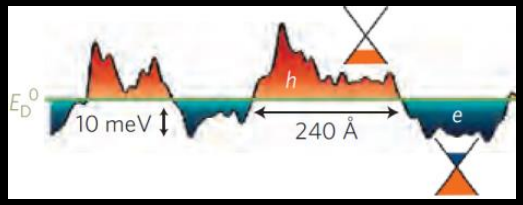
1. Enhance spin-momentum locking

Metric: Spin-Orbit Coupling (v_0)



2. Reduce scattering

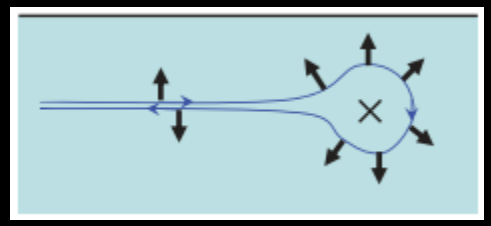
Metric: Mean Free Path (l_f)



H. Beidenkopf, Nat. Phys. 2011

3. Reduce vulnerability to external B & magnetic impurities:

Metric: *g*-factor

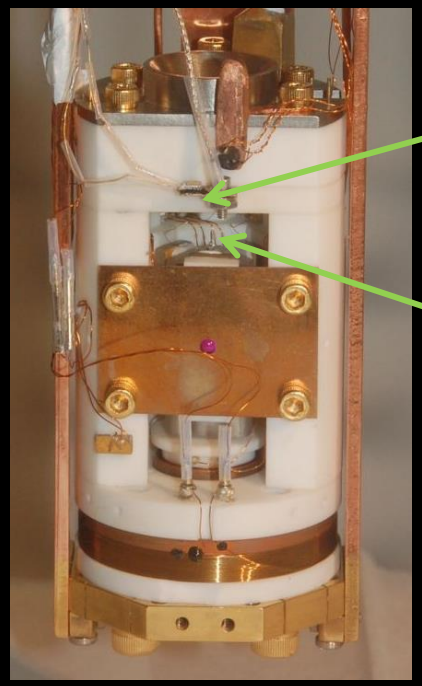


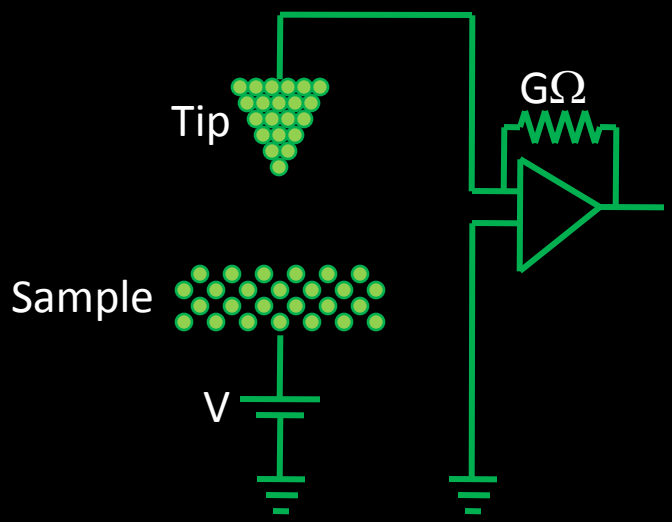
Need a probe which measures:
nanoscale, B-dependent, filled & empty states…

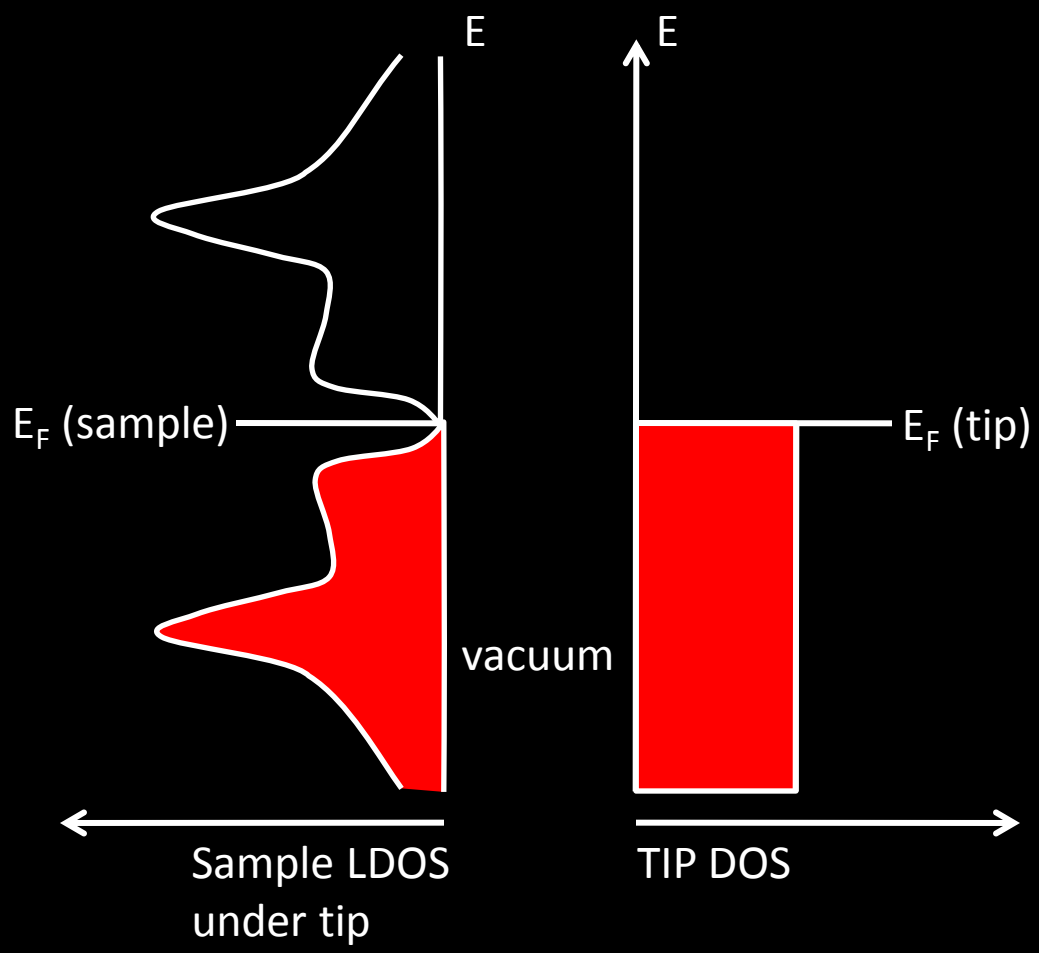
Outline

- Topological Insulators
- Scanning Tunneling Microscopy
- Nanoscale Band Structure
- Topological: Sb
- Insulator: SmB_6

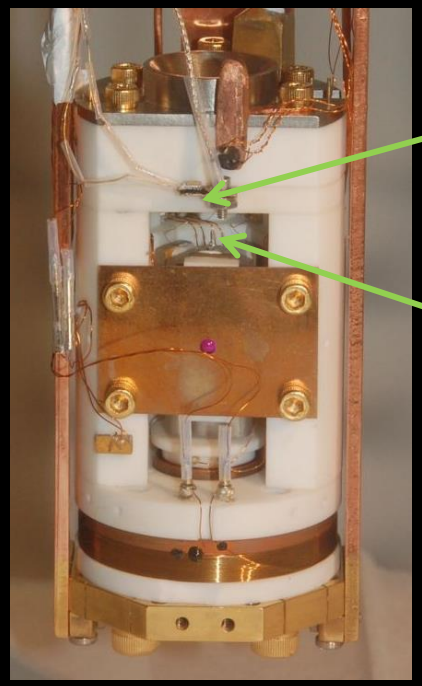
Scanning Tunneling Microscopy



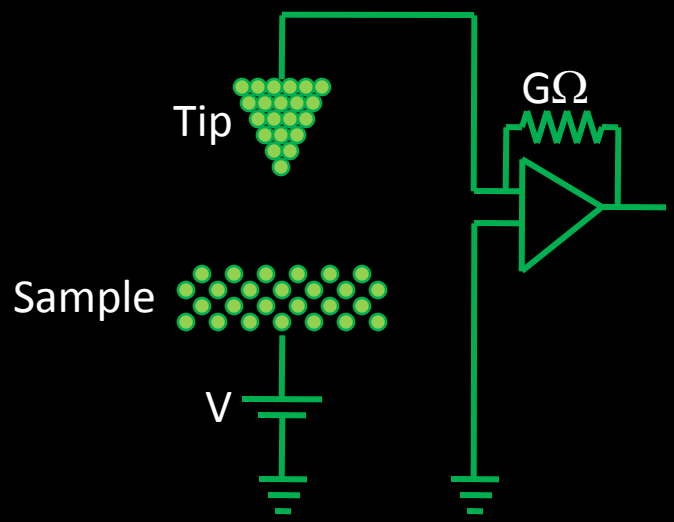


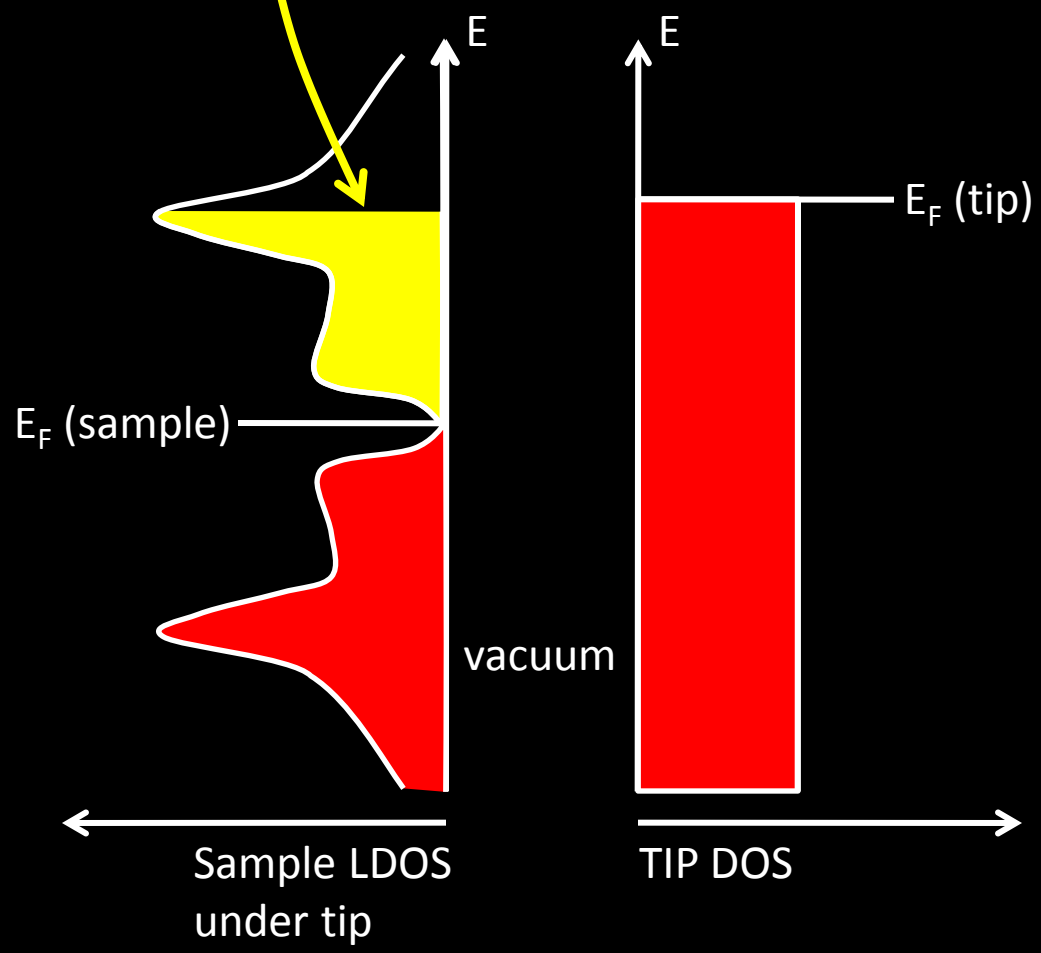


Scanning Tunneling Microscopy

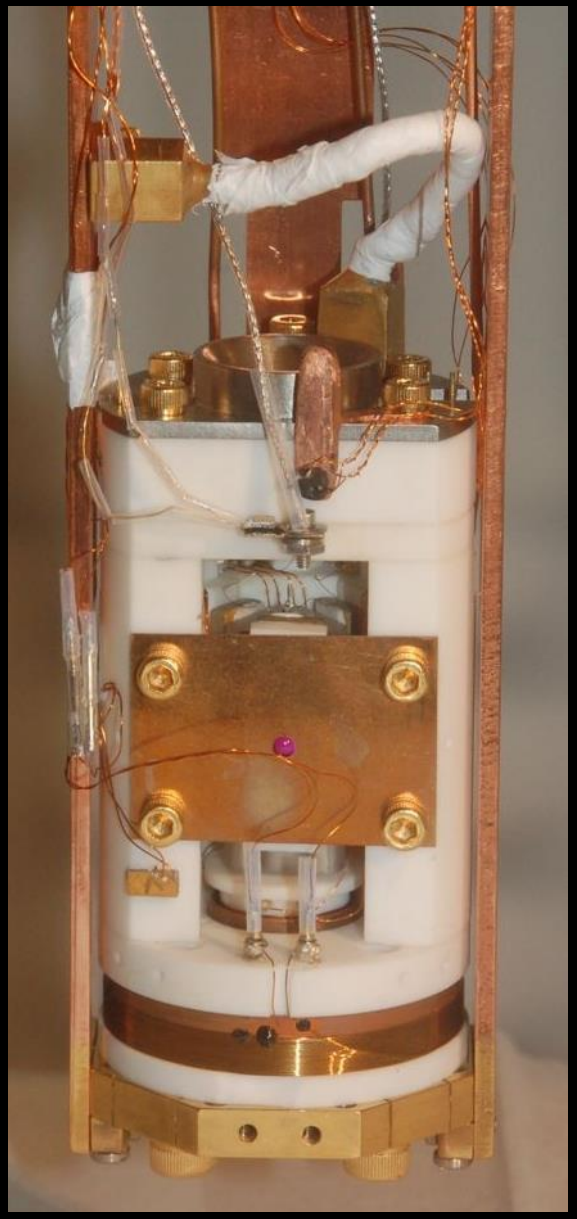


$$I(V) \propto \int_{E_F}^{eV} \mathrm{LDOS}(E)\,dE$$

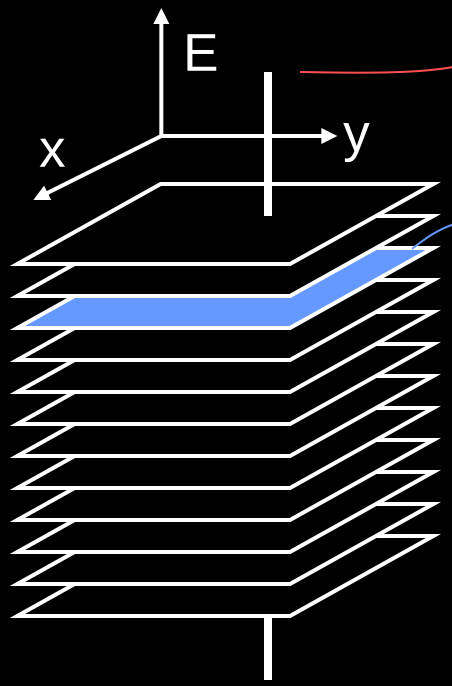




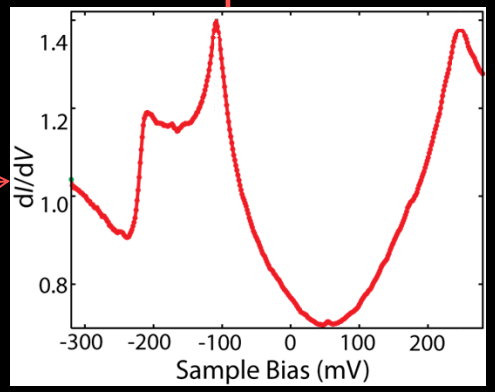
Types of STM Measurements



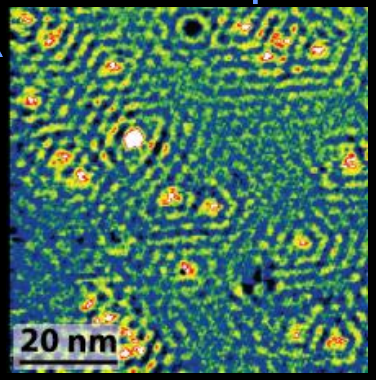
Local Density of States (x, y, E)



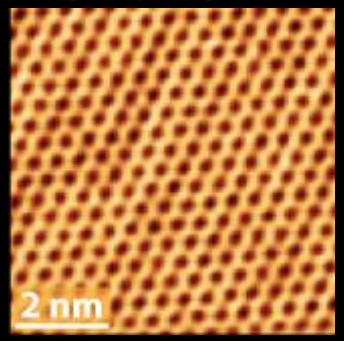
dI/dV Spectrum



dI/dV Map



Topography

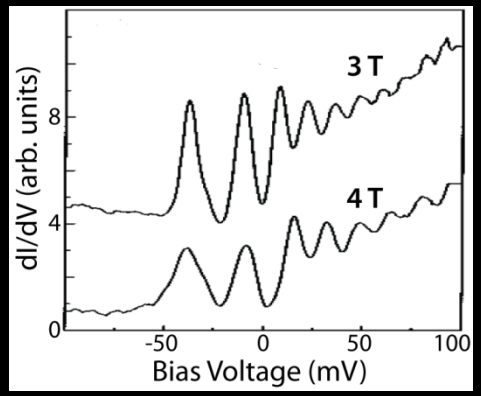


Constant current mode:

$$\int \frac{dI}{dV}$$

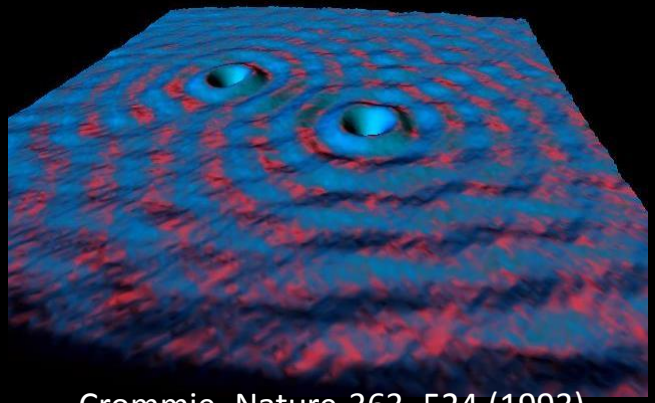
Momentum Information from STM?

Clean Samples → LLs

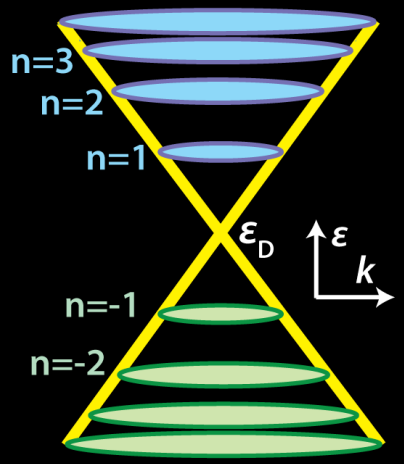


Wildöer, PRB 55, R16013 (1997)

Impurities → QPI

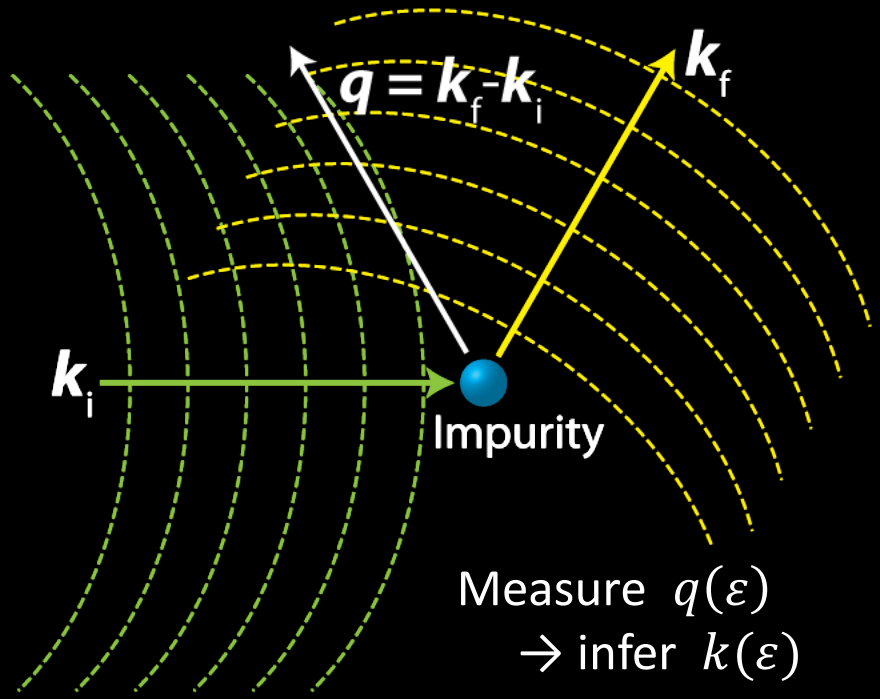


Crommie, Nature 363, 524 (1993)



Dirac dispersion

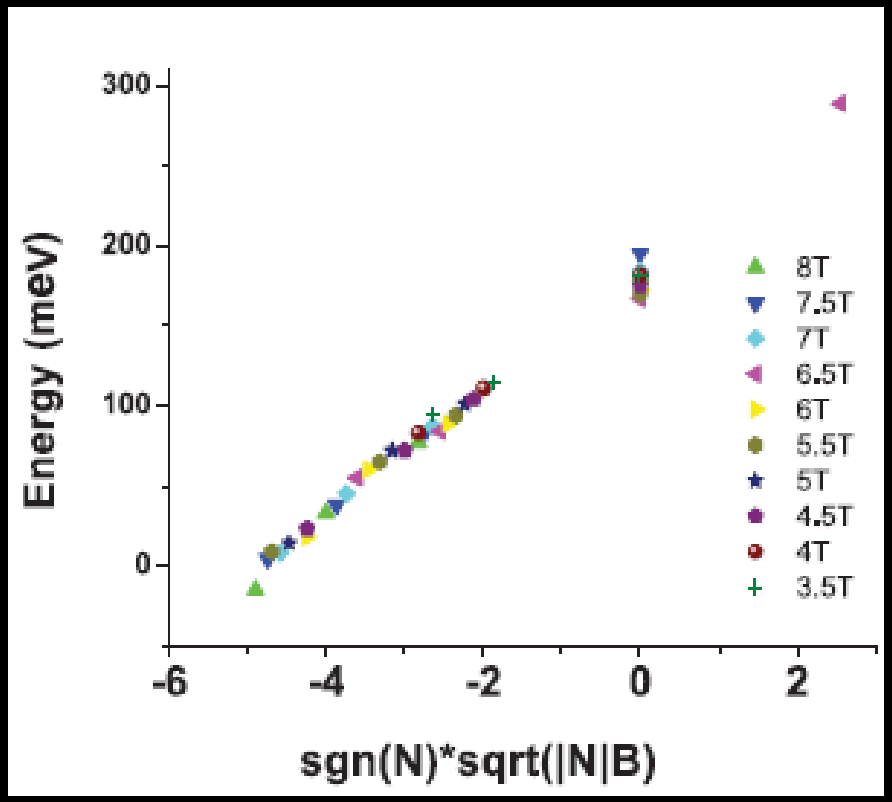
$$\rightarrow \varepsilon_N \propto \sqrt{e\hbar v_F N B}$$



Measure $q(\varepsilon)$
→ infer $k(\varepsilon)$

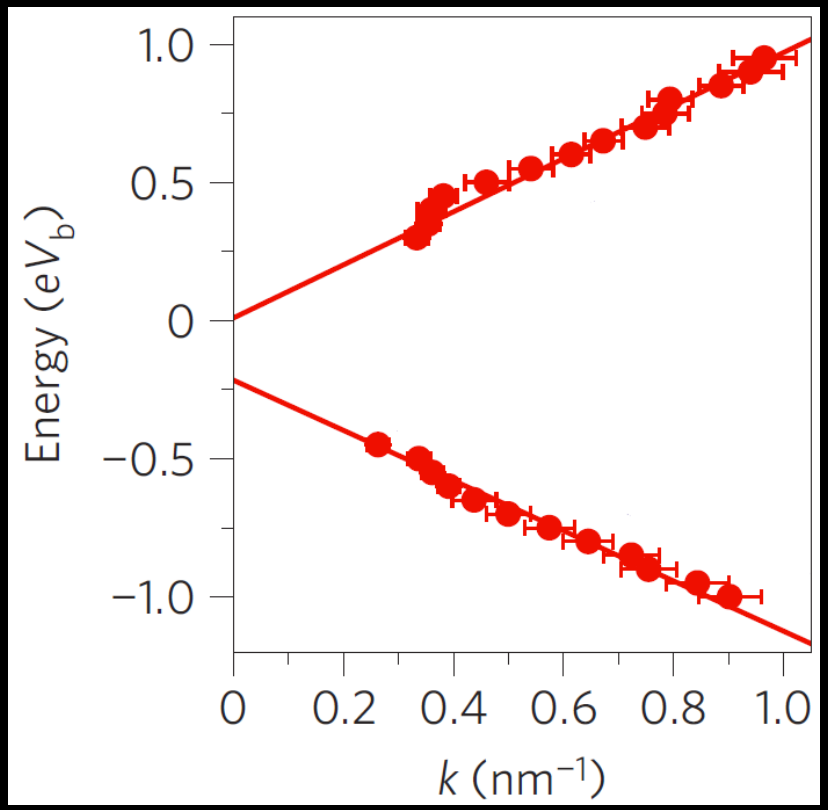
Single Layer Graphene

Landau levels



Luican+Andrei, PRB 83, 041405 (2012)

Quasiparticle interference



Zhang+Crommie, Nat. Phys. 5, 722 (2009)

40% Discrepancy!

$$v_{LL} = 1.07 \times 10^6 \text{ m/s} \longleftrightarrow v_{QPI} = 1.5 \times 10^6 \text{ m/s}$$

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- Topological Insulators
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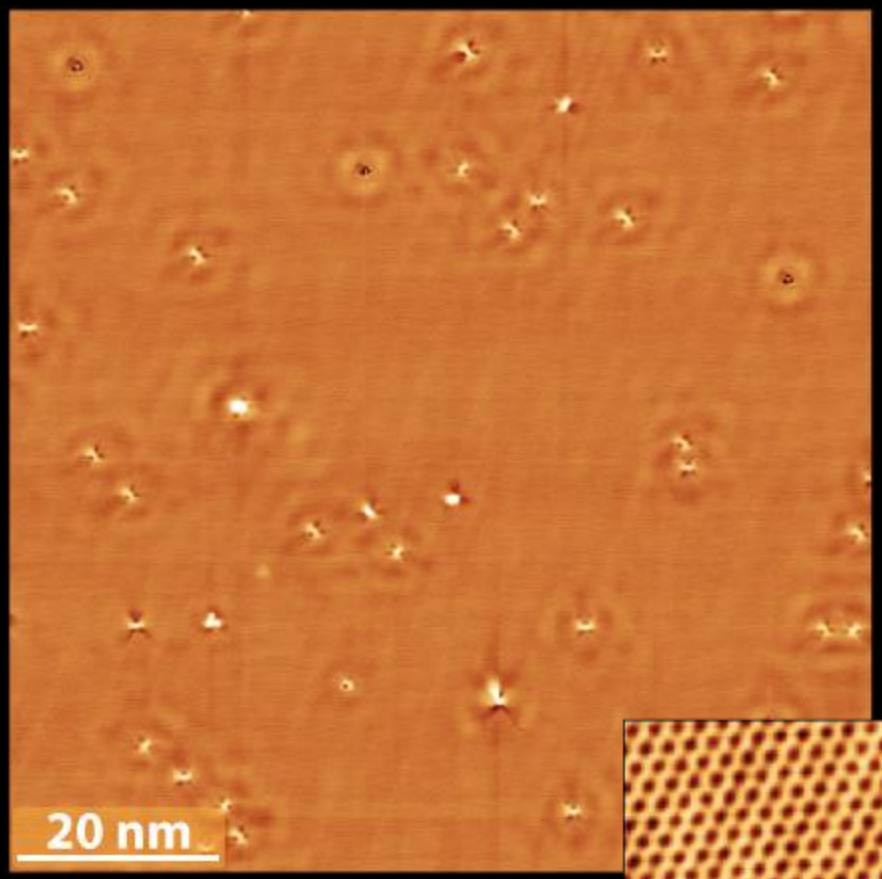
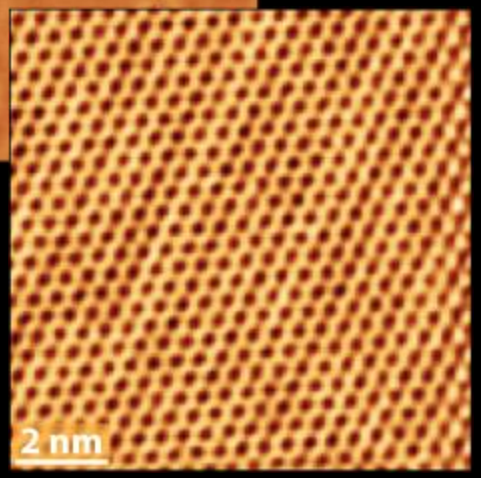
- Topological: Sb
- Insulator: SmB_6

Sb(111): Topography

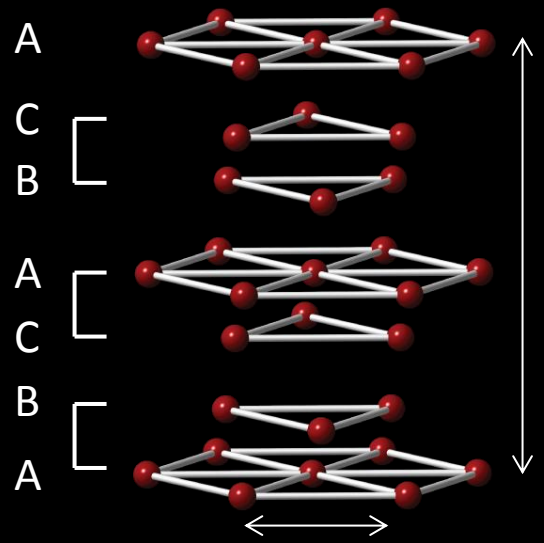


Z: low high

100 mV, 1 GΩ



100 mV, 1/8 GΩ



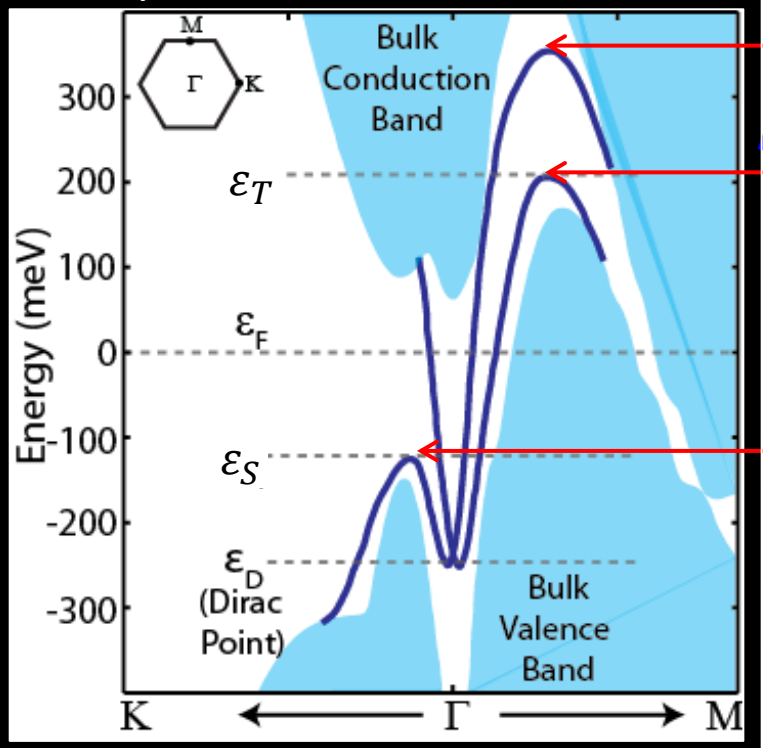
3 bilayers
$c = 11.3$ Å

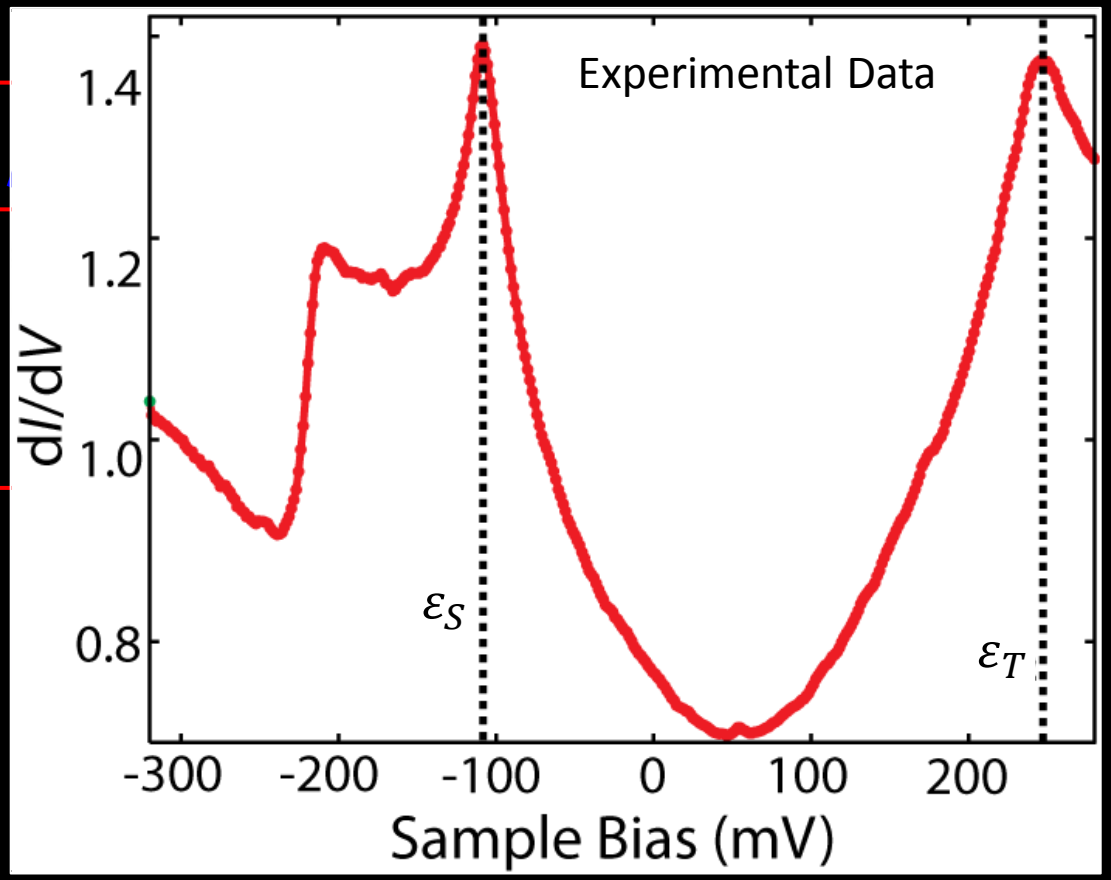
$a = 4.31$ Å

Sb(111): Spectroscopy and Band Structure

Surface states: $H = E_D + \frac{k^2}{2m^*} + (v_0 + \alpha k^2)(k_x\sigma_y - k_y\sigma_x) + \frac{1}{2}\lambda(k_+^3 + k_-^3)$

Theory





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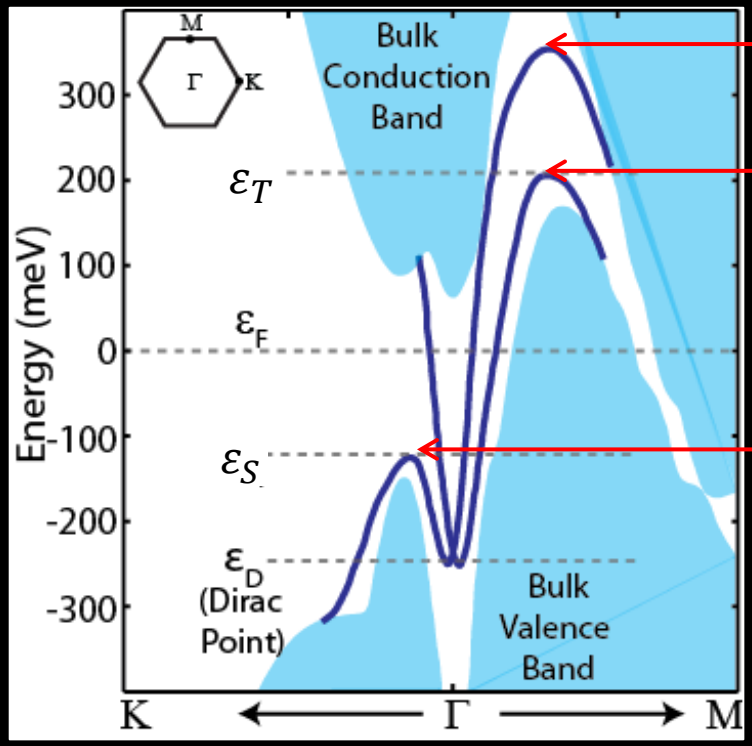
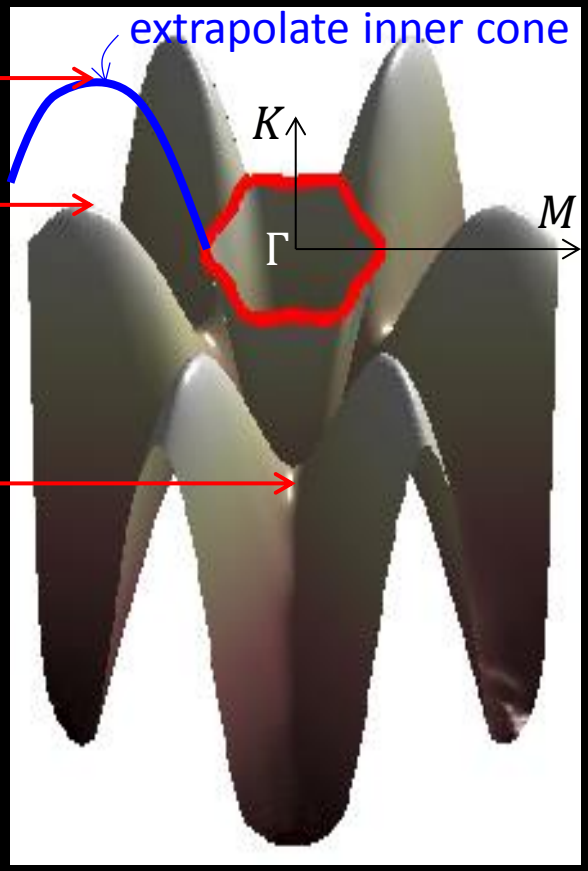
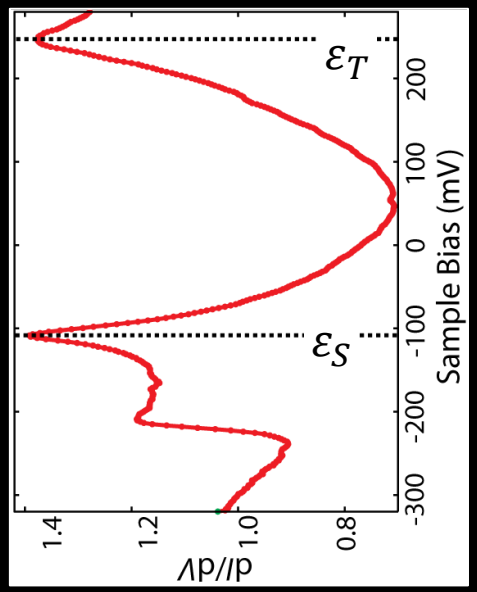
Theory

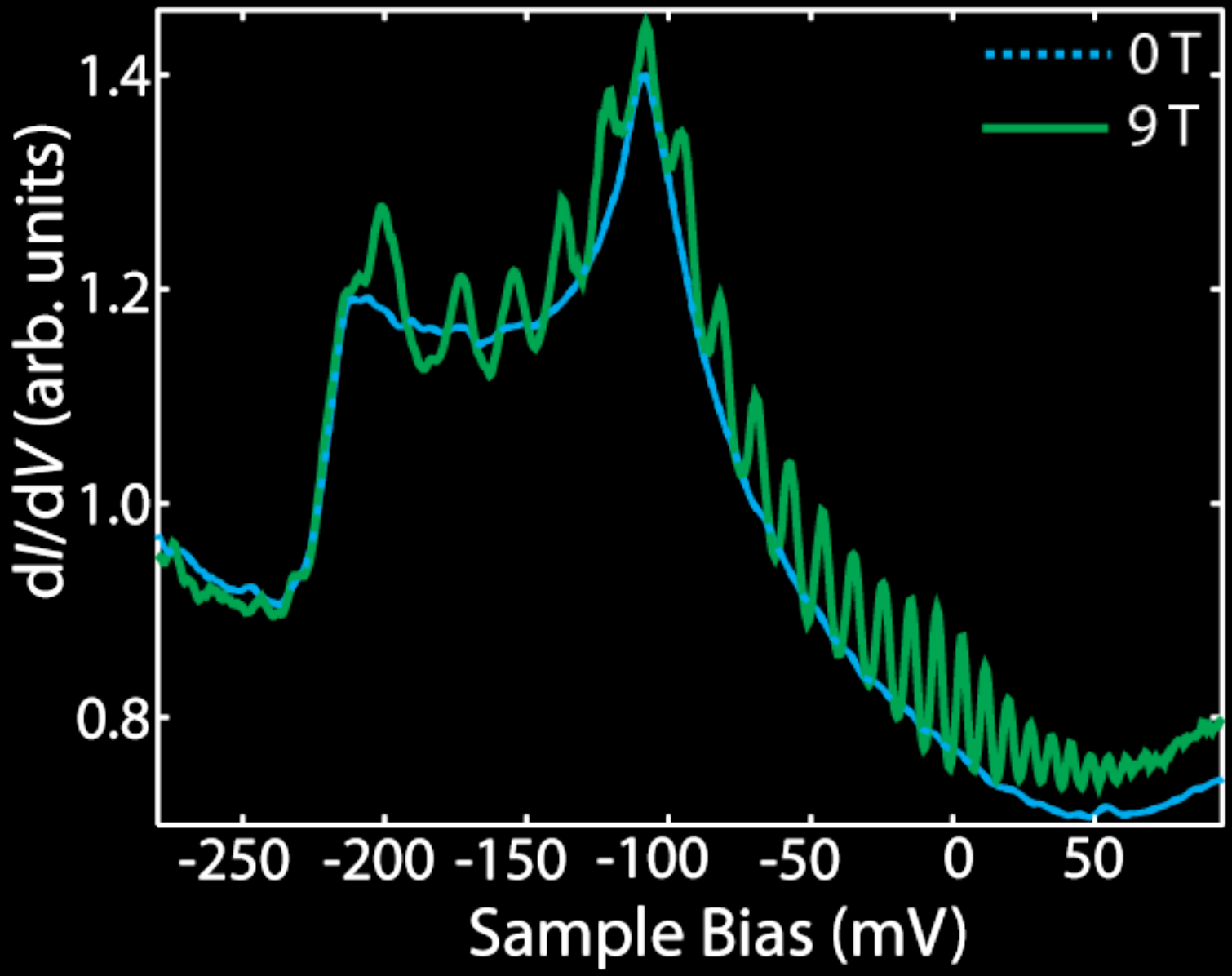




Data



Spectroscopy in Magnetic Field

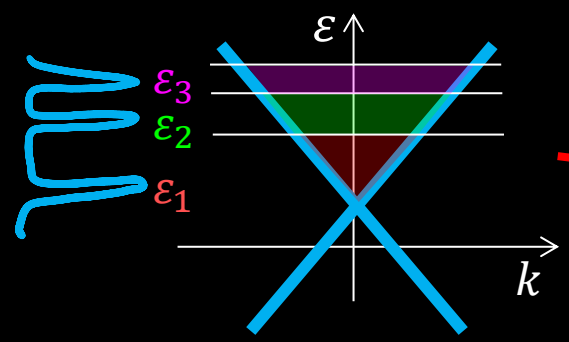


300 mV, 0.5 GΩ
100 mV, 0.2 GΩ

Landau Levels

Dirac Fermions: $\varepsilon = \hbar v_F k$

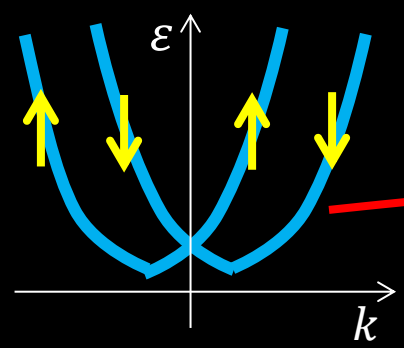
$$\varepsilon_N = \varepsilon_D + \sqrt{e\hbar v_F N B}$$

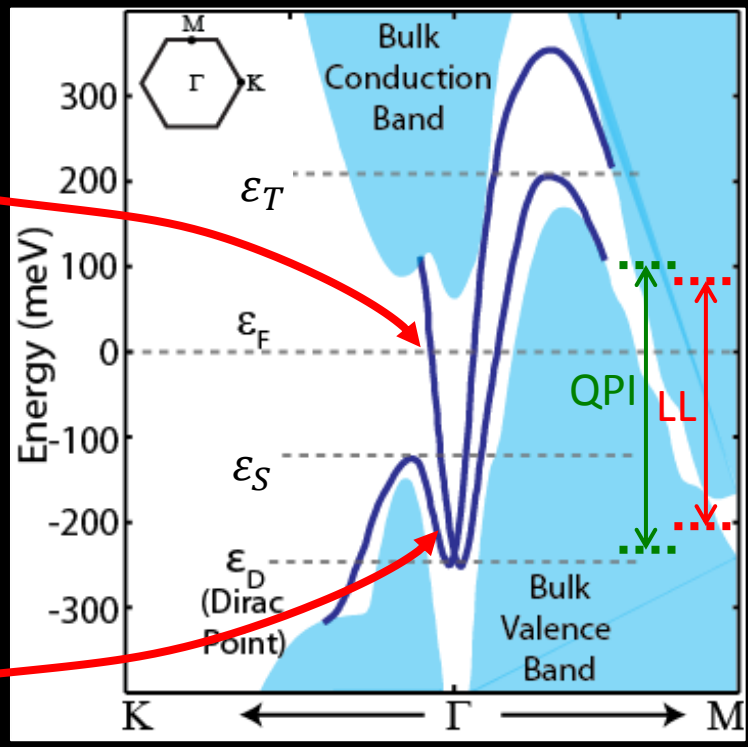


Rashba: 2 split parabolas

$$\omega_c = \frac{eB}{mc};\ \varepsilon_0 = \frac{1}{2}(\hbar\omega_c + g\mu_B B)$$

$$\varepsilon_n^{\pm} = \hbar\omega_c n \pm \sqrt{2nv_0^2 m\hbar\omega_c + \varepsilon_0^2}$$



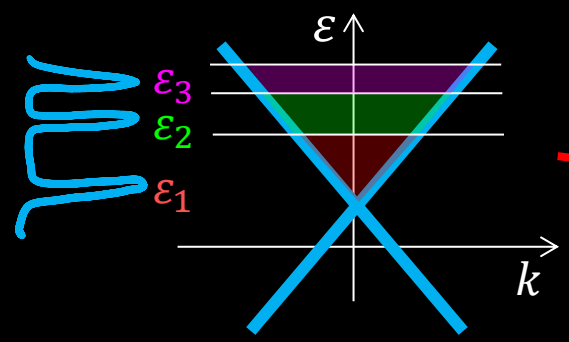


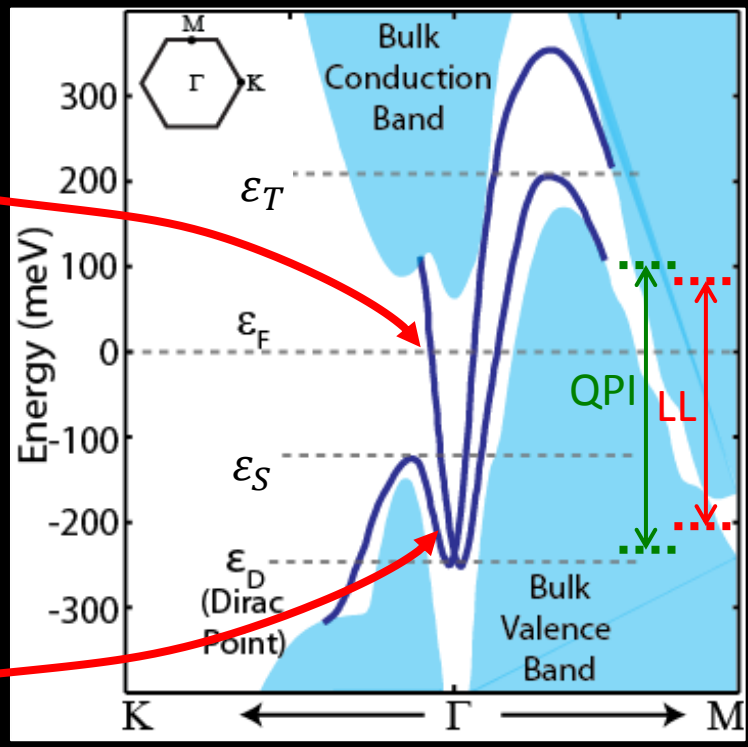
Landau Levels

Let's focus on Dirac-like first…

Dirac Fermions: $\varepsilon = \hbar v_F k$

$$\varepsilon_N = \varepsilon_D + \sqrt{e\hbar v_F N B}$$





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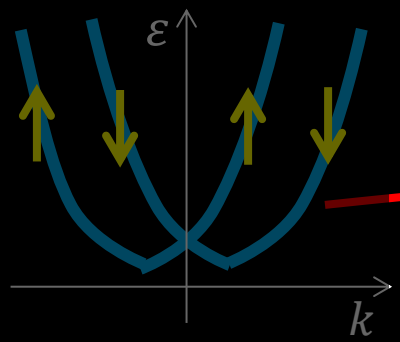
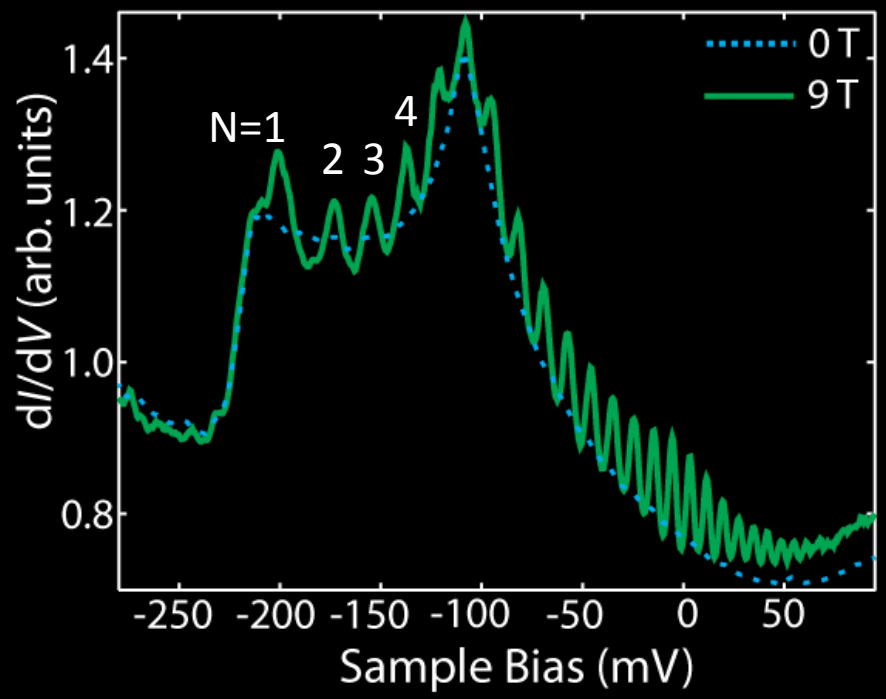
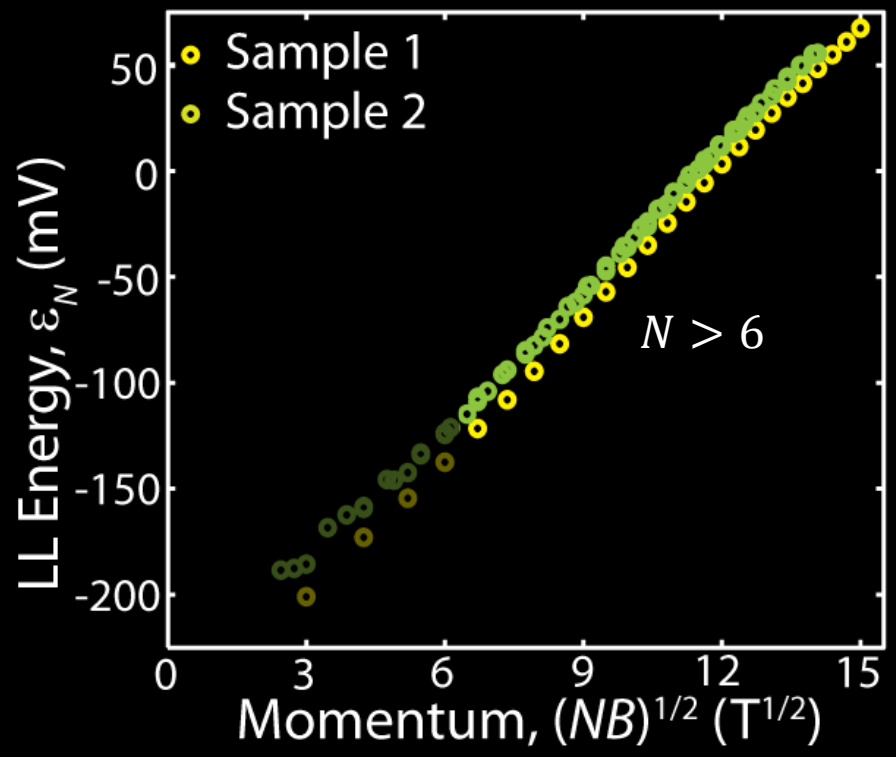


Landau Levels: Data





Hold that thought…

$$\varepsilon_N = \varepsilon_D + \sqrt{e\hbar v_{LL} NB}$$

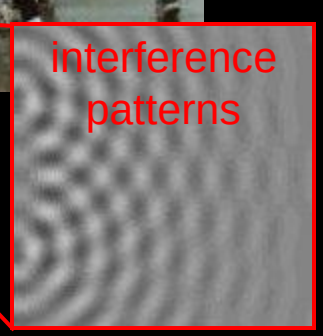
$$v_{LL} = 6.38 \times 10^5 \text{ m/s}$$

Quasiparticle Interference Imaging

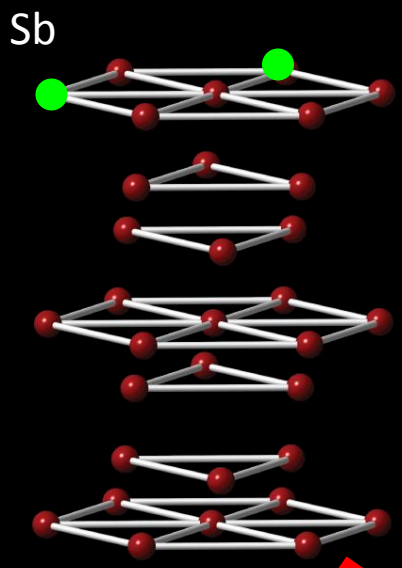
unperturbed H_2O

ME
(experimentalist)

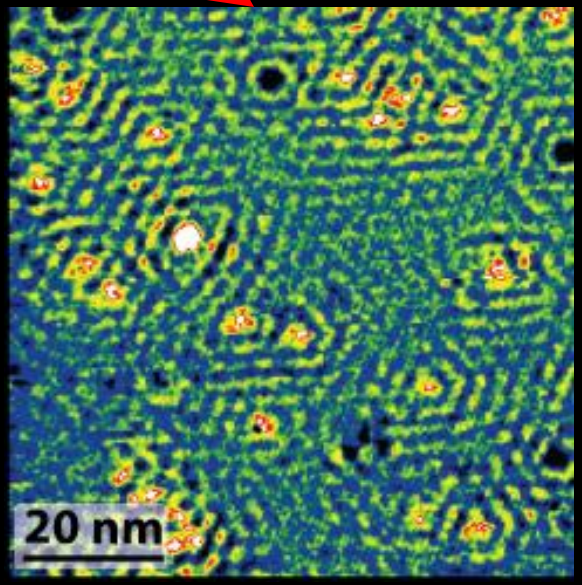
perturbation



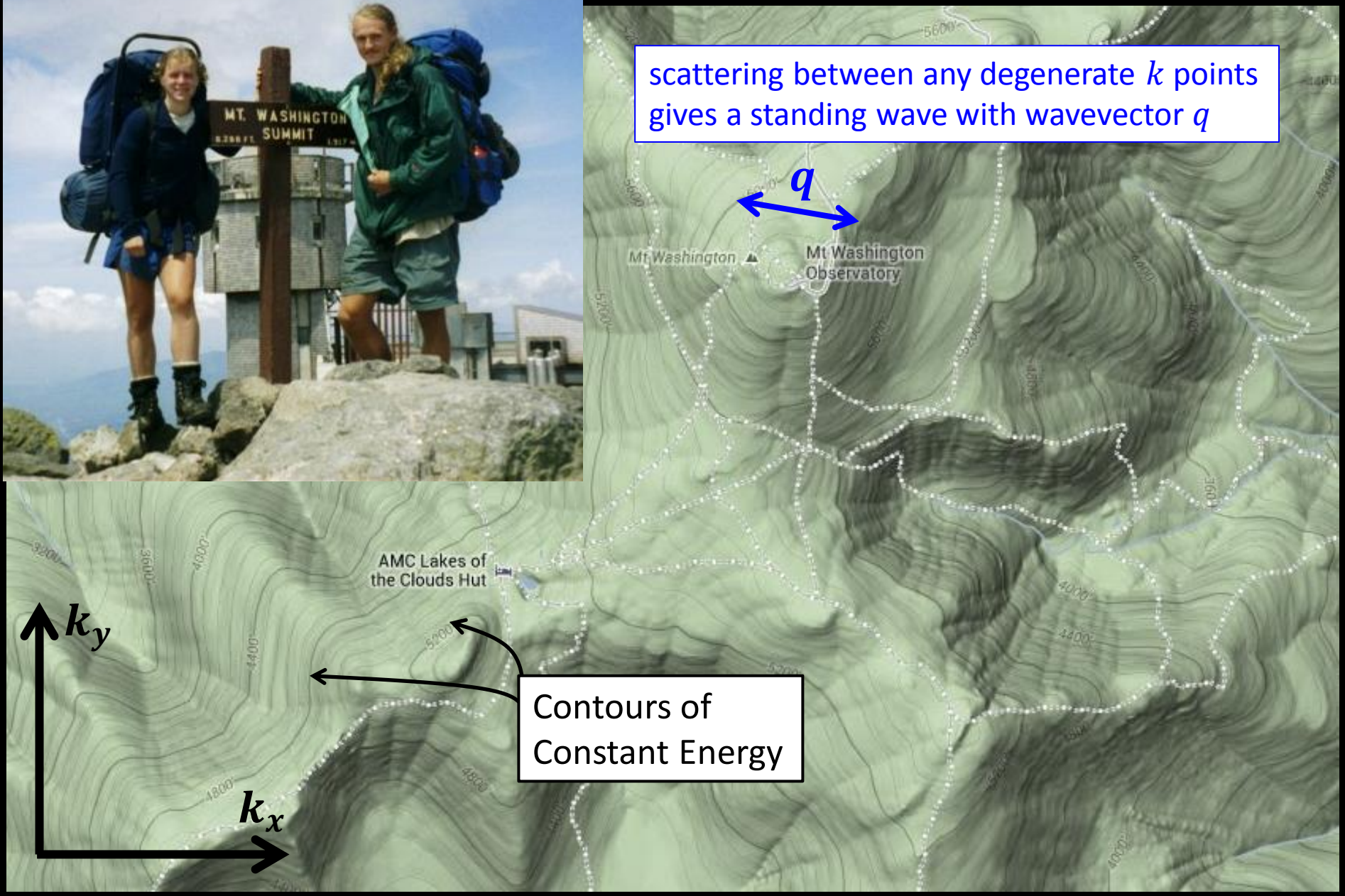
interference
patterns



defects

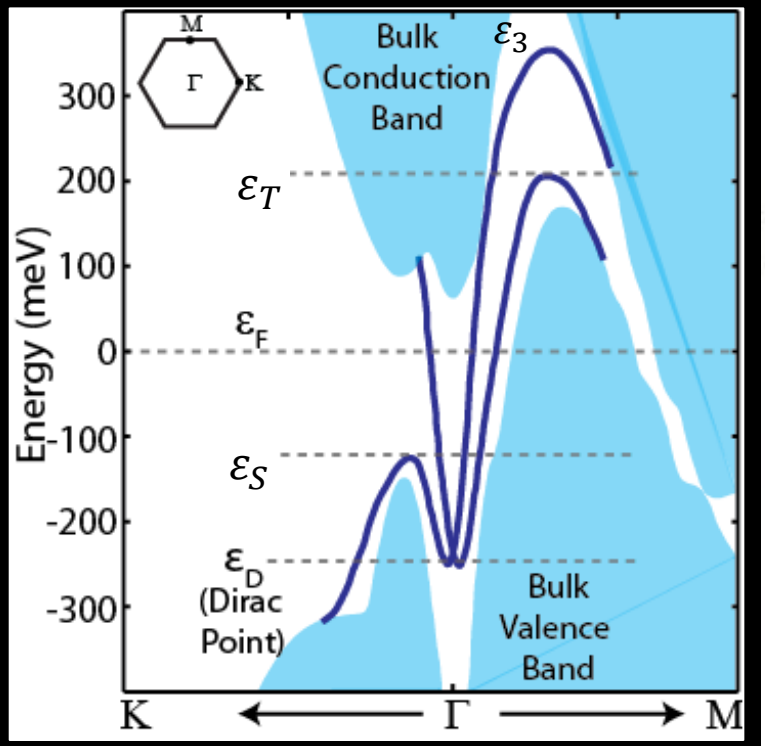


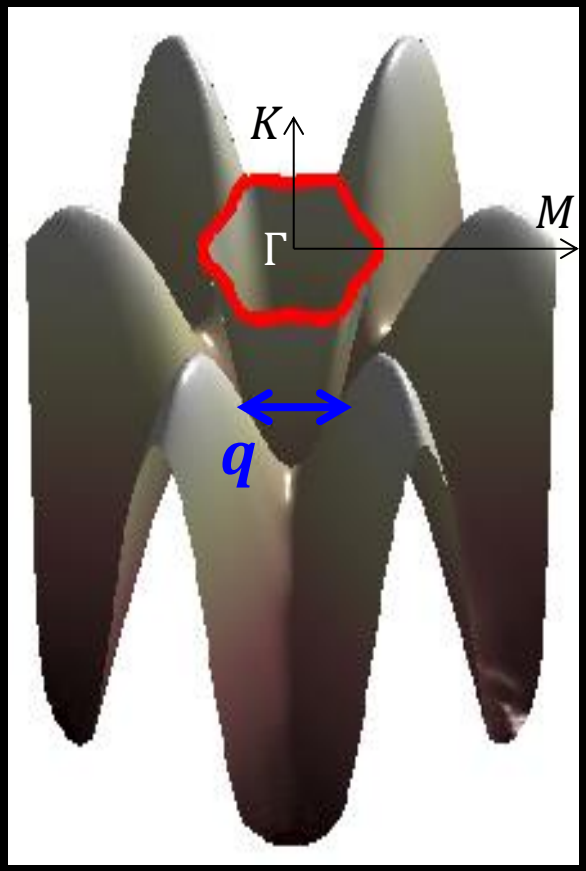
2-dim band structure: topographic map for e^-



QPI in Sb(111)

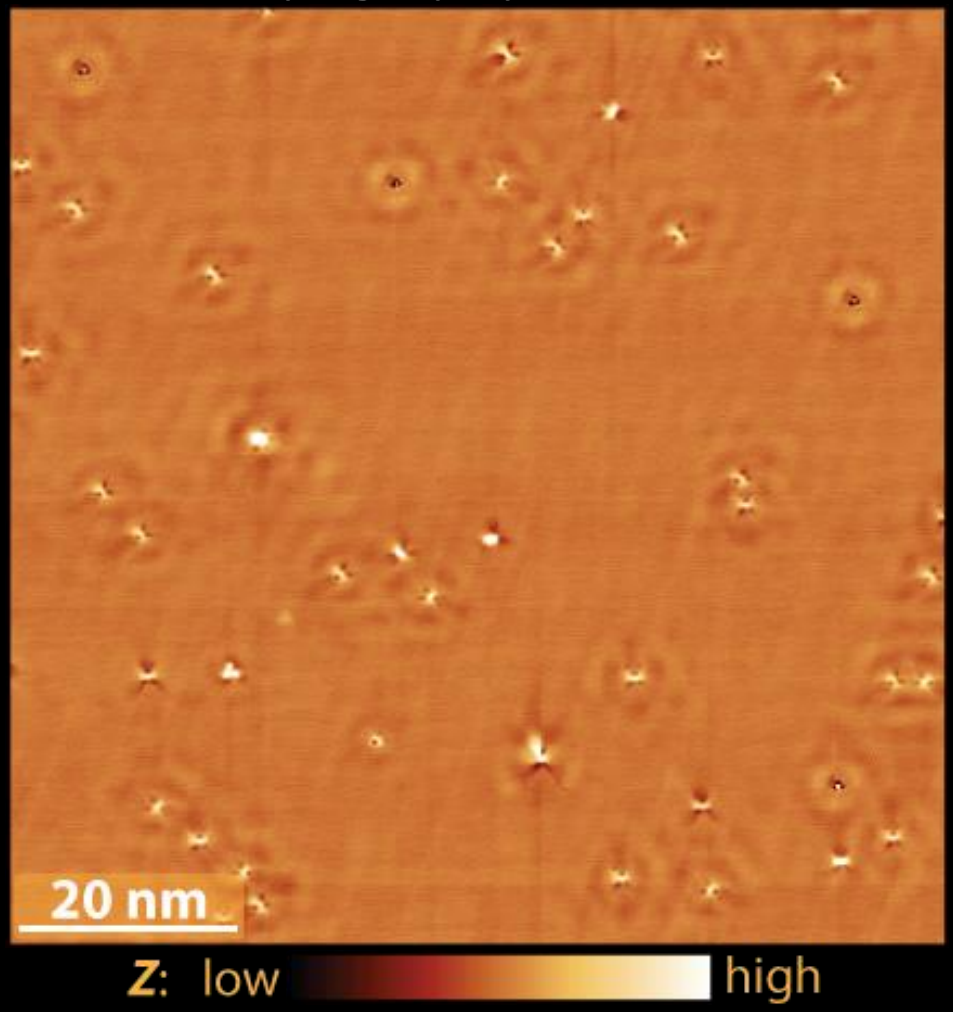
Surface states: $H = E_D + \frac{k^2}{2m^*} + (v_0 + \alpha k^2)(k_x\sigma_y - k_y\sigma_x) + \frac{1}{2}\lambda(k_+^3 + k_-^3)$



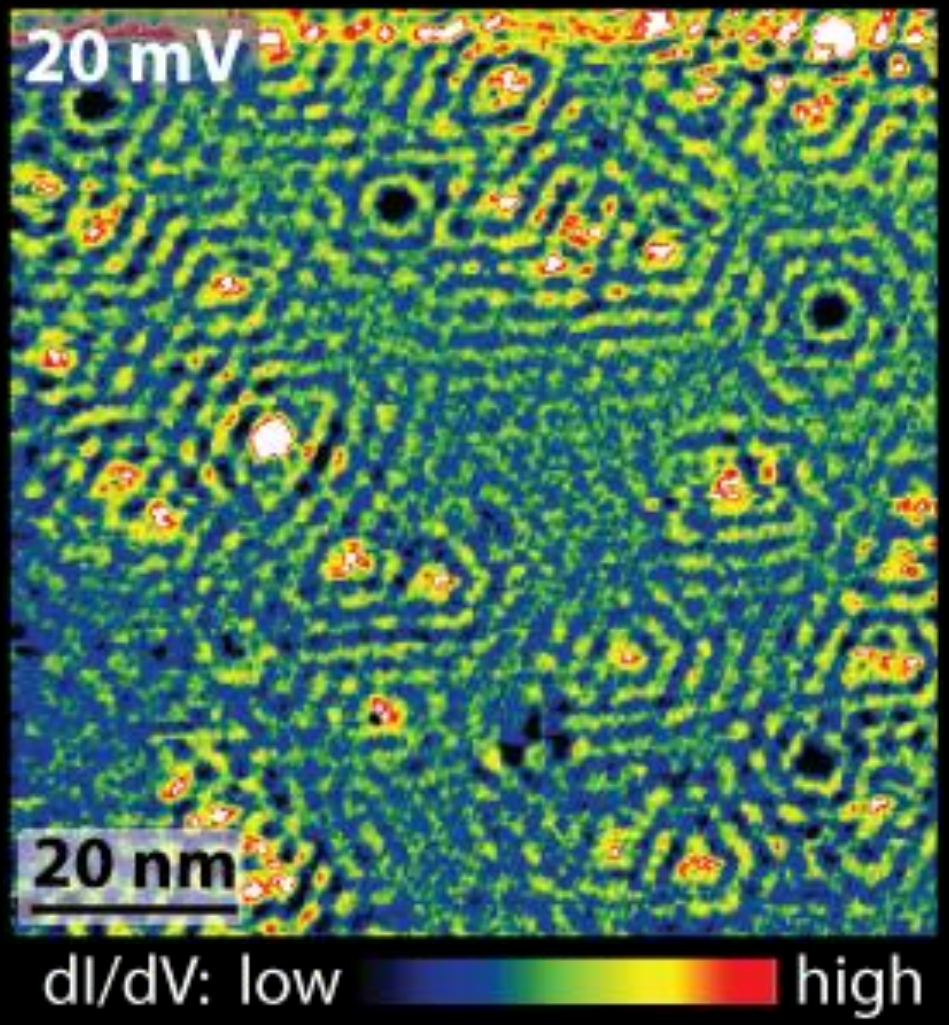


Quasiparticle Interference on Sb(111)

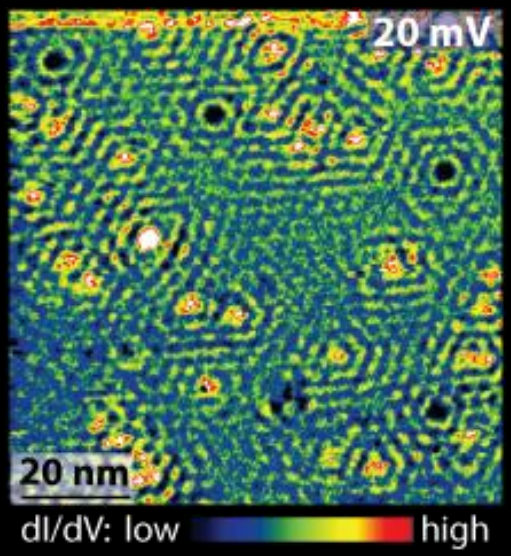
Sb(111) Topography



dI/dV (density of states)

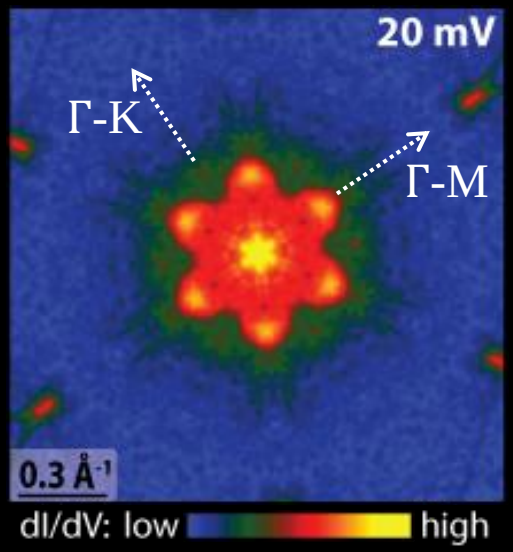


Quasiparticle Interference on Sb(111)

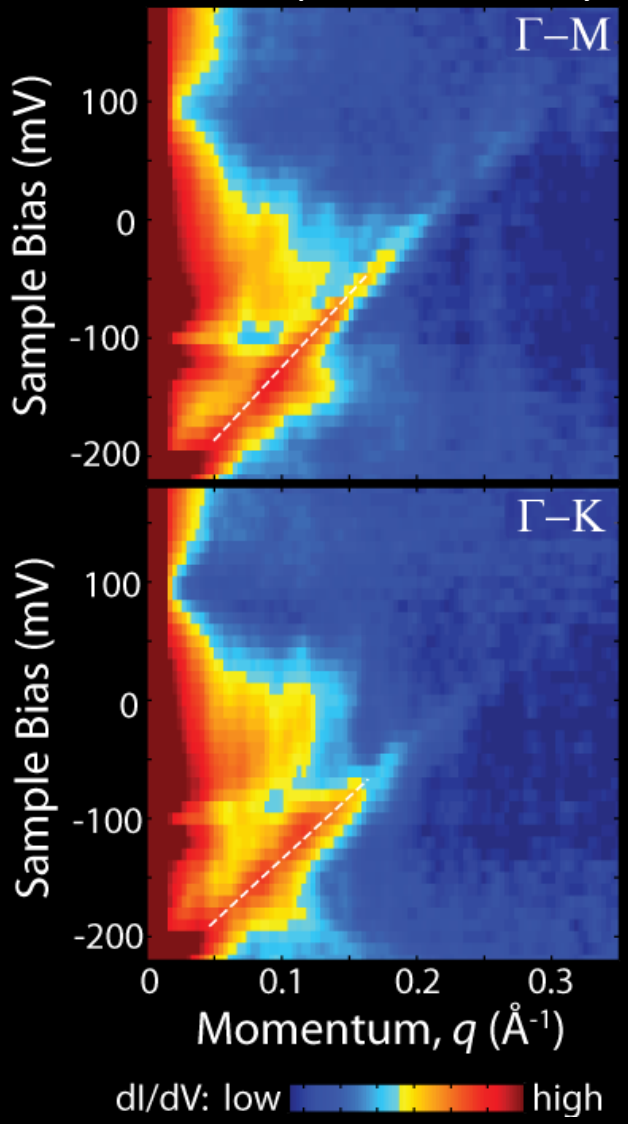


Fourier transform →

Dominant modes along $\Gamma - M$ and $\Gamma - K$

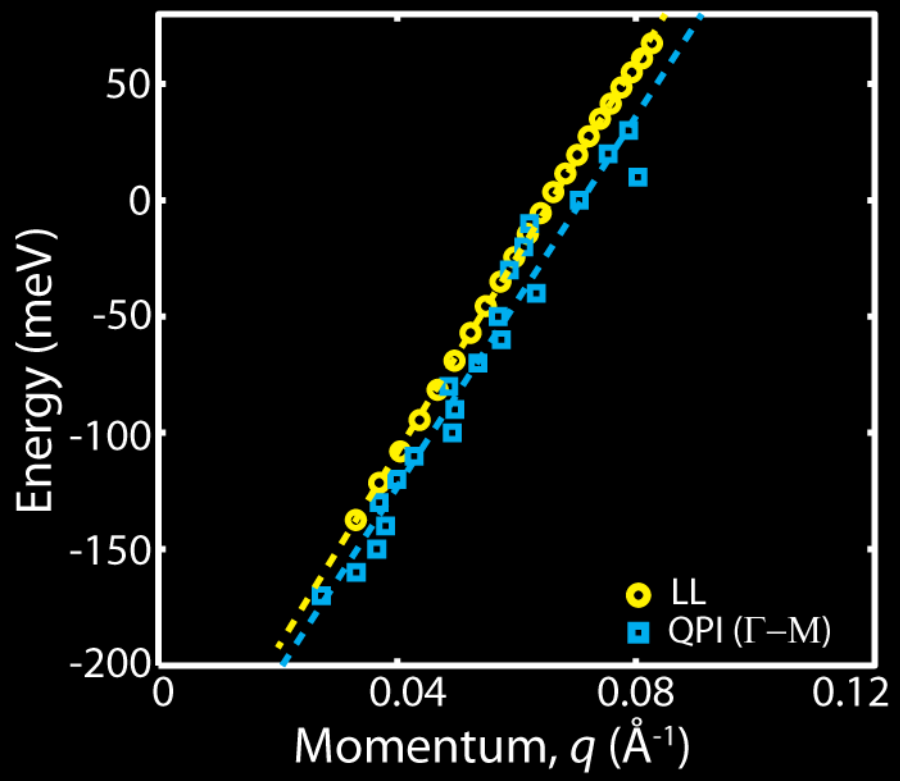


QPI disperses ~linearly



Will this agree with Landau levels??

LL & QPI: Dispersion Comparison



$$v_{QPI} = 6.08 \times 10^5 \text{ m/s}$$

$$v_{LL} = 6.38 \times 10^5 \text{ m/s}$$

→ agree within 3%

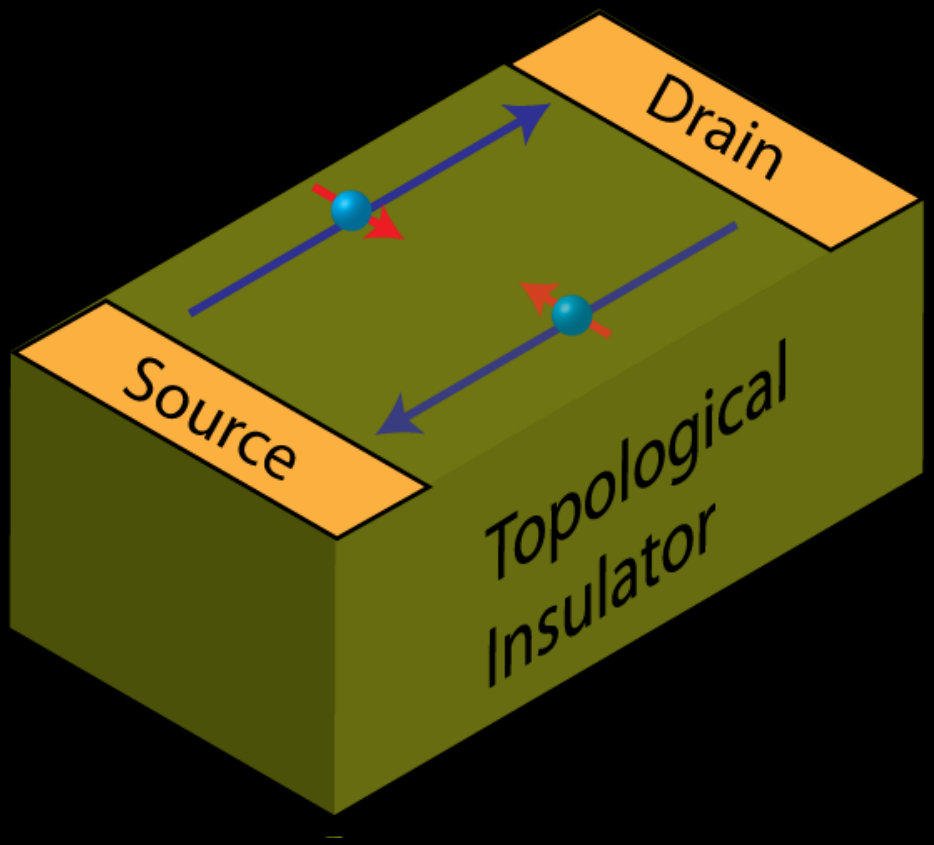
- STM Advantages
  - Filled and empty states
  - Nontrivial band structure
  - sub-meV energy resolution
  - B-field dependence
  - Nanoscale spatial resolution

arxiv:1311.1758

Outline

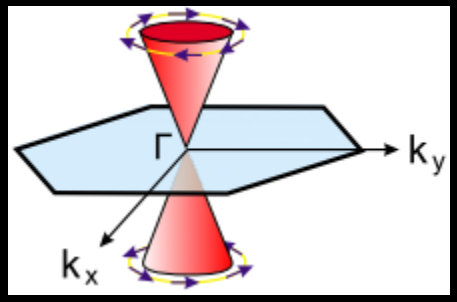
- Topological Insulators
- Scanning Tunneling Microscopy
- Nanoscale Band Structure
- Topological: Sb
- Insulator: SmB_6

Metrics for topological devices



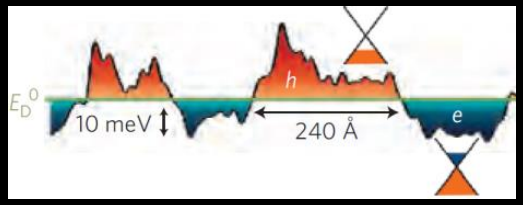
1. Enhance spin-momentum locking

Metric: Spin-Orbit Coupling (v_0)



2. Reduce scattering

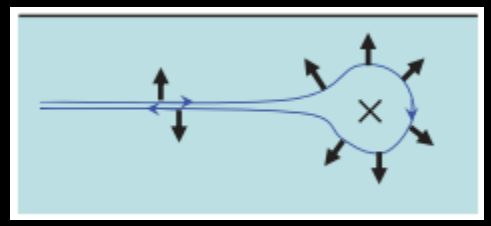
Metric: Mean Free Path (l_f)



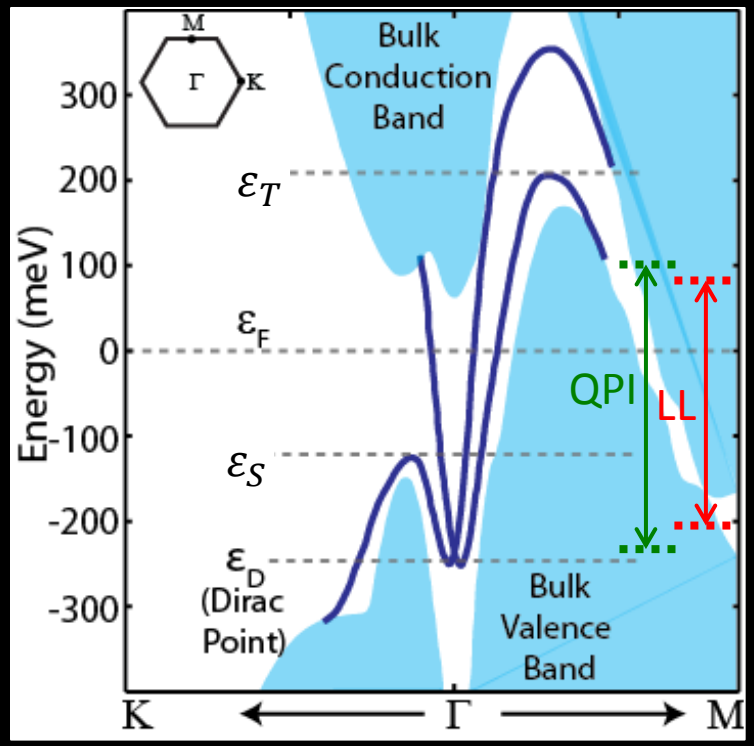
H. Beidenkopf, Nat. Phys. 2011

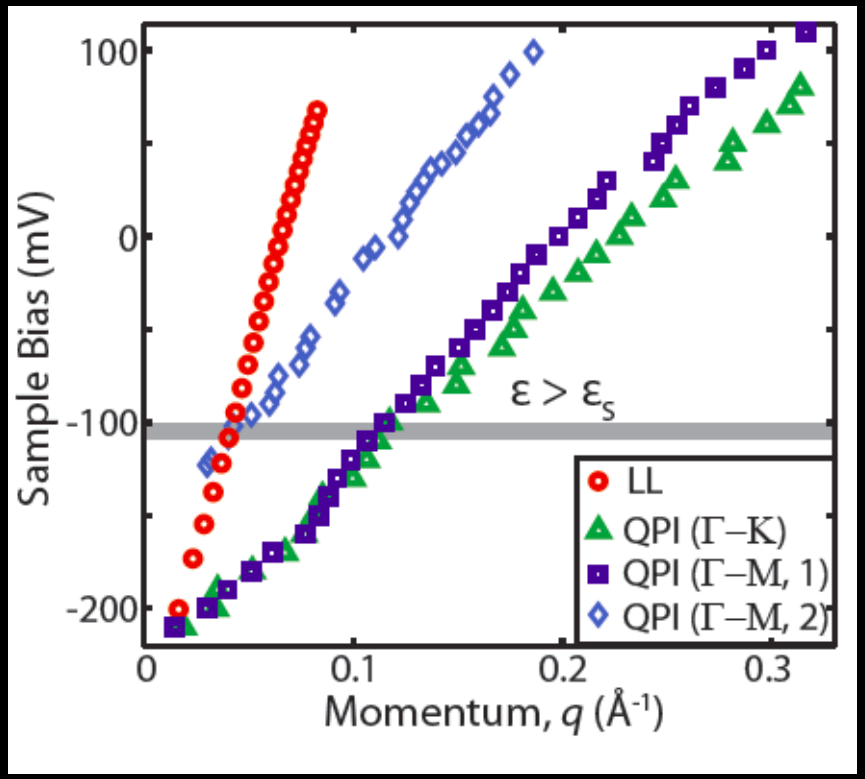
3. Reduce vulnerability to external B & magnetic impurities:

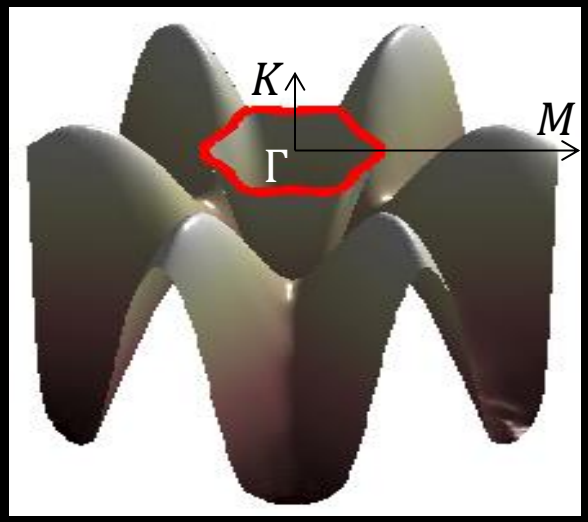
Metric: *g*-factor

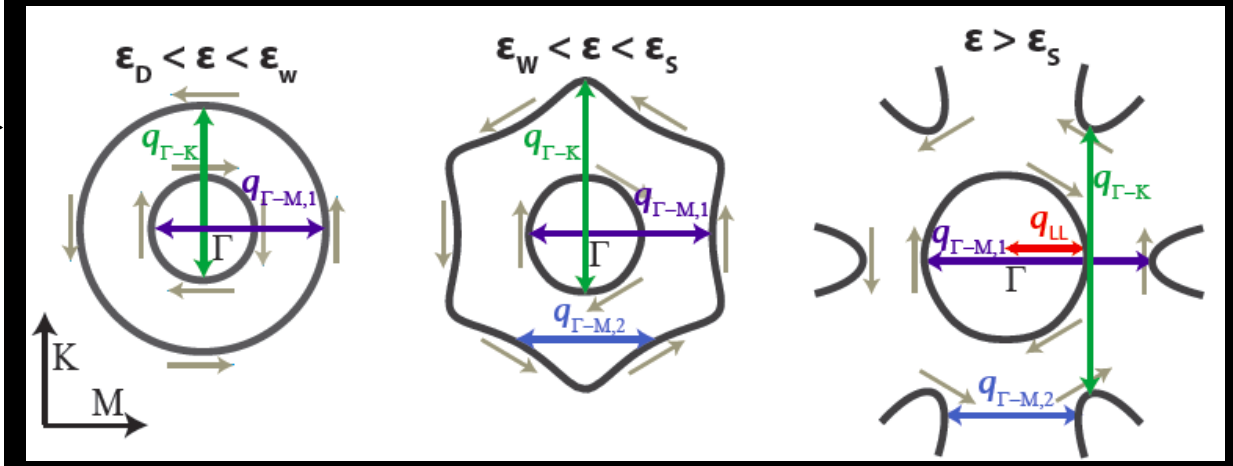


Reconstruct multi-component band structure

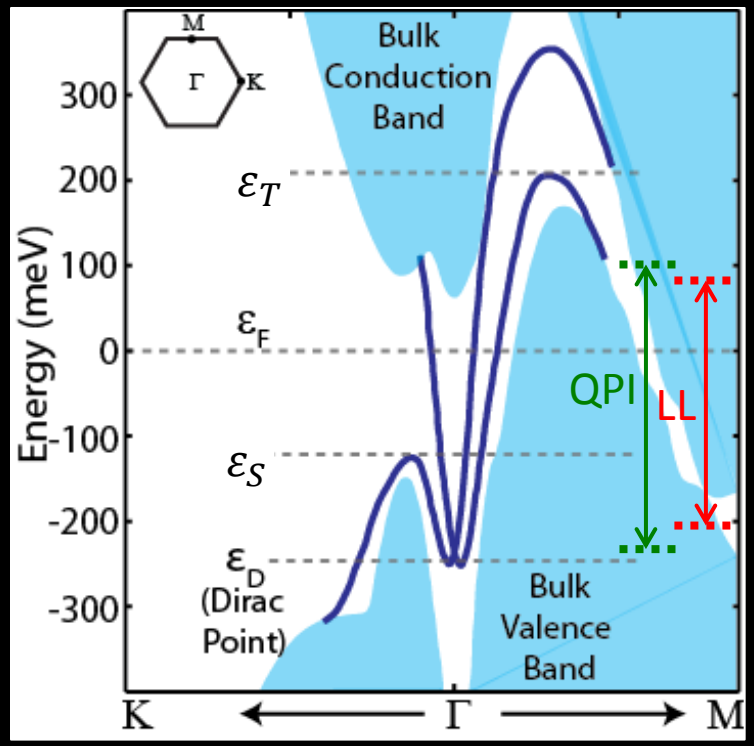


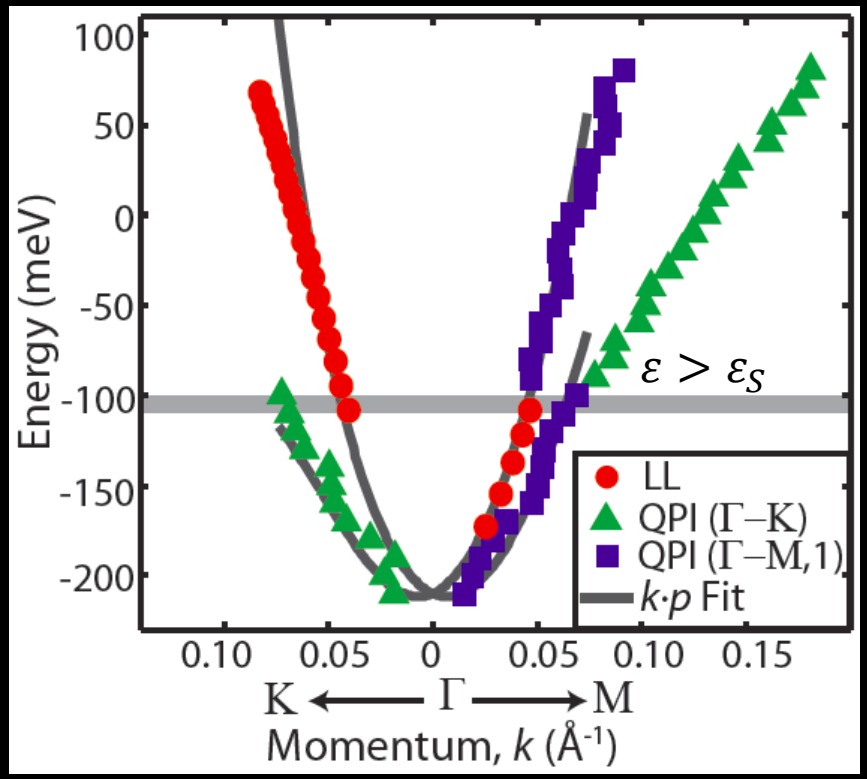


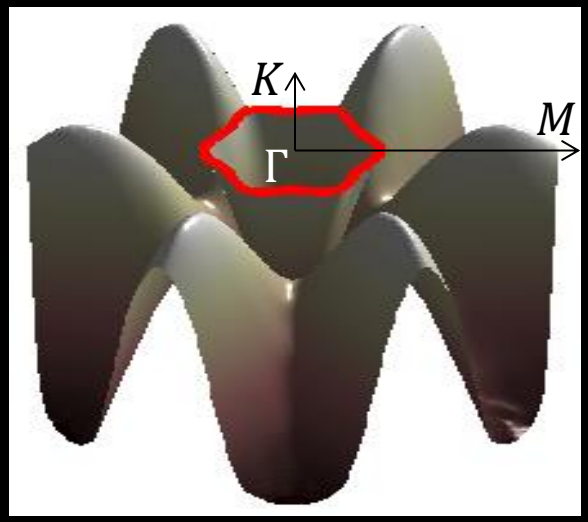


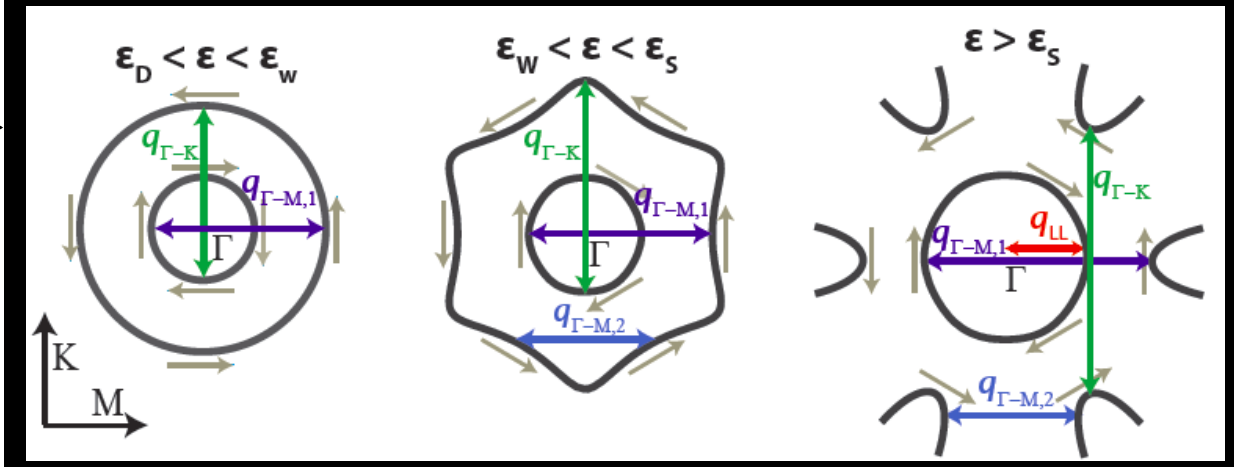


Reconstruct multi-component band structure









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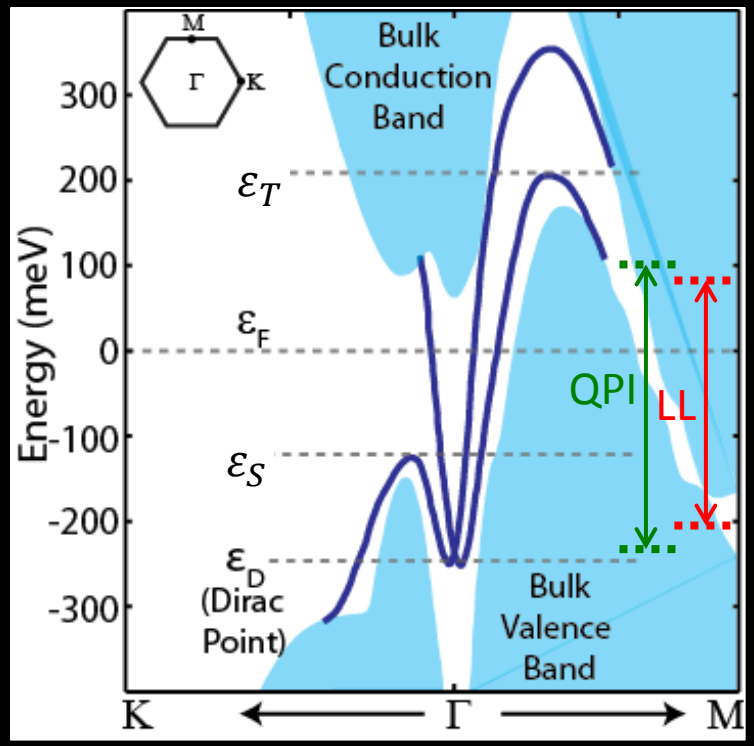
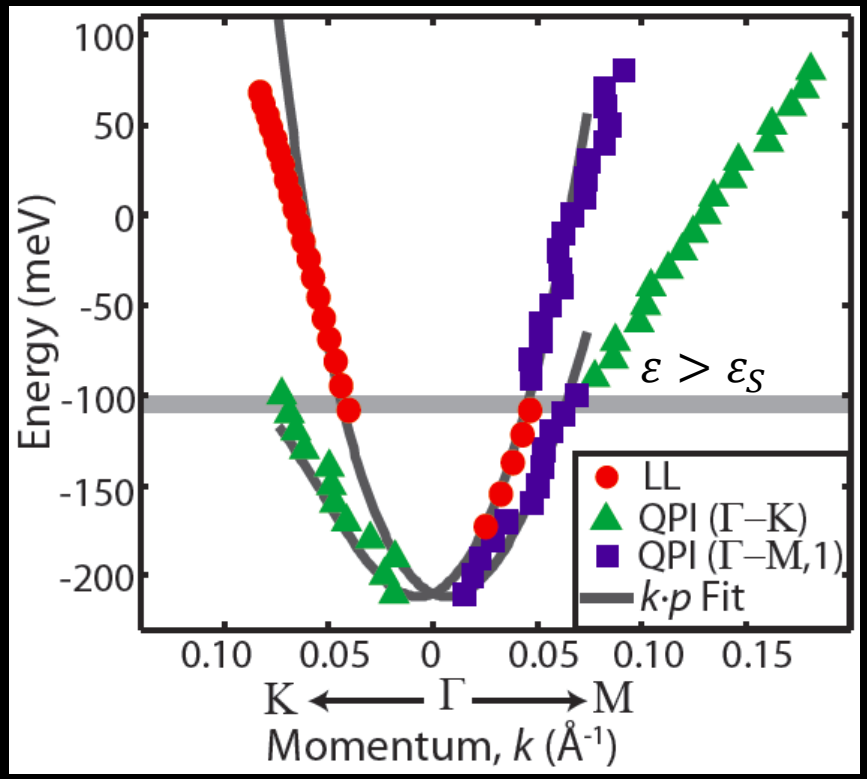


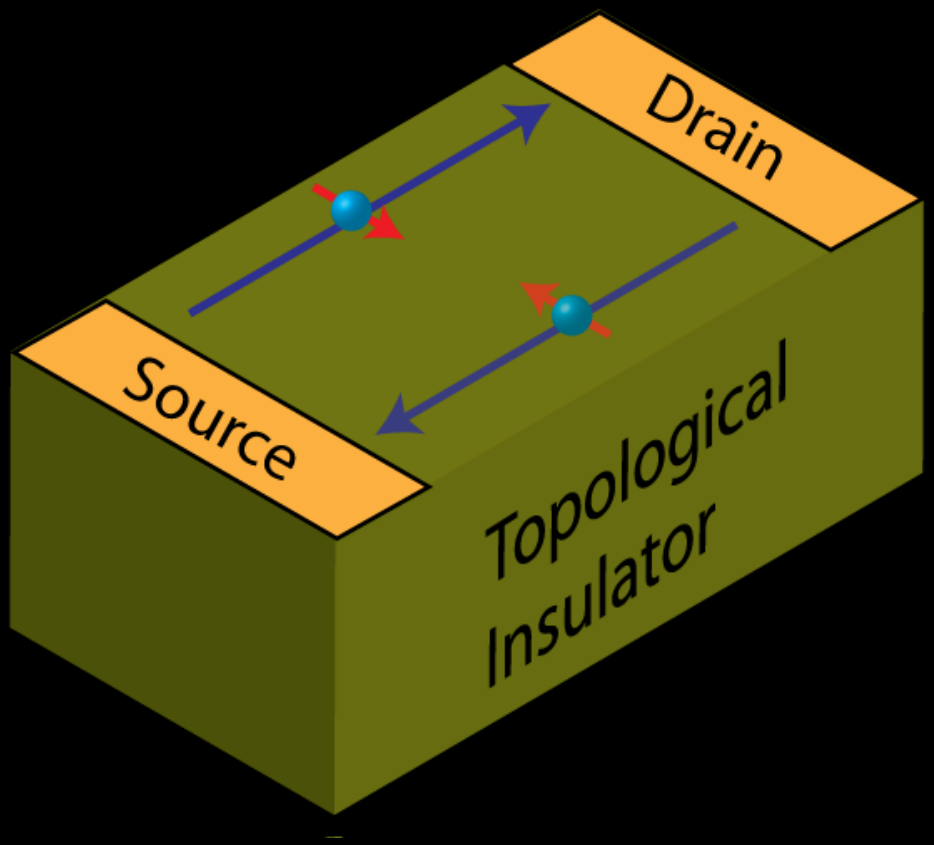


$$H = E_D + \frac{k^2}{2m^*} + (v_0 + \alpha k^2)(k_x\sigma_y - k_y\sigma_x) + \frac{1}{2}\lambda(k_+^3 + k_-^3)$$

$E_D = -210$ mV; $m^* = 0.1m_e$; $v_0 = 0.51$ eV·Å;

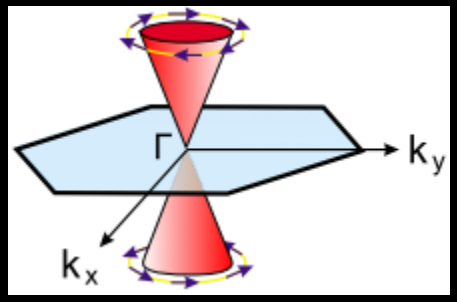
$\alpha = 110$eV·Å^3; $\lambda = 230$ eV·Å^3

Metrics for topological devices



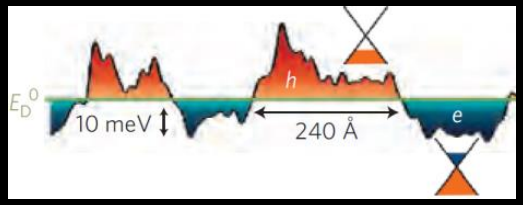
1. Enhance spin-momentum locking

Metric: Spin-Orbit Coupling (v_0=0.5 eV·Å)



2. Reduce scattering

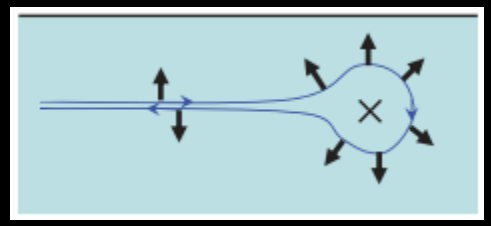
Metric: Mean Free Path (l_f)



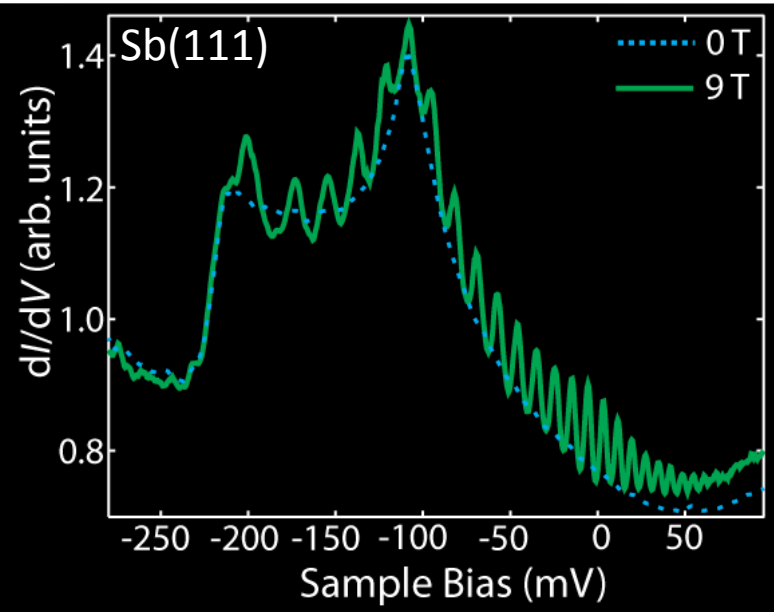
H. Beidenkopf, Nat. Phys. 2011

3. Reduce vulnerability to external B & magnetic impurities:

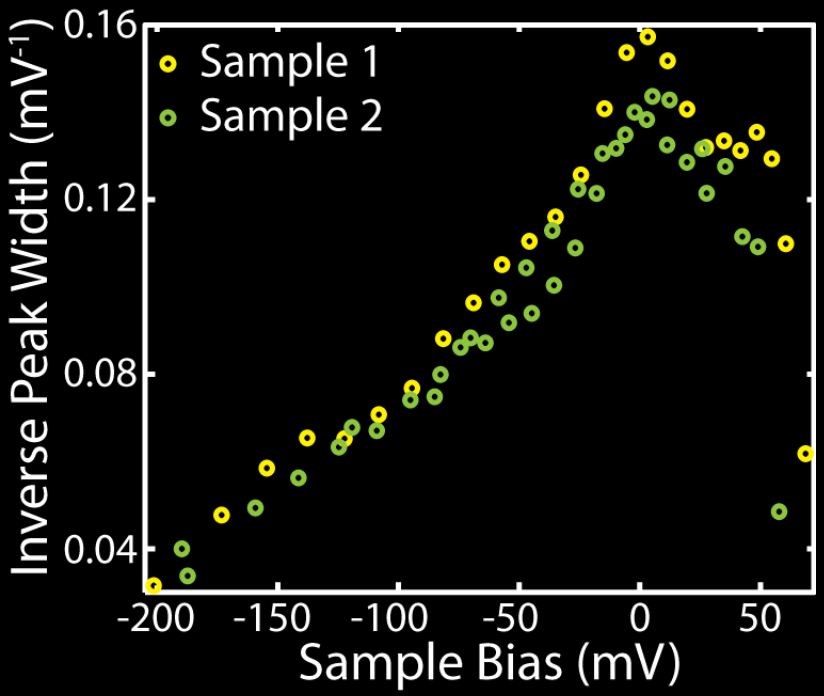
Metric: *g*-factor



LL 'Sharpness' & Lifetime Broadening



- LLs are sharpest at ε_F



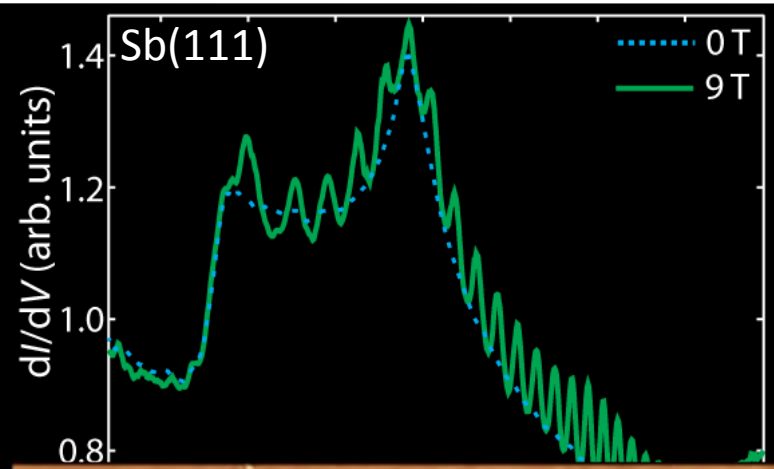
- Sb(111) mean free path

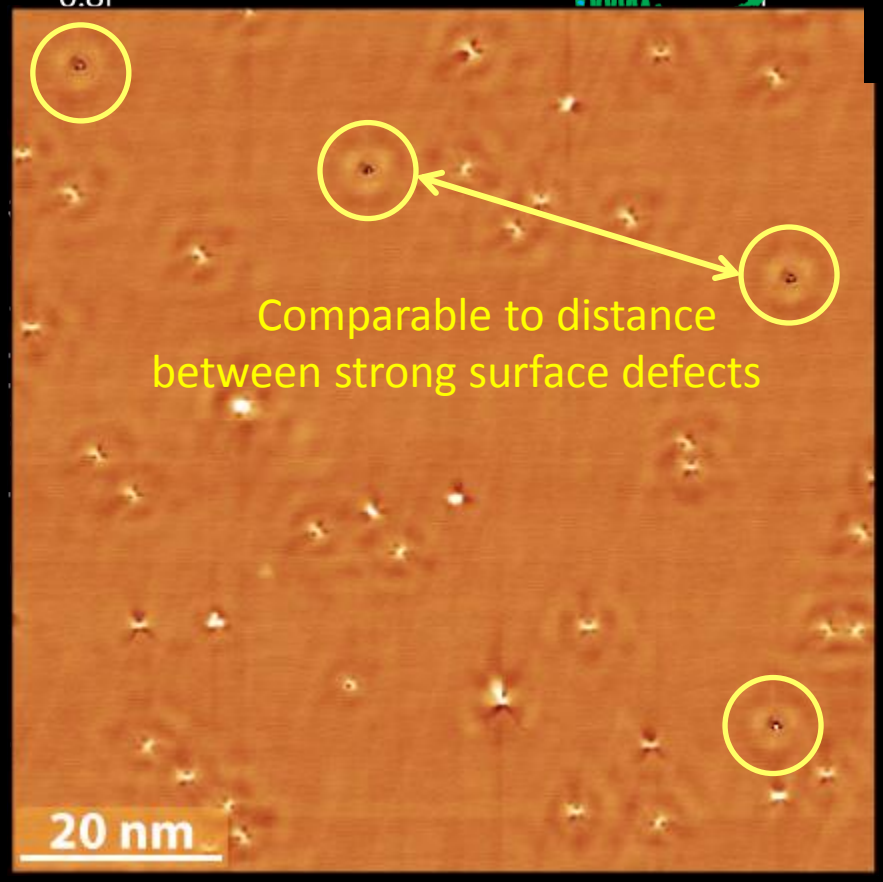
$$\ell \sim \frac{\hbar}{\Gamma(\varepsilon_F)} \cdot v_F$$

Sample 1: λ_F ~ 65 nm

Sample 2: λ_F ~ 59 nm

LL 'Sharpness' & Lifetime Broadening





- LLs are sharpest at ε_F

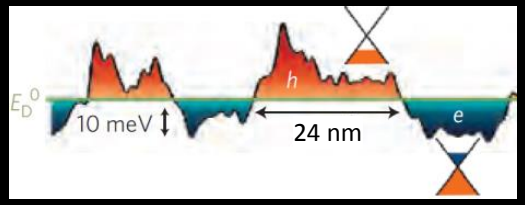
- Sb(111) mean free path

$$\ell \sim \frac{\hbar}{\Gamma(\varepsilon_F)} \cdot v_F$$

Sample 1: λ_F ~ 65 nm

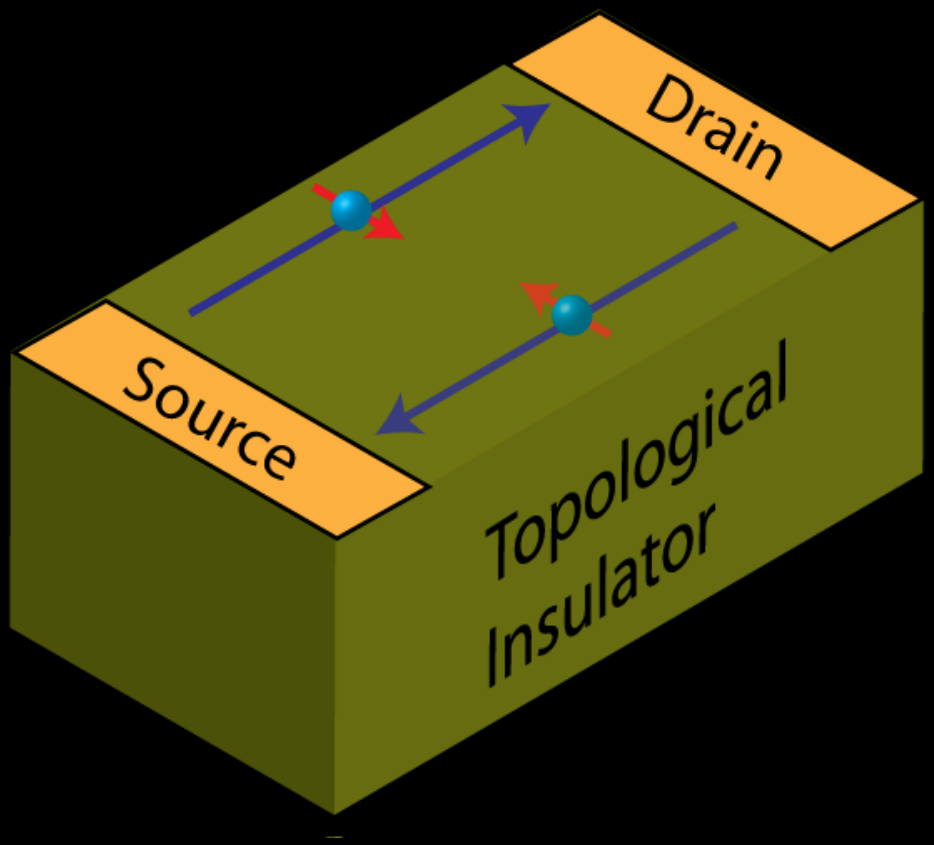
Sample 2: λ_F ~ 59 nm

c.f. Bi_2Se_3
Bi_2Te_3



H. Beidenkopf, Nat. Phys. 2011

Metrics for topological devices



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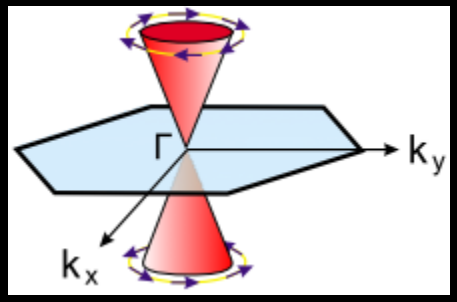
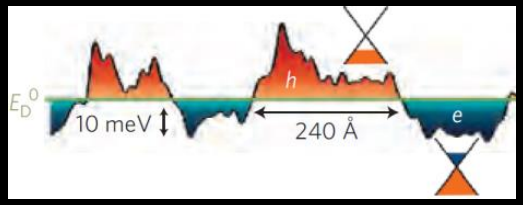


2. Reduce scattering

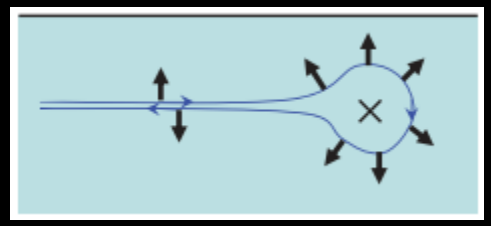
Metric: Mean Free Path (l_f~60 nm)



H. Beidenkopf, Nat. Phys. 2011

3. Reduce vulnerability to external B & magnetic impurities:

Metric: *g*-factor

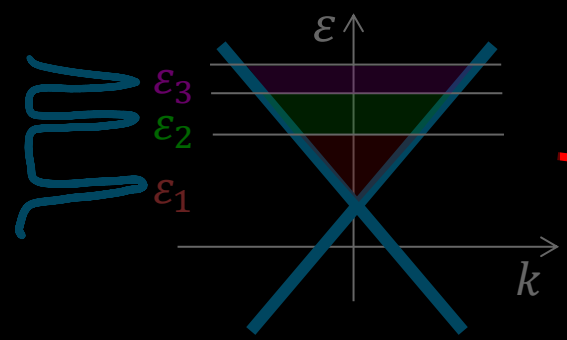


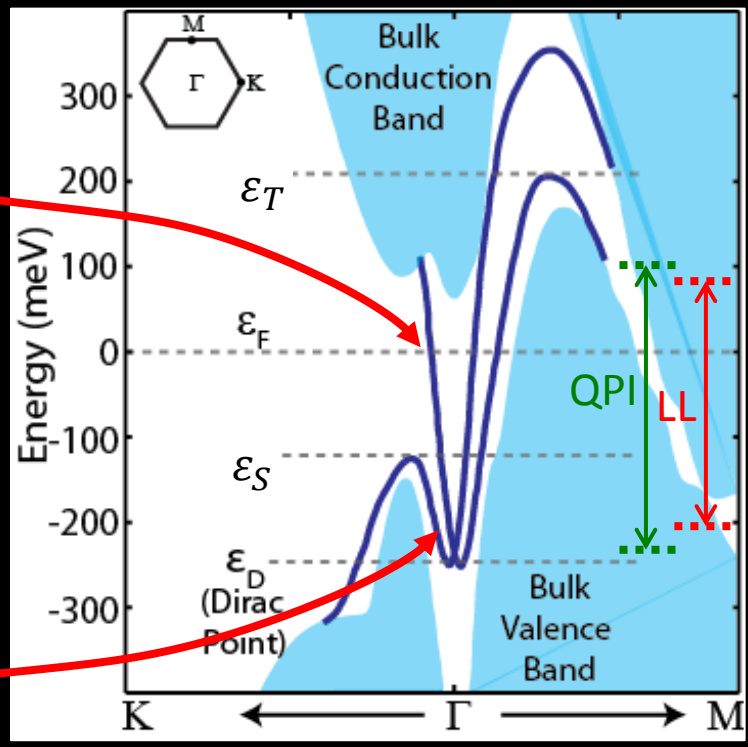
Quantify g-factor from low-energy LLs

Need to look at low N to get the g-factor…

Dirac Fermions: $\varepsilon = \hbar v_F k$

$$\varepsilon_N = \varepsilon_D + \sqrt{e\hbar v_F N B}$$



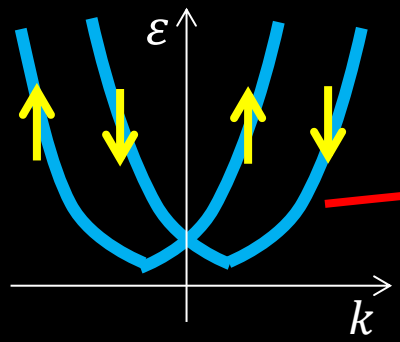


Rashba: 2 split parabolas

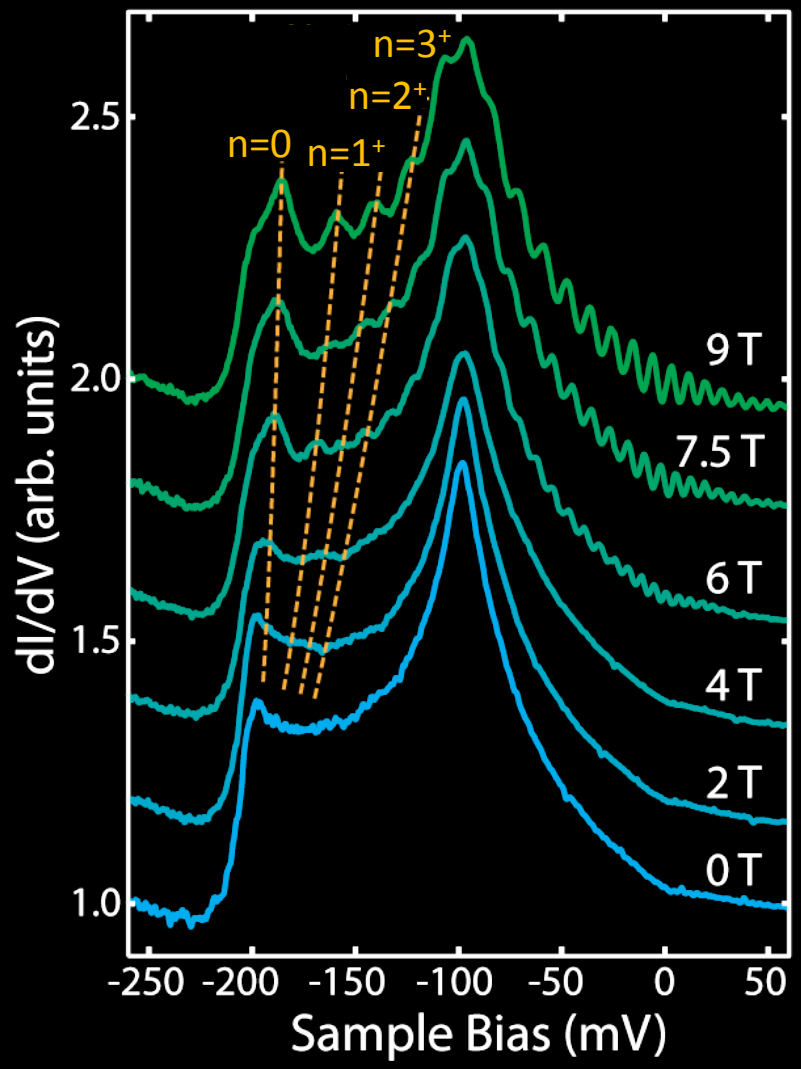
$$\varepsilon_0 = \tfrac{1}{2}(\hbar\omega_c + g\mu_B B)$$

$$\varepsilon_n^{\pm} = \hbar\omega_c n \pm \sqrt{2nv_0^2 m\hbar\omega_c + \varepsilon_0^2}$$

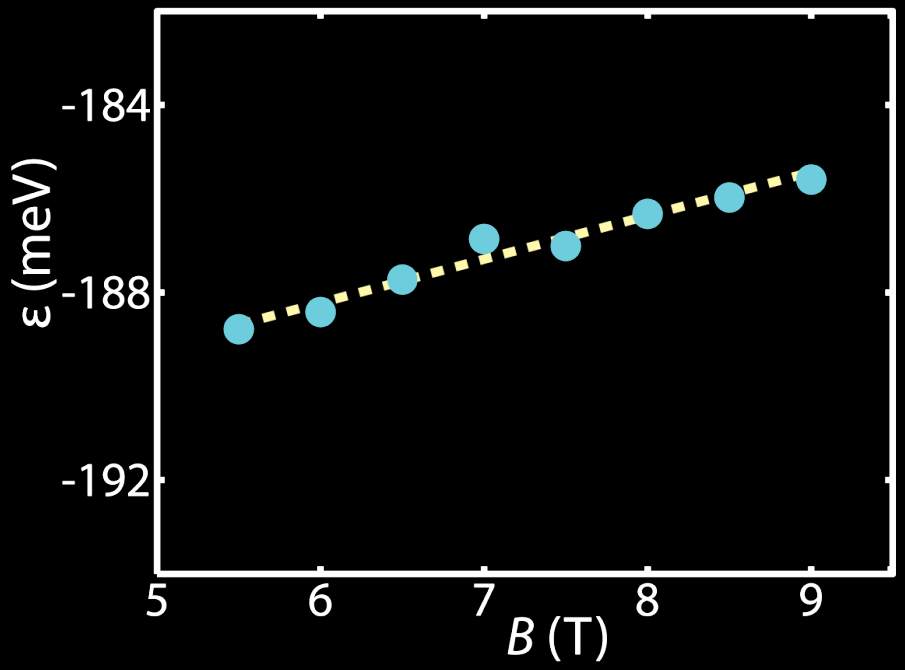
(where $\omega_c = \frac{eB}{mc}$)



Landau level identification in Sb(111)

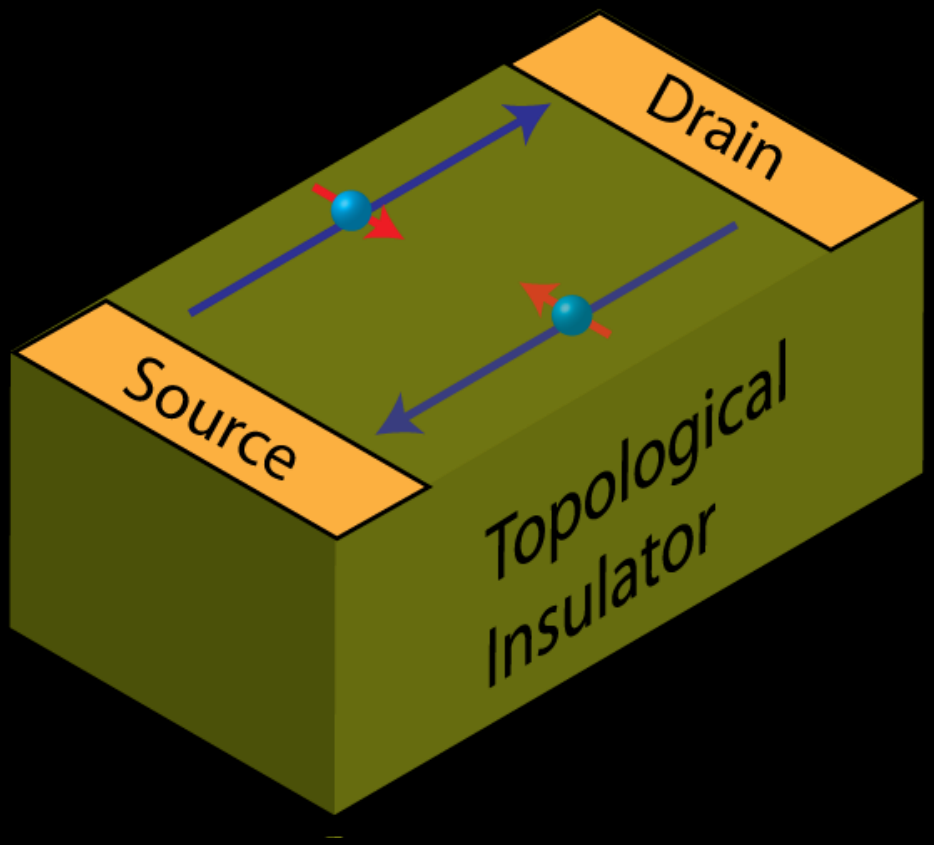


$$\varepsilon_0 = \frac{1}{2}(\hbar\omega_c + g\mu_B B)$$



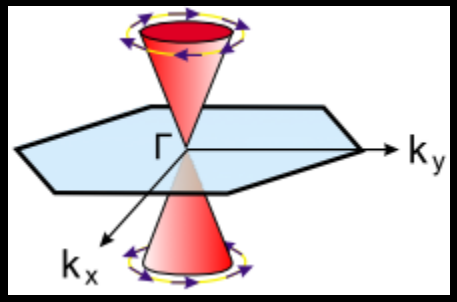
$\rightarrow g = 12.8$

Metrics for topological devices



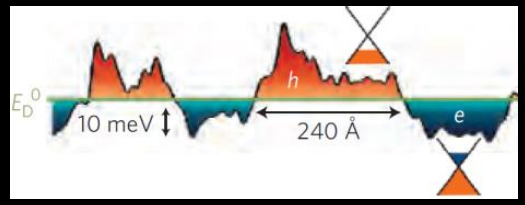
1. Enhance spin-momentum locking

Metric: Spin-Orbit Coupling (v_0=0.5 eV·Å)



2. Reduce scattering

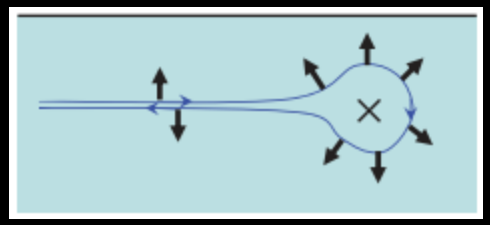
Metric: Mean Free Path (l_f~60 nm)



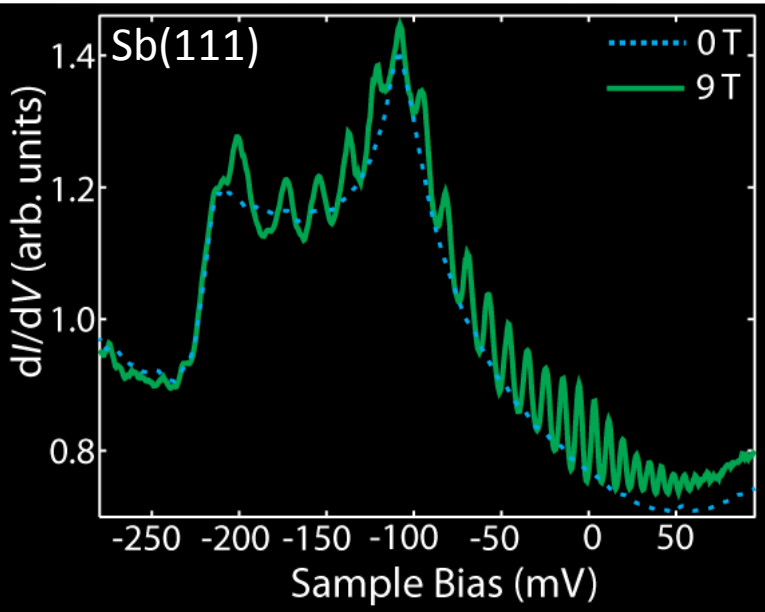
H. Beidenkopf, Nat. Phys. 2011

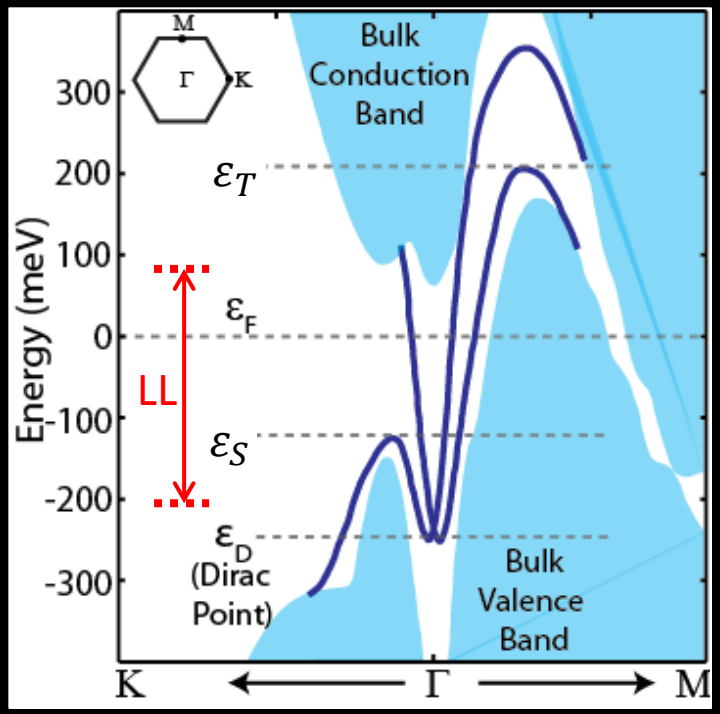
3. Reduce vulnerability to external B & magnetic impurities:

Metric: g-factor ($g = 12.8$)



Robust Surface States in Semimetal Sb





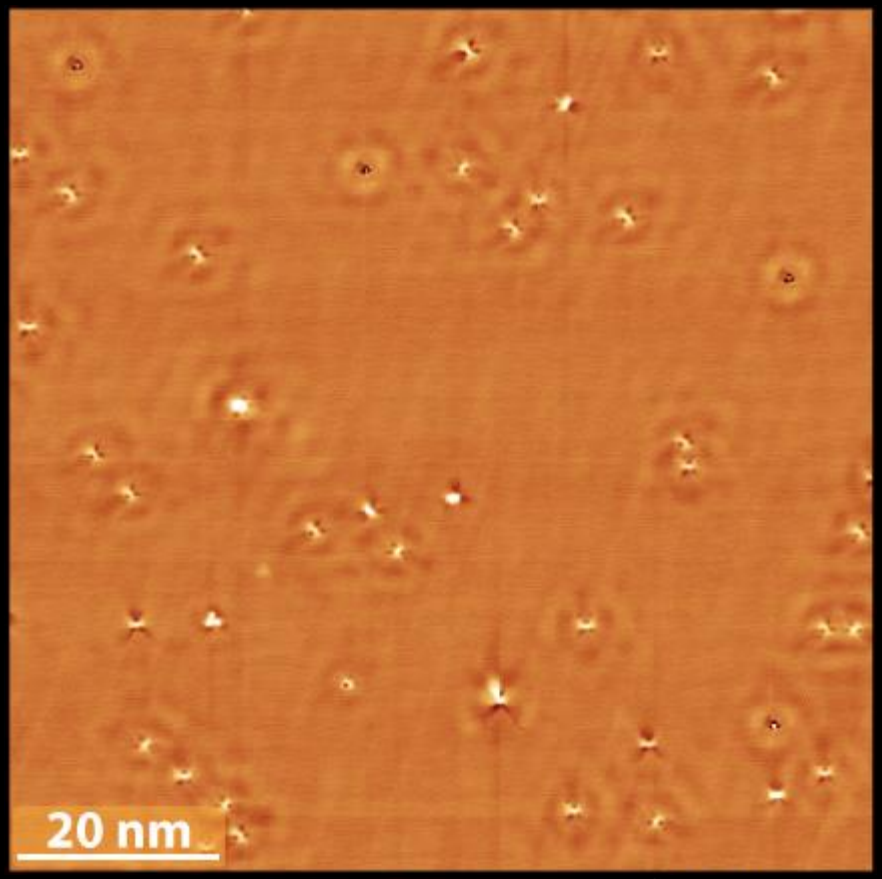
Material (Group)	LL Range (N)	Bulk Overlap (N)
Bi_2Se_3 (RIKEN) PRB 82, 081305 (2010)	0 : 22 (9 T)	~ 18 (VB)
Sb_2Te_3 (MBE, CAS) PRL 108, 016401 (2012)	-4 : 8 (7 T)	~ -3 (VB), ~6 (CB)
Bi_2Te_3 (BC) PRL 109, 166407 (2012)	~ 0 : 14 (7 T)	~ N = 0-15
$Pb_{1-x}Sn_xSe$ (BC) Science 341, 1496 (2013)	-2 :18 (3-7.5T)	~ N = 7-18
Bi_2Te_2Se (RIKEN) ACS Nano 7, 4105 (2013)	~ 0 : 17 (11 T)	~ N = 0
Sb (Harvard)	**1 : 27 (4 – 9 T)**	**Full**

→ suggests to shift focus from topological insulators to topological semimetals

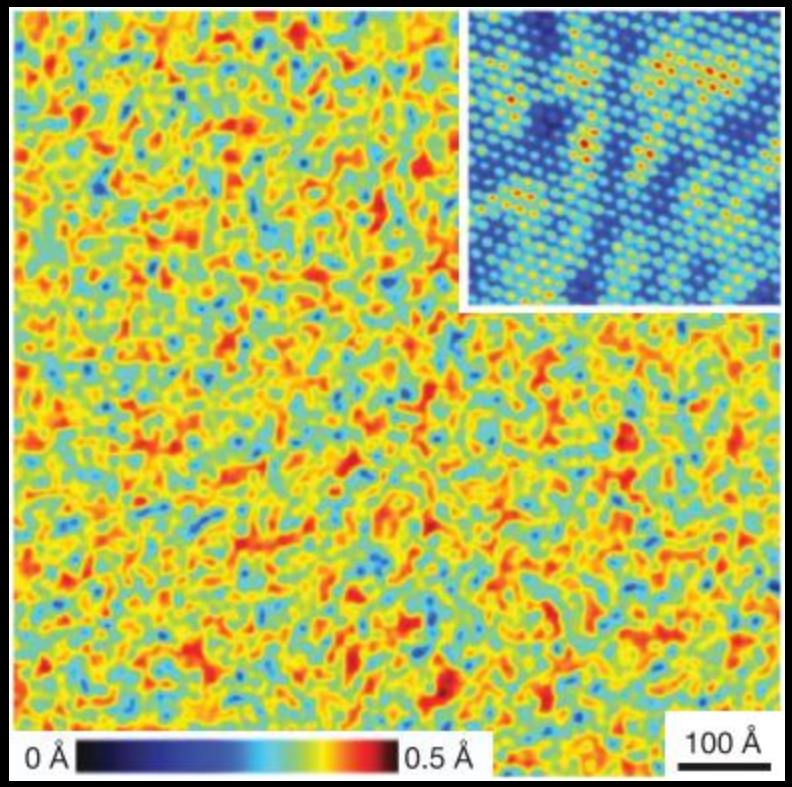
Topological Semimetal vs. Insulator

Sb: bulk semimetal
Flat topography, electronic modulations primarily around impurities

$Bi_{0.92}Sb_{0.08}$: bulk insulator
Large chemical potential fluctuations



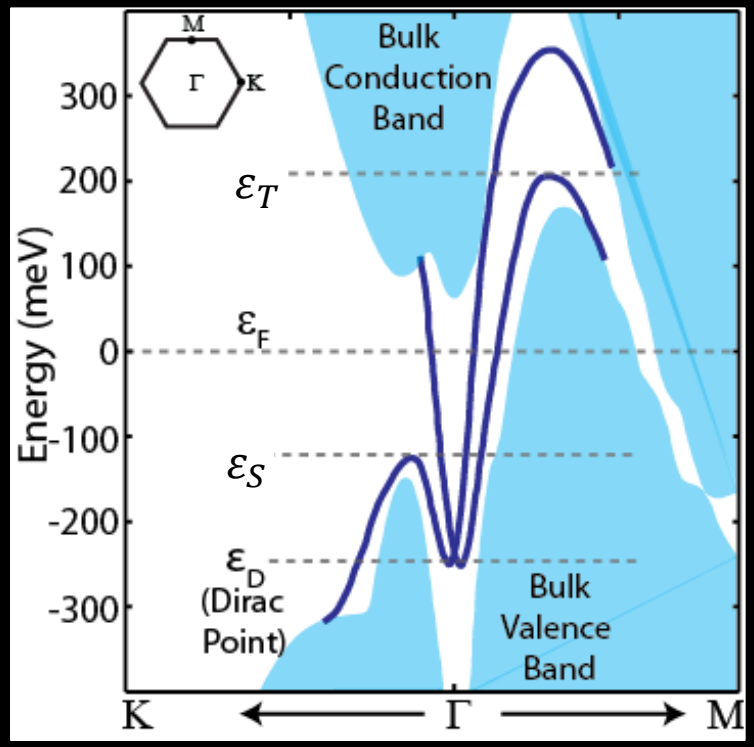
100 mV, 1 GΩ



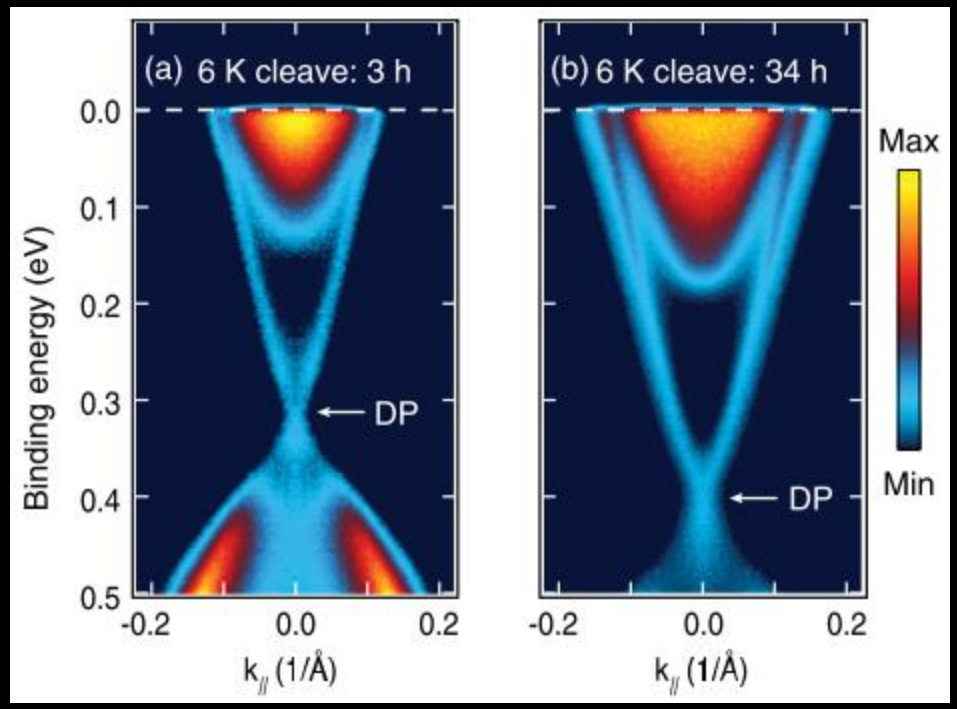
Roushan, Nature 460, 1106 (2009)

Sb vs. "canonical" Bi_2Se_3

Sb



Bi_2Se_3



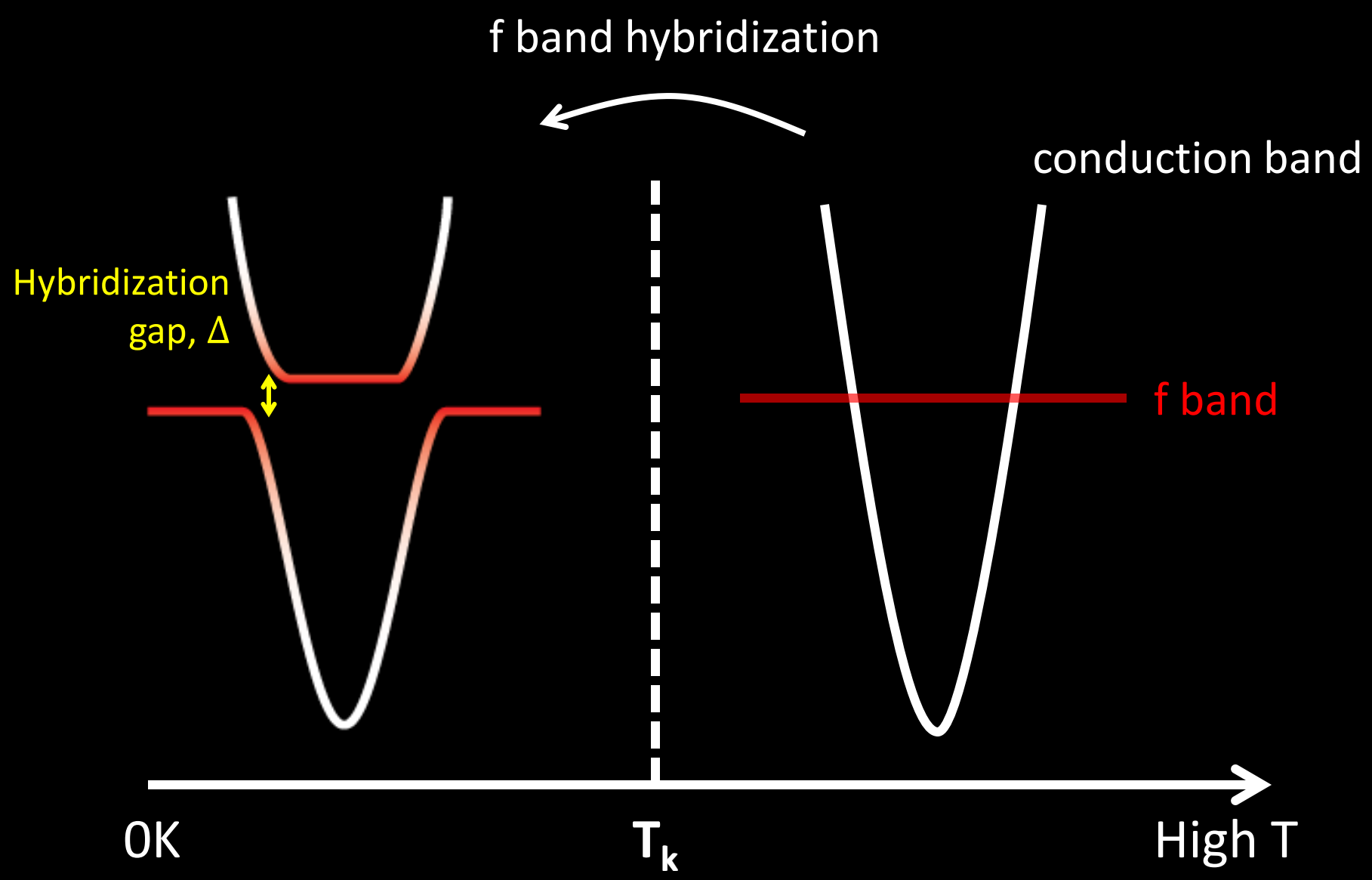
Zhu, … Elfimov, Damascelli, PRL 107, 186405 (2011)
Zhu, … Elfimov, Damascelli, PRL 110, 216401 (2013)

→ Sb is an excellent platform for exploring topological proximity effects

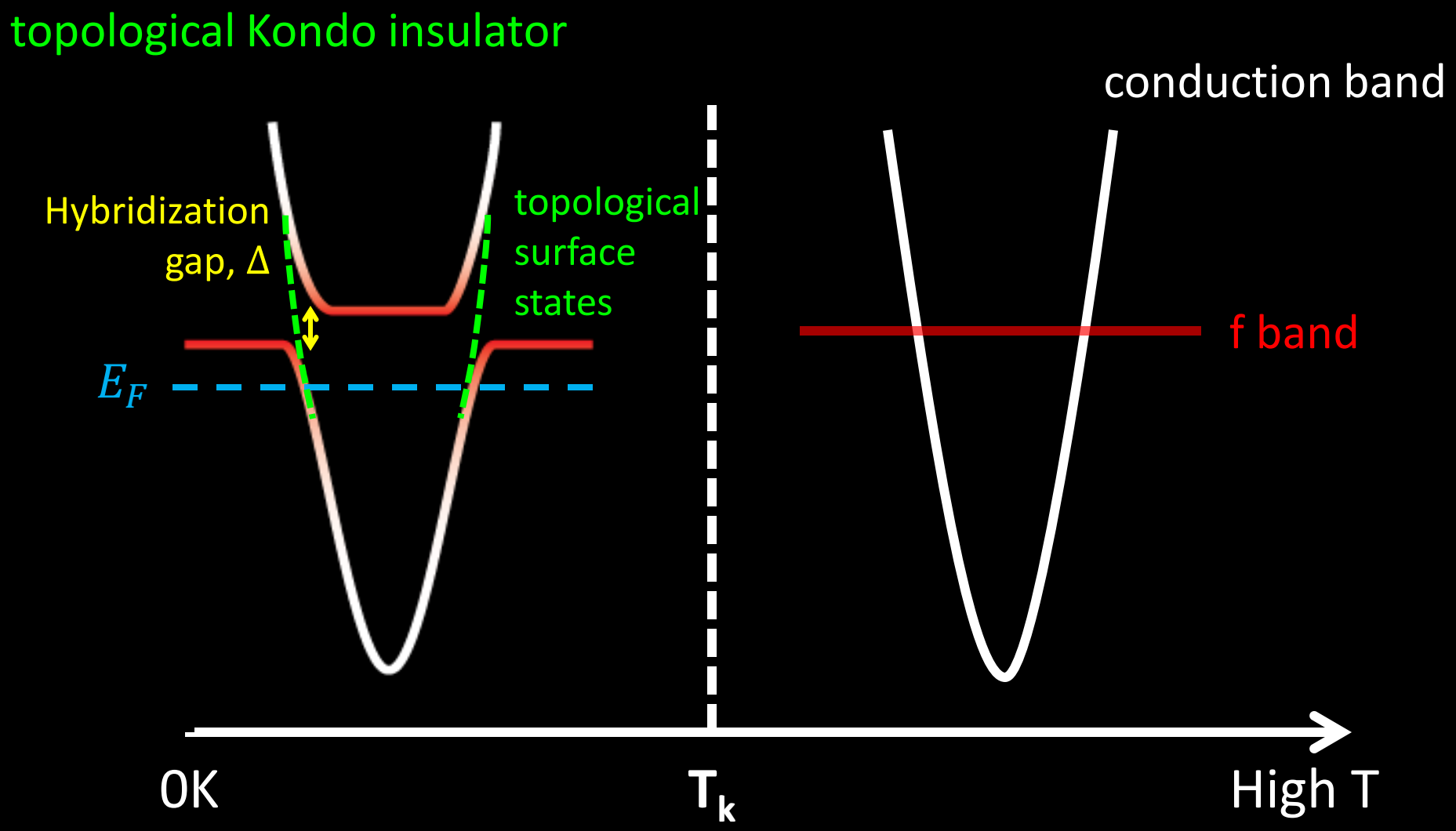
Outline

- Topological Insulators
- Scanning Tunneling Microscopy
- Nanoscale Band Structure
- Topological: Sb
- Insulator: SmB_6

Topological Kondo Insulator

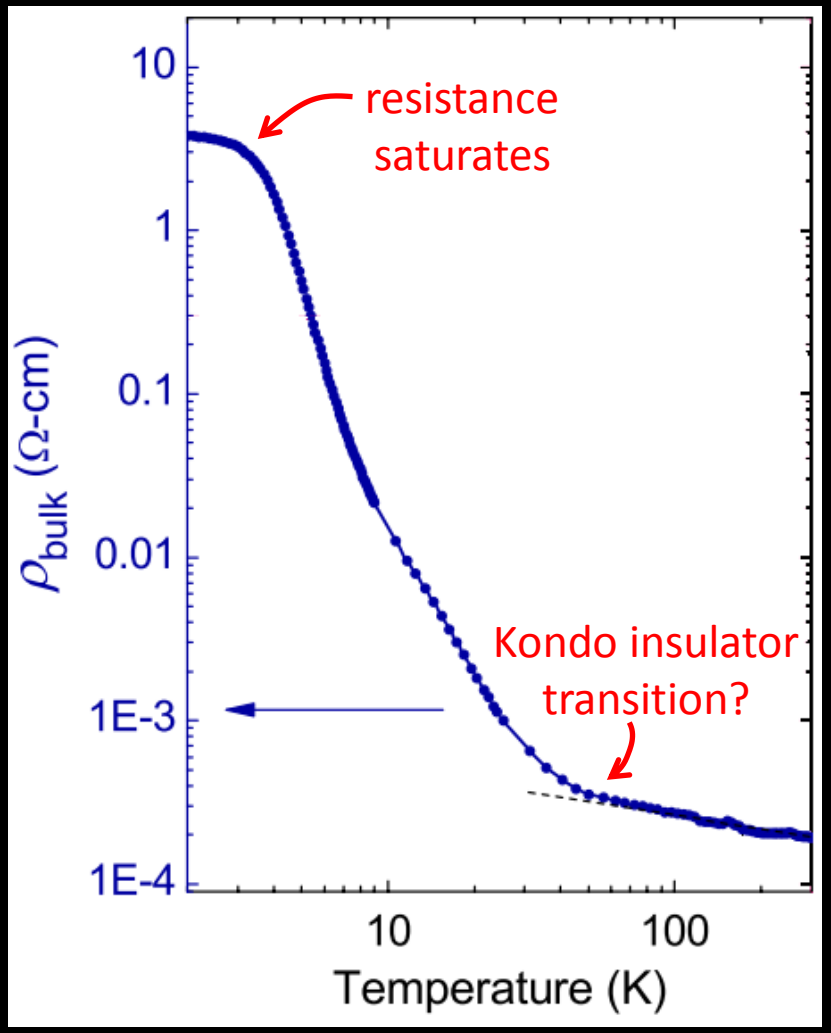


Topological Kondo Insulator

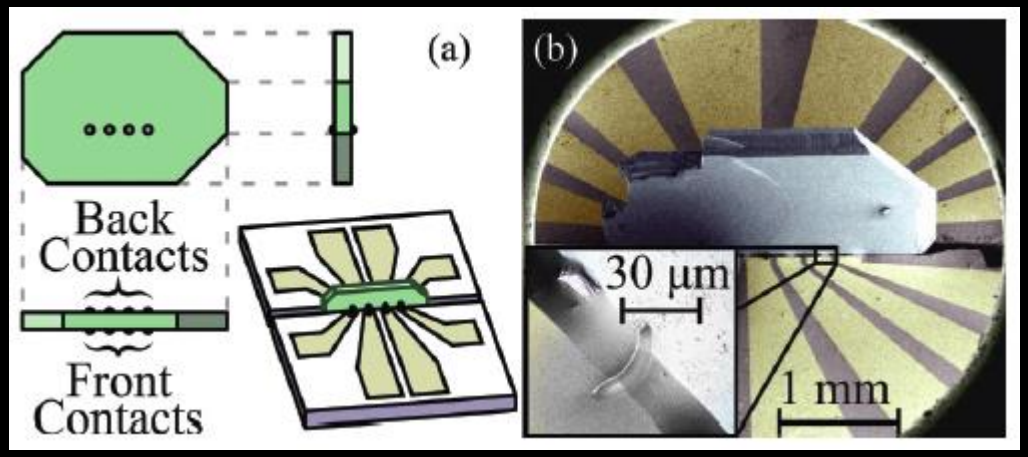


SmB_6 as possible TKI

Resistivity

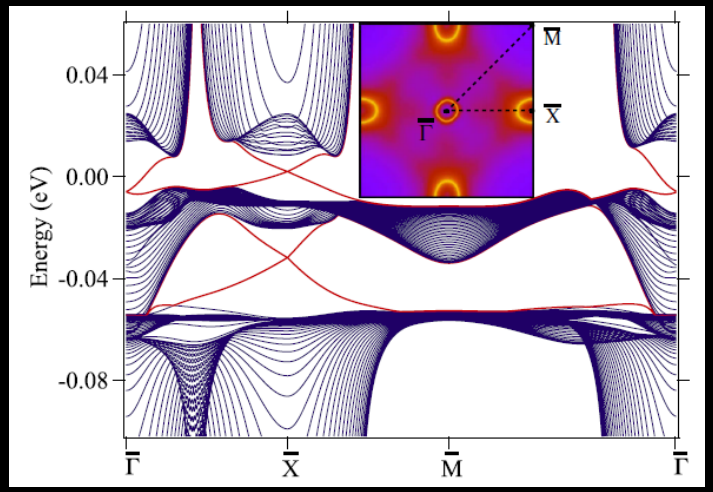


Zhang, PRX 3, 011011 (2013)



Wolgast, PRB 88, 180405 (2013)

LDA



Lu, PRL 110, 096401 (2013)

Hybridization gap in SmB_6

Transport:

Δ = 4.6 meV ..... *Menth, PRL 22, 295 (1969)*

Δ = 11.2 meV .....*Flachbart, PRB 64, 085104 (2001)*

Δ = 3.47 meV .....*Wolgast, PRB 88, 180405 (2013)*

Reflectivity & transmissivity:

Δ = 4.7 meV .....*Travaglini, PRB 29, 893 (1984)*

Δ = 19 meV .....*Gorshunov, PRB 59, 1808 (1999)*

Raman spectroscopy:

Δ = 36 meV .....*Nyhus, PRB 52, R14308 (1995)*

Planar tunneling / point contact spectroscopy:

Δ = 2.7 meV .....*Güntherodt, PRL 49, 1030 (1982)*

Δ = 14 meV .....*Amsler, PRB 57, 8747 (1998)*

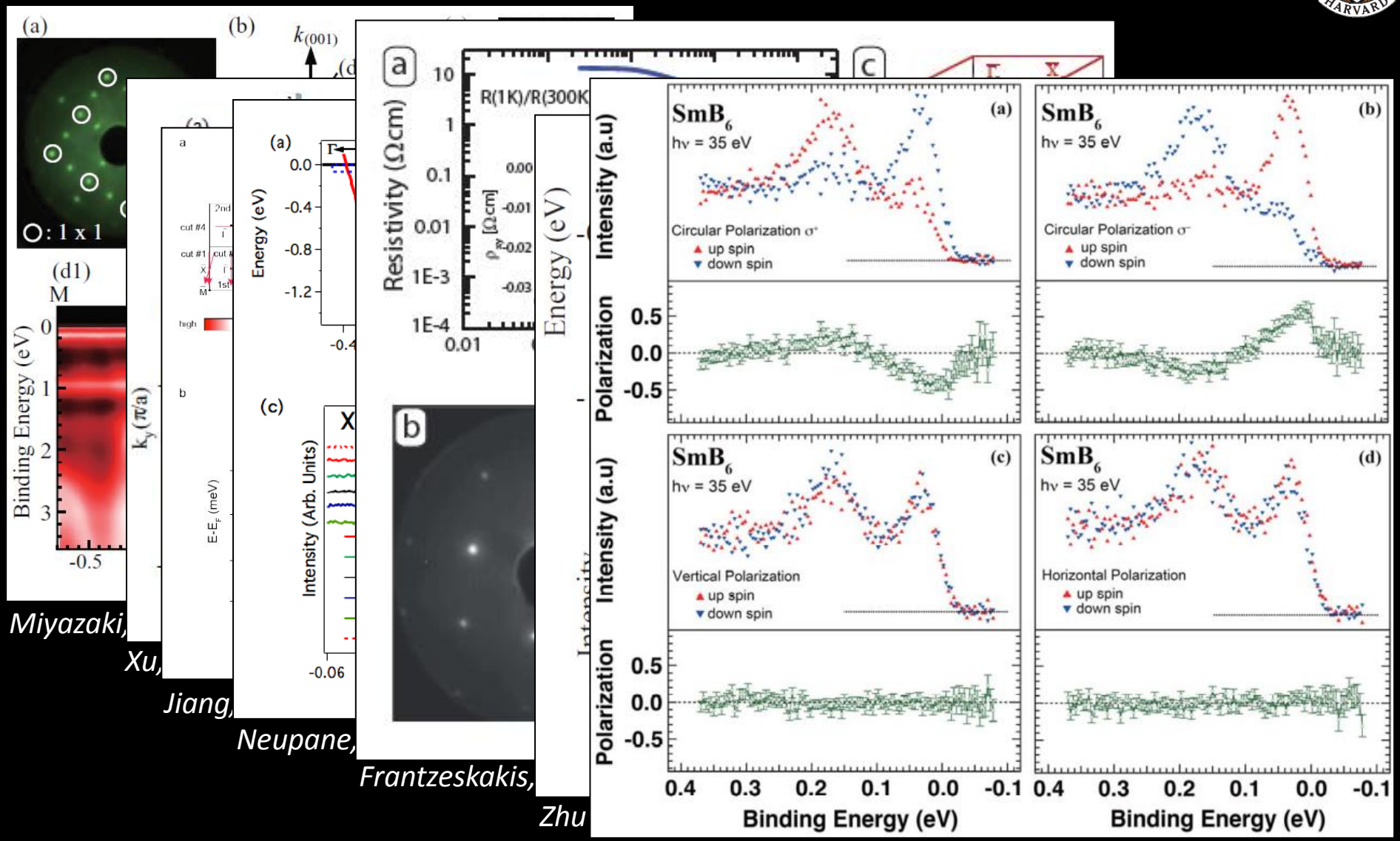
Δ = 22 meV .....*Flachbart ,PRB 64, 085104 (2001)*

Δ = 18 meV .....*Zhang, PRX 3, 011011 (2013)*

ARPES: (seven contradictory papers in last few months!)

Δ ranges from < 5 meV (entirely below E_F) to > 20 meV (spanning E_F)

SmB_6 ARPES



Miyazaki,

Xu,

Jiang,

Neupane,

Frantzeskakis,

Zhu

Suga, JPSJ 83, 014705 (2014)

But where is the hybridization gap??

SmB_6 ARPES

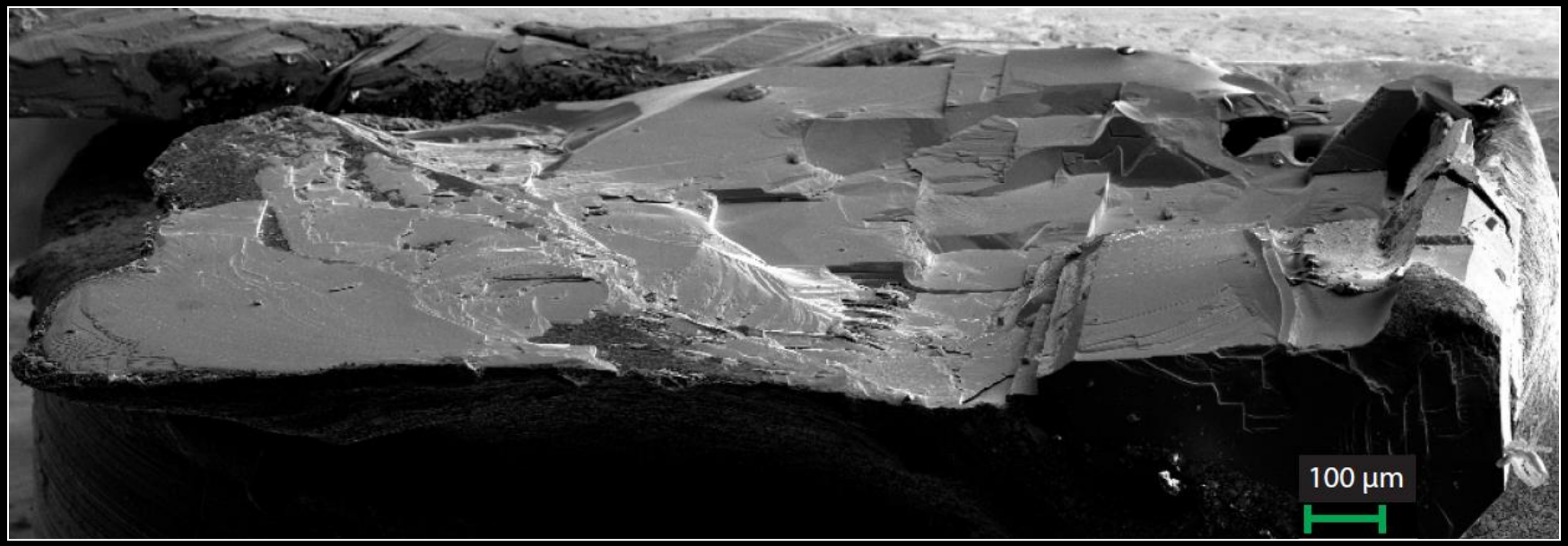
$^6H_{7/2}$ (meV)	$^6H_{5/2}$ (meV)	Δ (meV)	Spans E_F?	In-gap state?	Reference
-200	-15 (X) to -20 (Γ)	~ 15	YES	-4 to -8 meV, weakly dispersing	Miyazaki, *PRB 86, 075105 (2012)*
-160	-20	~ 20	YES	2 dispersing bands	Xu (H. Ding), *PRB 88, 121102 (2013)*
-150	-18	> 18	YES	2 dispersing bands, circular dichroism	Jiang (D.L. Feng), *Nat Com 4, 3010 (2013)*
-150	-15	14	**NO**	-4 meV, non-dispersing	Neupane (Z. Hasan), *Nat Com 4, 2991 (2013)*
-170	-40	< 5 meV	**NO**	cannot resolve	Frantzeskakis (M. Golden), *PRX 3, 041024 (2013)*
-150	-20			$\sim E_F, \sim -2$ eV dispersing	Zhu (A. Damascelli), *PRL 111, 216402 (2013)*
-150	-18				Suga, *JPSJ 83, 014705 (2014)*

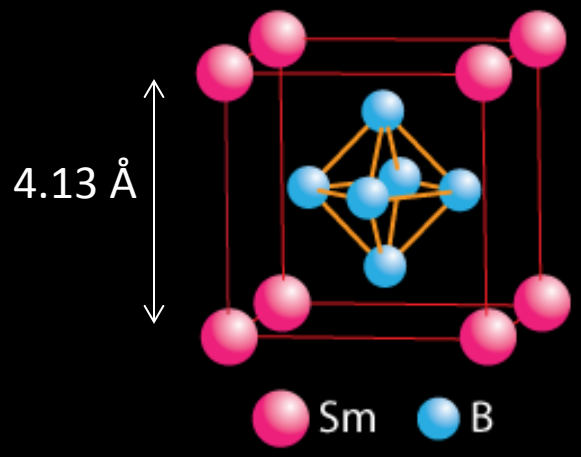
f band energies

SmB_6 is not even a Kondo insulator !?!?!

→ Need reliable, spatially resolved, empty + filled state measure of Δ

SmB_6 single crystal



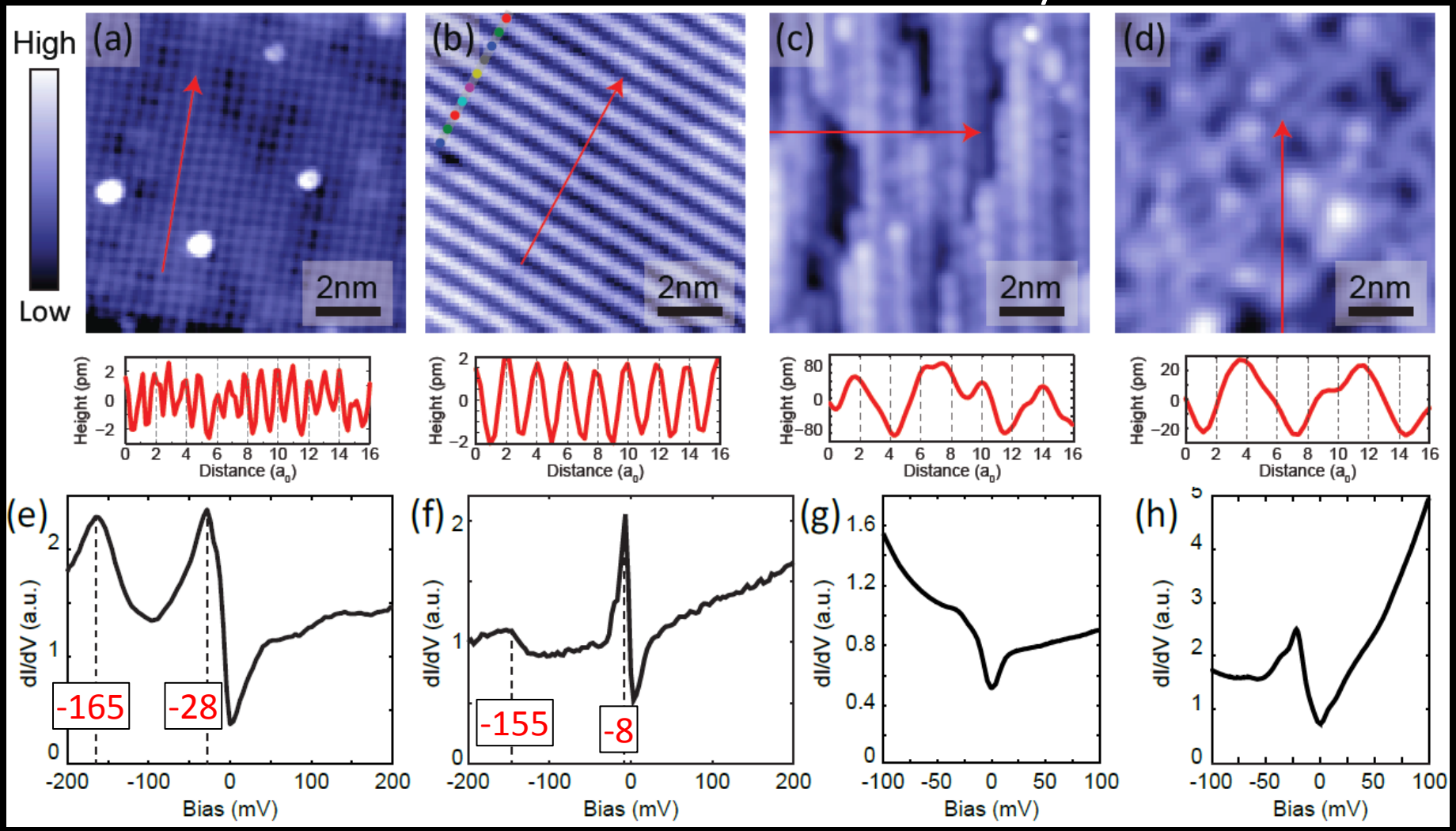


- grown by Al flux method
- cleaved in cryogenic UHV
- exposes (001) plane
- surface B:Sm ratio > 6:1

→ insert into STM

SmB_6 atomic surface morphologies

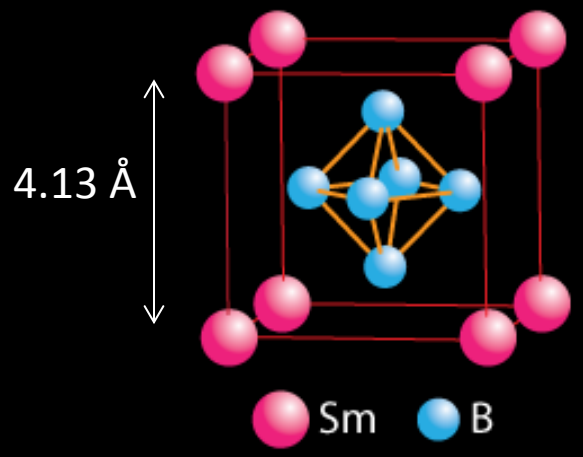
Sm 1 x 1 | Sm 2 x 1 | B filamentary | disordered

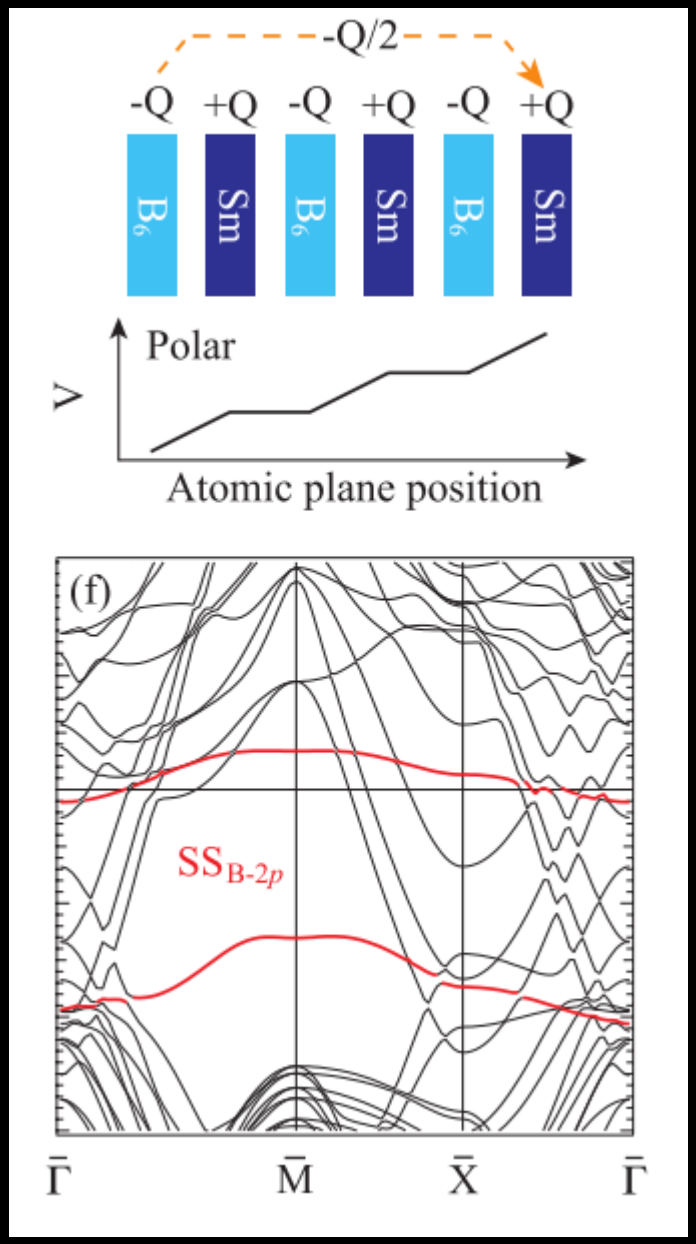


c.f. ARPES: $^6H_{7/2}$ ~ -160 to -150
$^6H_{5/2}$ ~ -20 to -14

→ band bending at this polar 1 x 1 surface

1x1 surfaces: Polarity-driven surface states?

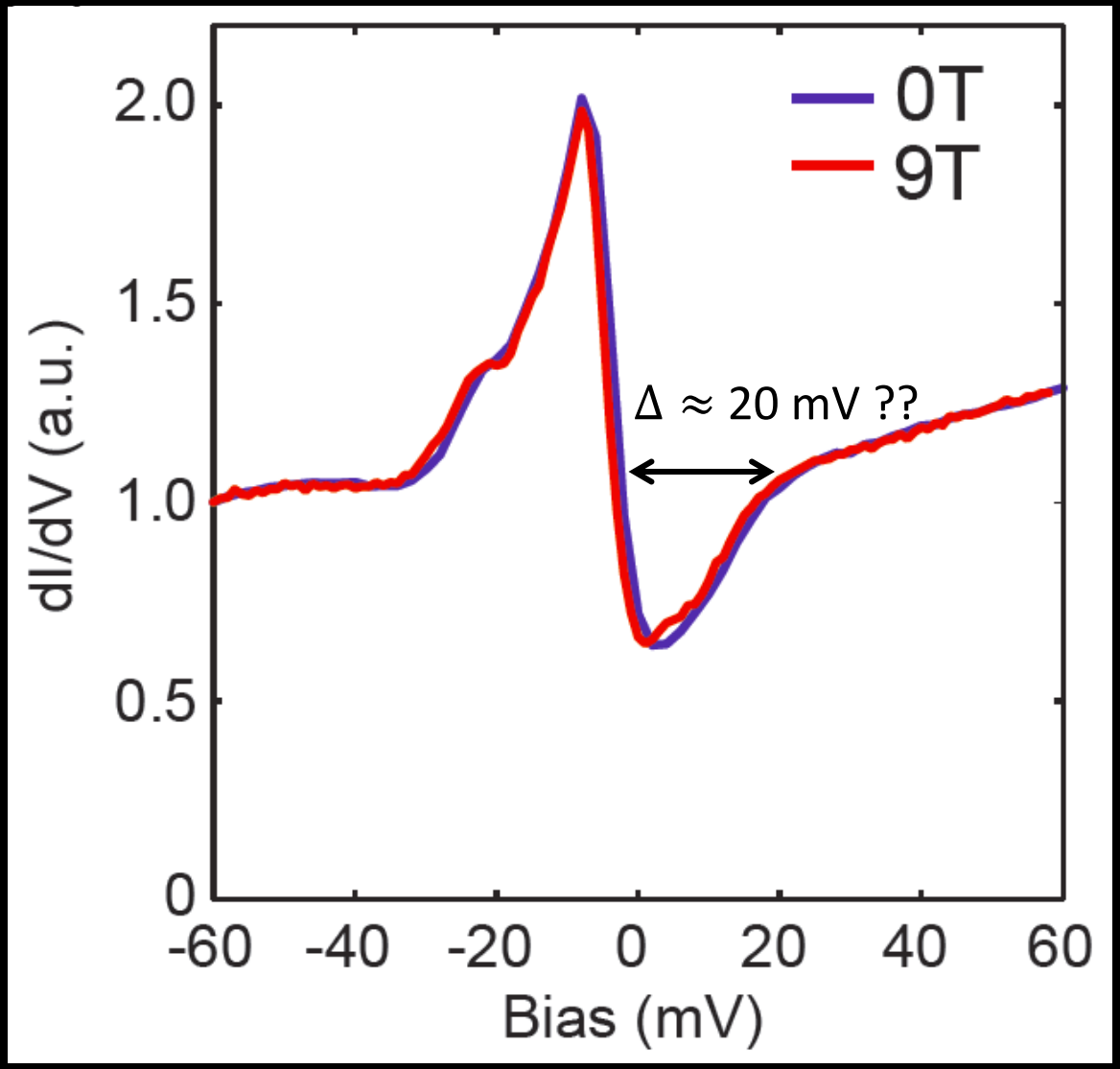




Zhu & Damascelli, PRL 111, 216402 (2013)

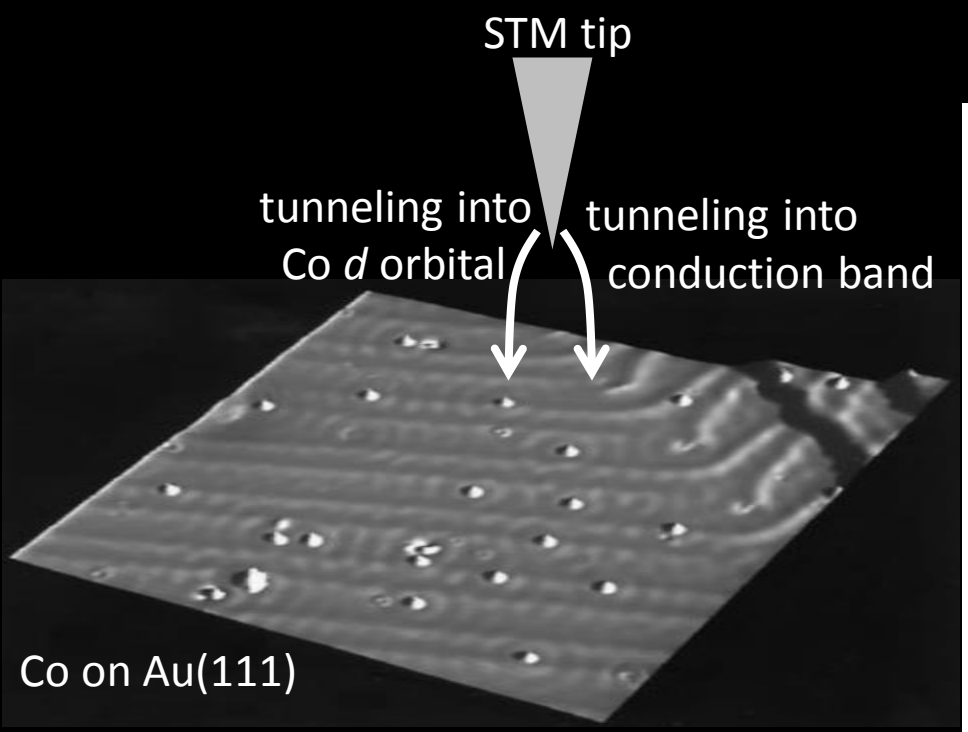
2x1 non-polar: SmB_6 hybridization gap?

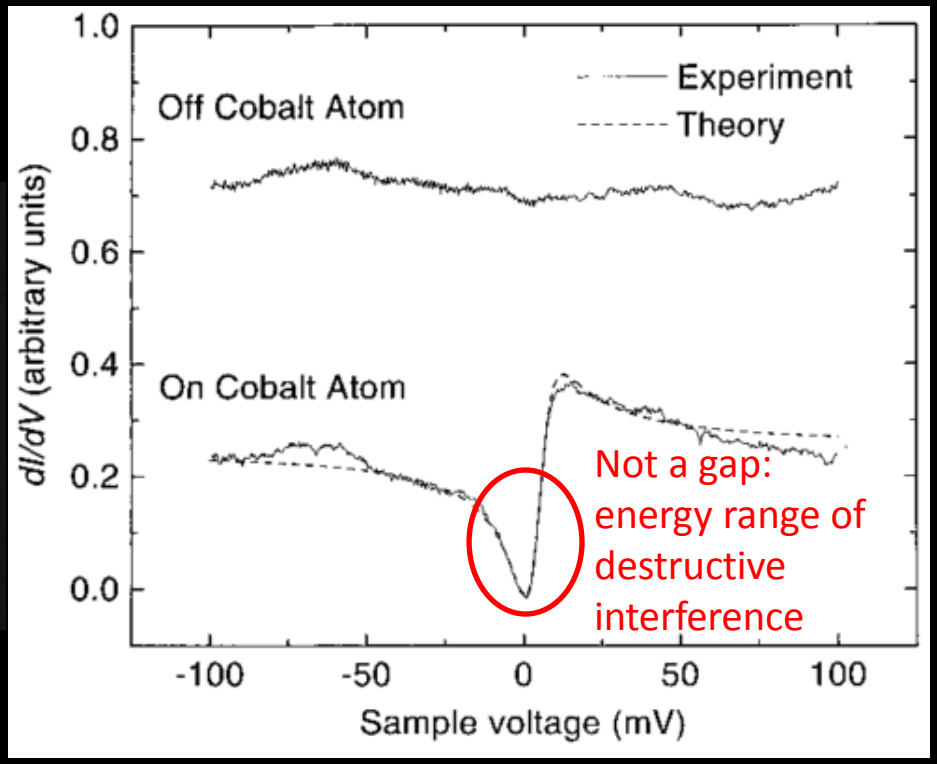
Can we just read Δ off from the spectrum?



Not so fast…

Tunneling into Kondo impurity: Fano resonance





Madhavan, Science 280, 567 (1998)

Interference between two tunneling channels gives Fano resonance:

$$\frac{dI}{dV}(\mathrm{V}) \propto \frac{(q+\epsilon)^2}{1+\epsilon^2}$$

q = ratio between tunneling channels
$\epsilon = (\mathrm{eV} - \epsilon_0)/w$;
ϵ_0 = bare resonance; w = resonance width

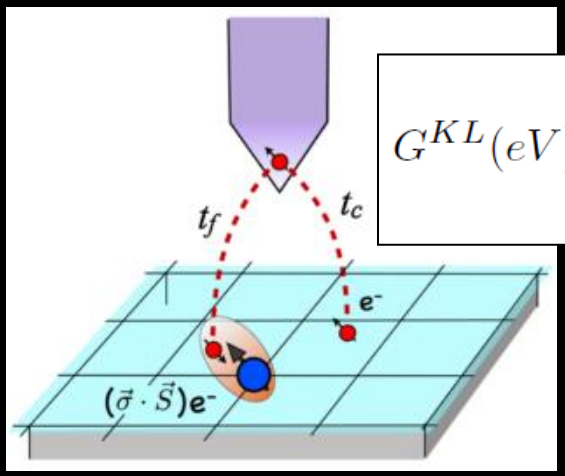
Tunneling into a Kondo Lattice

Dirty Kondo lattice: Fano is the limiting case

$$\frac{dI}{dV}(V) \propto \frac{(q+\epsilon)^2}{1+\epsilon^2}$$

Yang, PRB 79, 241107 (2009)
Wolfle, Dubi & Balatsky, PRL 105, 246401 (2010)

Clean Kondo lattice: analytic model, structureless conduction band

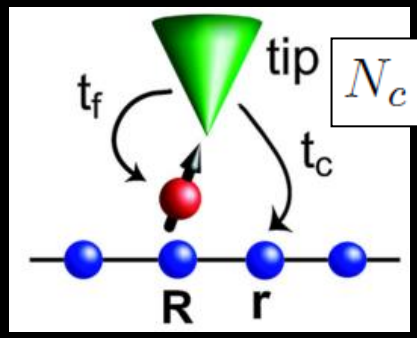


$$G^{KL}(eV) = \left(1 + \frac{v}{eV - E_0^f}\frac{t_f}{t_c}\right)^2 \ln\left[\frac{eV + D_1 - \frac{v^2}{eV - E_0^f}}{eV - D_2 - \frac{v^2}{eV - E_0^f}}\right] + \frac{D_1 + D_2}{eV - E_0^f}\left(\frac{t_f}{t_c}\right)^2$$

$$\frac{dI}{dV}(V) \propto \mathrm{Im}\left[G^{KL}(eV - i\gamma)\right]$$

Maltseva, Dzero & Coleman, PRL 103, 206402 (2009)

Clean Kondo lattice: computational model, realistic conduction band



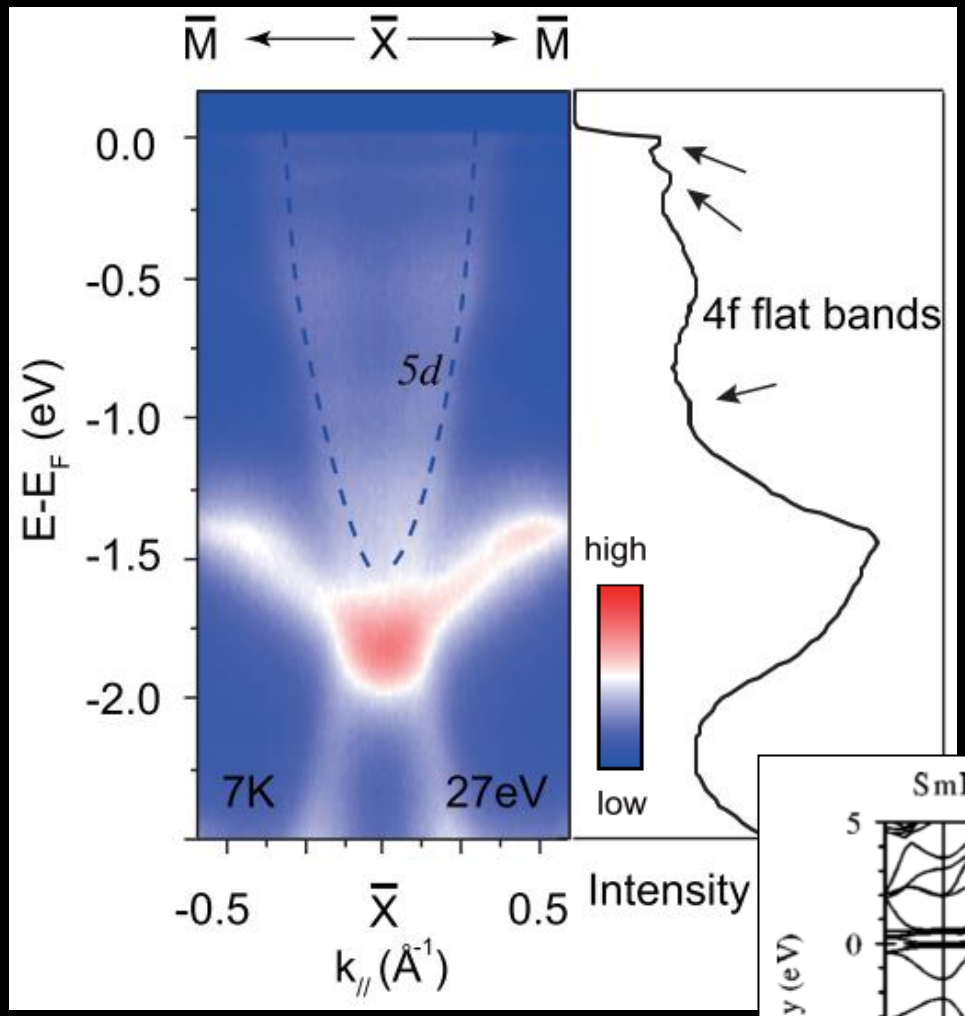
$$N_c = \mathrm{Im}\left[G_c(k,\omega)\right]; \quad N_f = \mathrm{Im}\left[G_f(k,\omega)\right]; \quad N_{cf} = \mathrm{Im}\left[G_{cf}(k,\omega)\right]$$

$$\frac{dI}{dV} \propto N_c + \left(\frac{t_f}{t_c}\right)^2 N_f + 2\left(\frac{t_f}{t_c}\right) N_{cf}$$

Figgins & Morr, PRL 104, 187202 (2010)

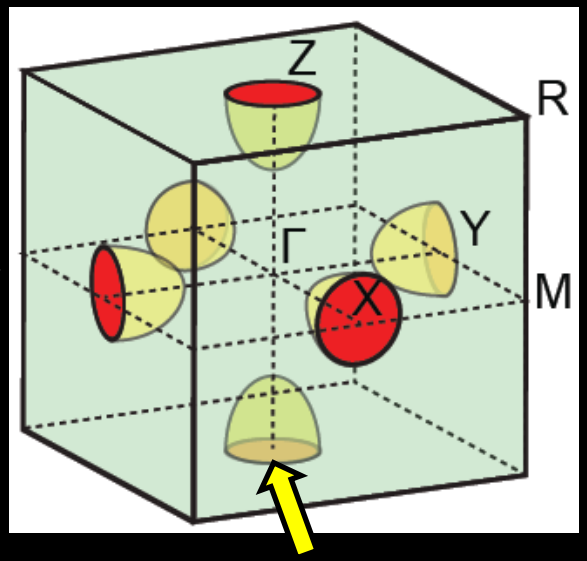
SmB_6 bands from ARPES

ARPES filled states



Jiang, Nat Comm 4, 3010 (2013)

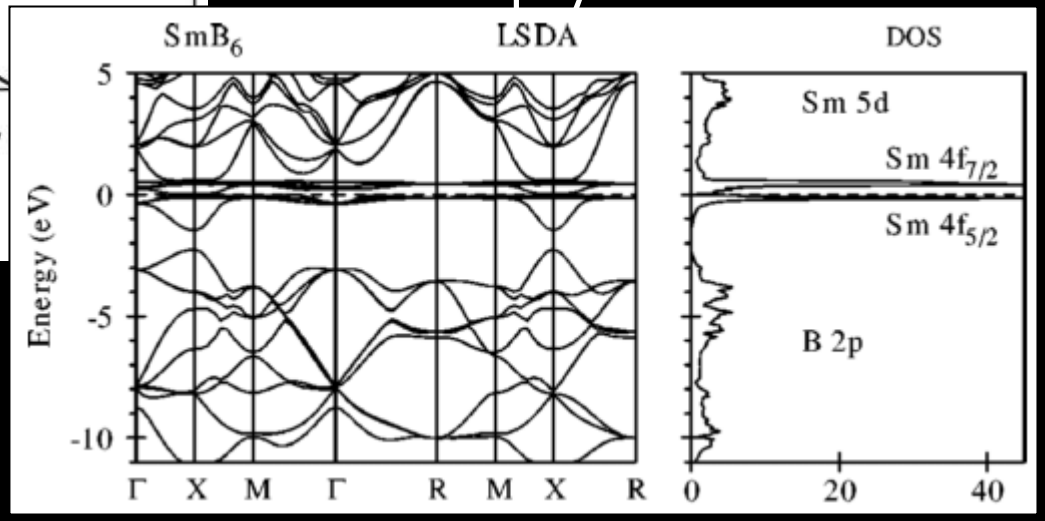
our model



Sm *5d* conduction band

$-D_1 = -1.6$ eV ; $D_2 = 3$ eV

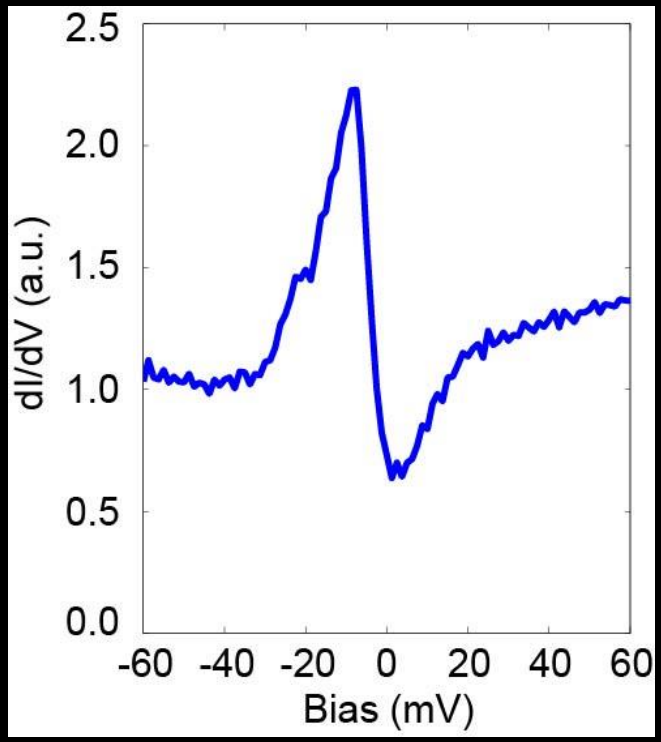
LDA for empty states



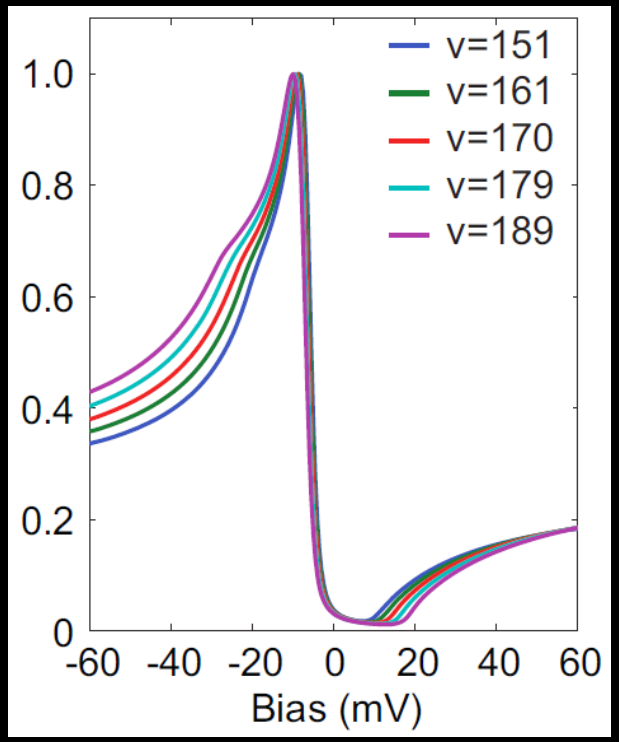
Antonov, PRB 66, 165209 (2002)

Figgins vs. Maltseva Models

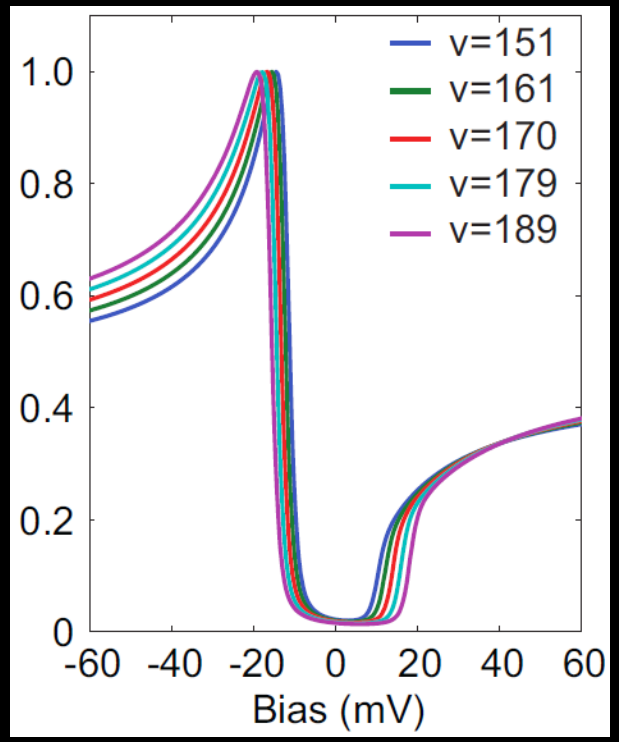
Raw dI/dV data



Figgins



Maltseva



Both models: $\gamma = k_B T$ ($T = 8$ K)

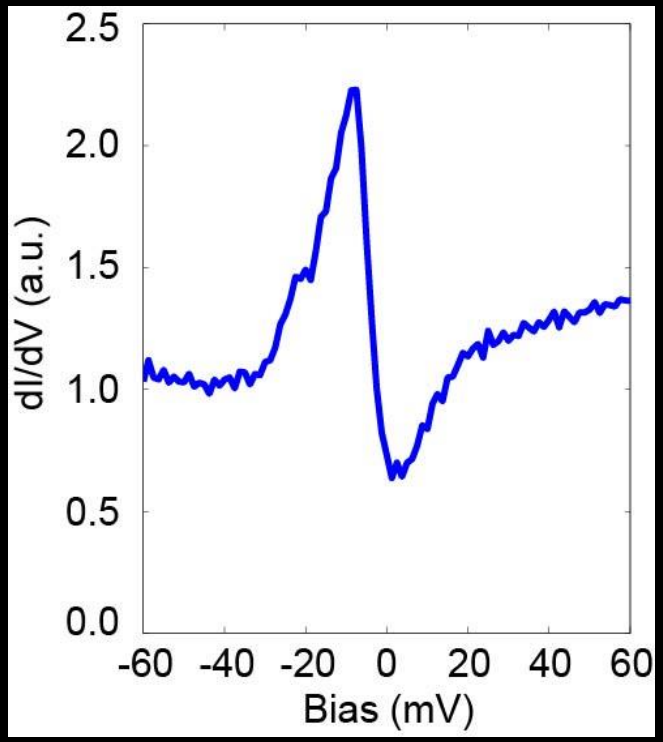
$$\frac{t_f}{t_c} = -0.055$$

$\Rightarrow v \sim 155$ meV in both models

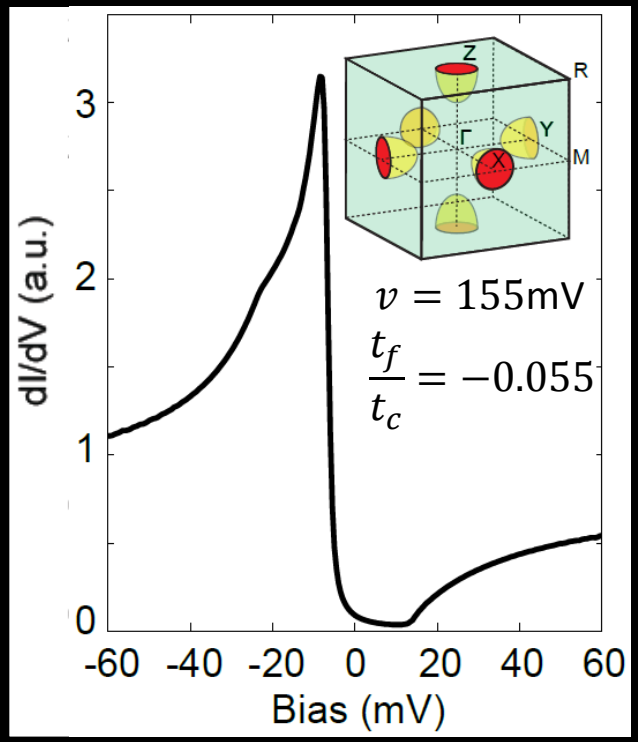
$$E_k^{\pm} = \frac{1}{2}\left(E_k^c + E_k^f\right) \pm \sqrt{\frac{1}{2}\left(E_k^c - E_k^f\right)^2 + v^2}$$

Recapturing the band structure from dI/dV

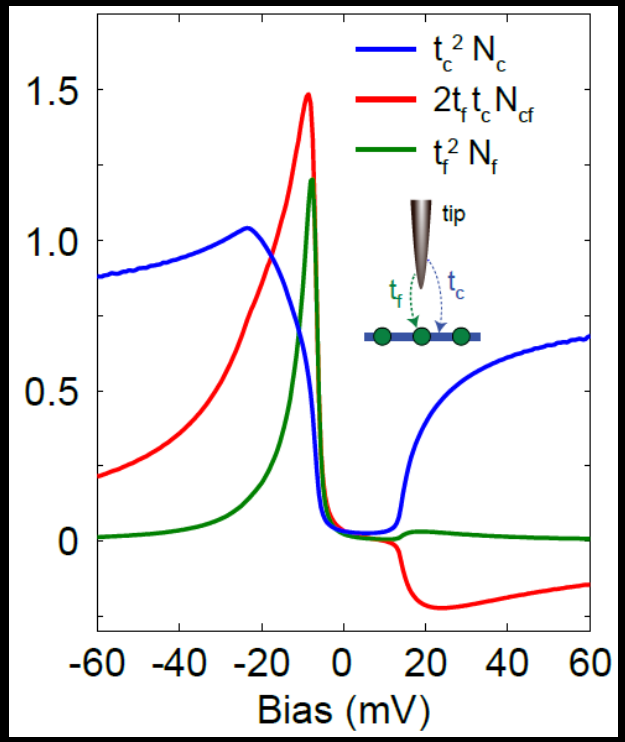
Raw dI/dV data



Figgins



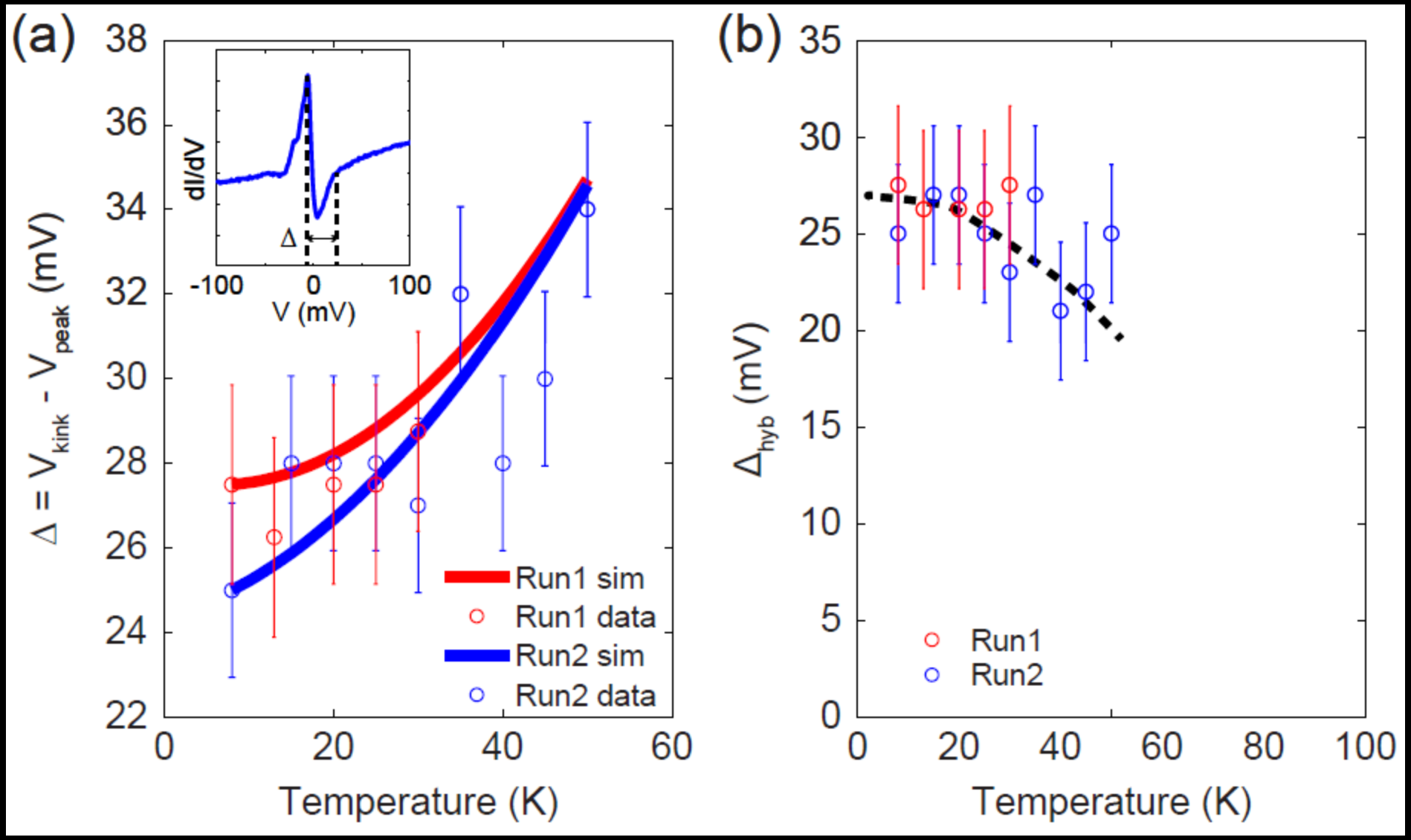
Figgins decomposition



→ dI/dV is dominated by the bare conduction band

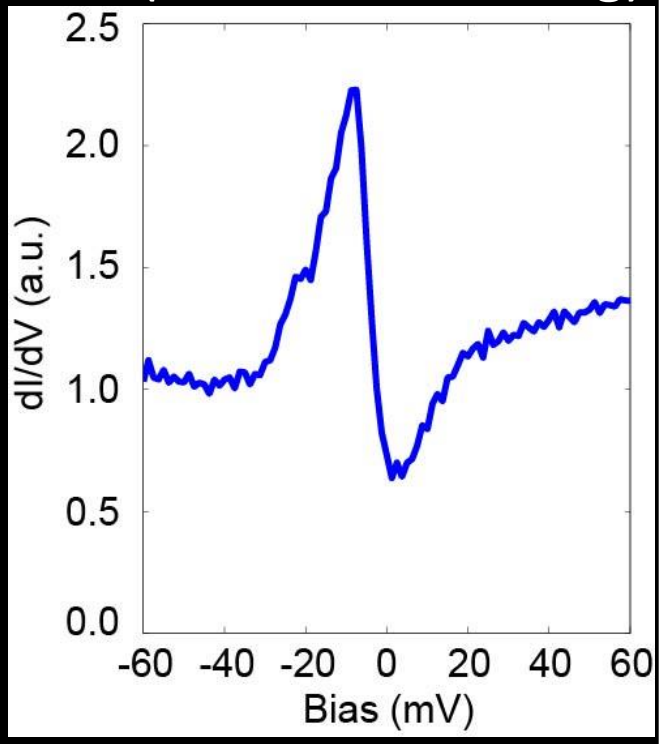
→ gap in STM dI/dV is the true hybridization gap

Kondo gap closes at T > 50K

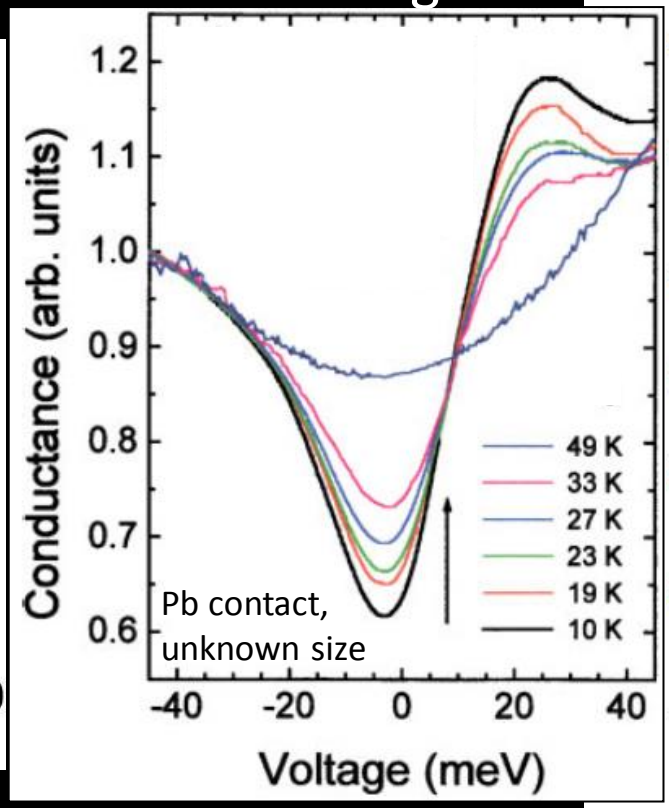


Comparison to "Point Contact Spectroscopy"

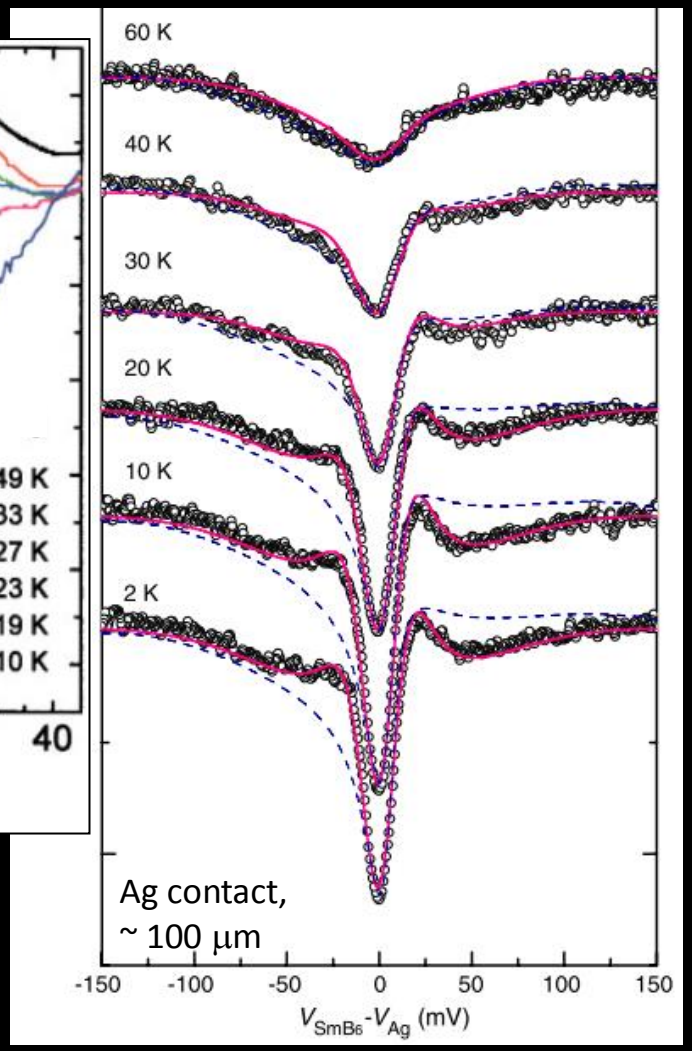
STM (vacuum tunneling)



Planar tunneling



Amsler, PRB 57, 8747 (1998)



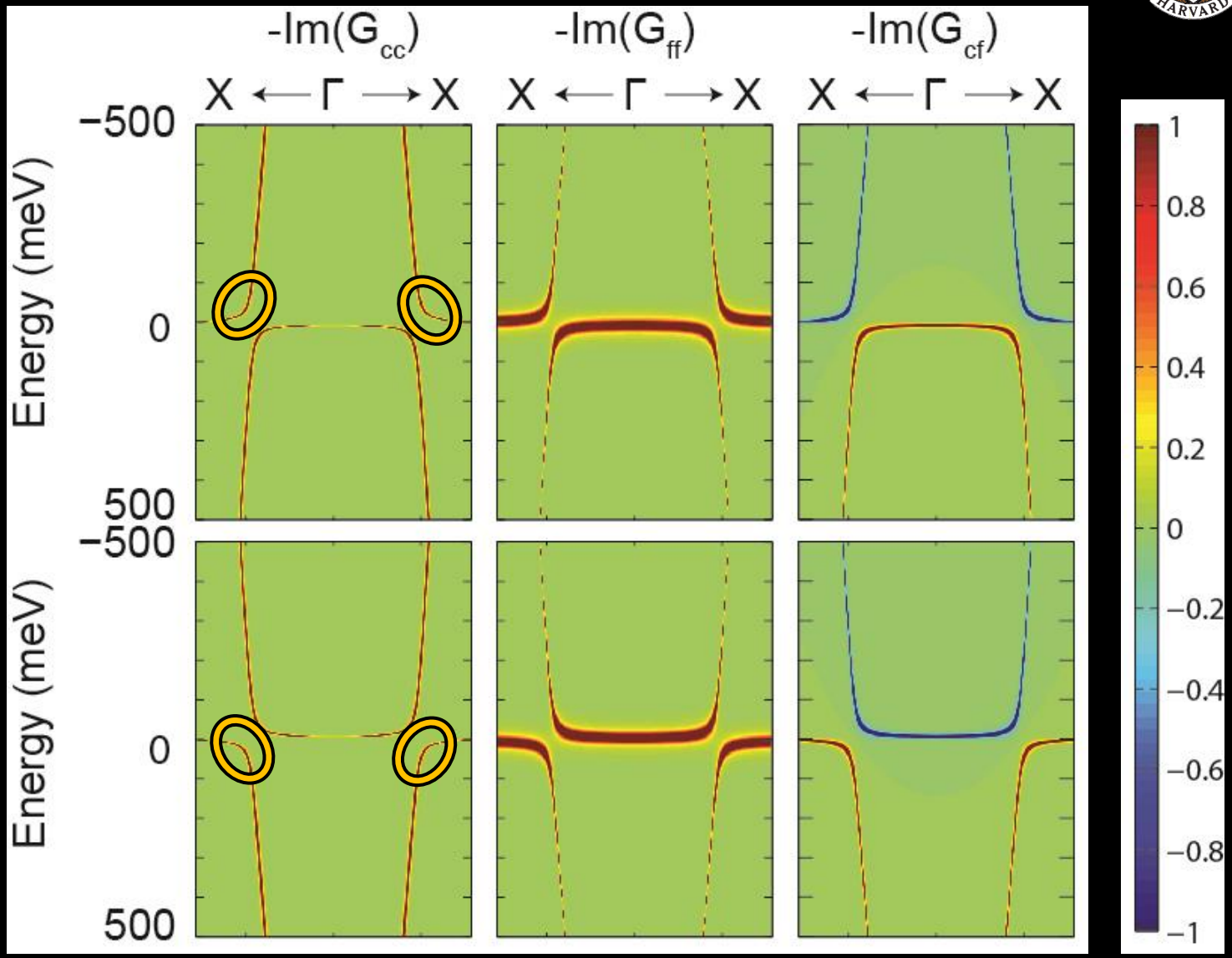
Zhang, PRX 3, 011011 (2013)

→ prominent peak is on opposite side

Electron vs. hole

Hole-like conduction band

Electron-like conduction band

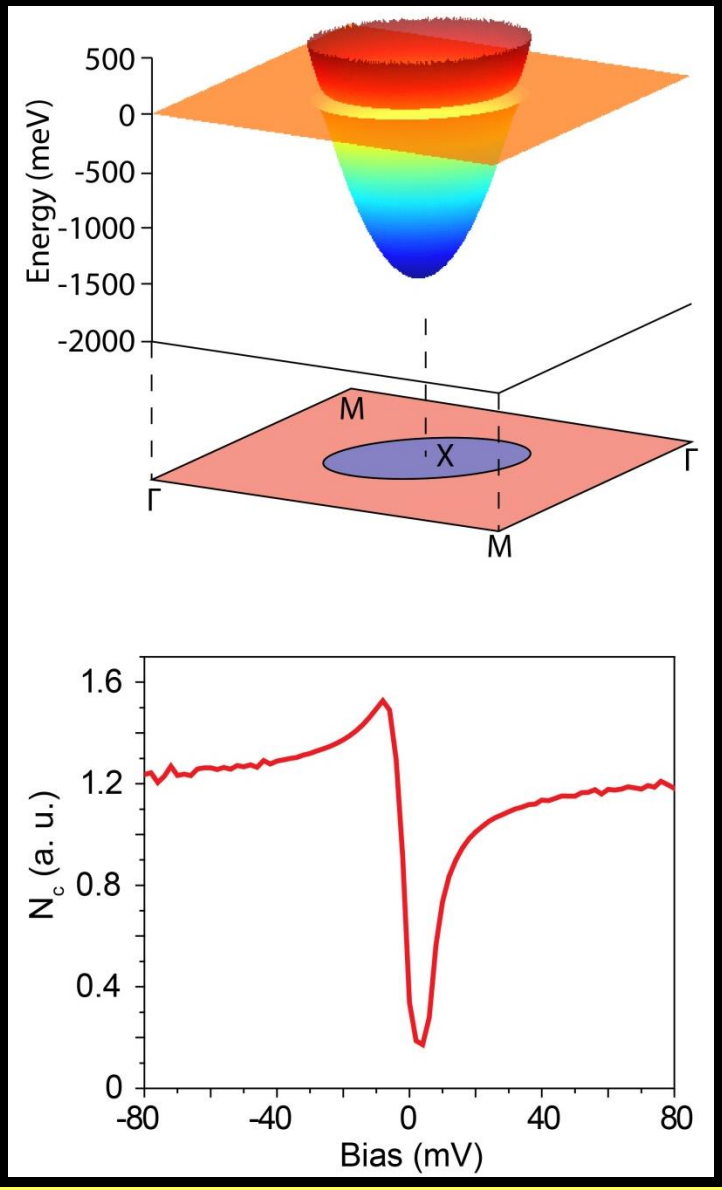


In 3-dim, "outside shell" will give more prominent peak than "inside shell"

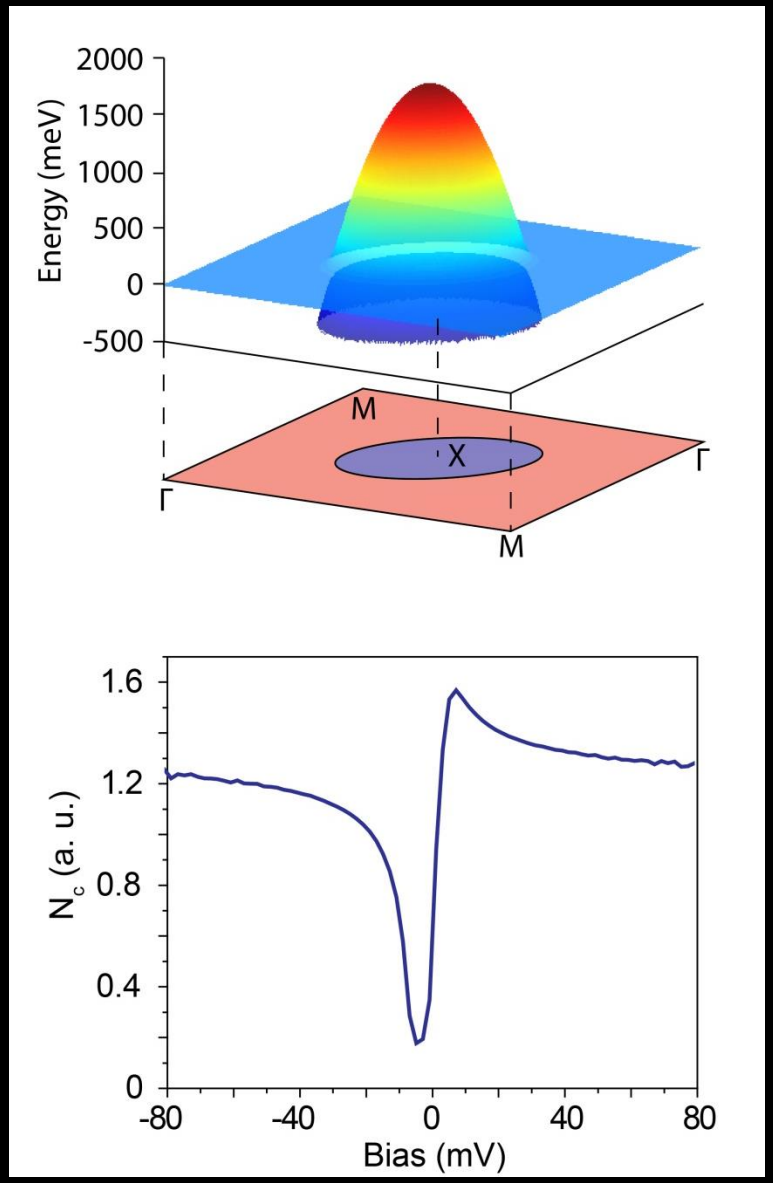
→ Expect conduction band peak on negative side

Electron vs. Hole

Electron-like conduction band

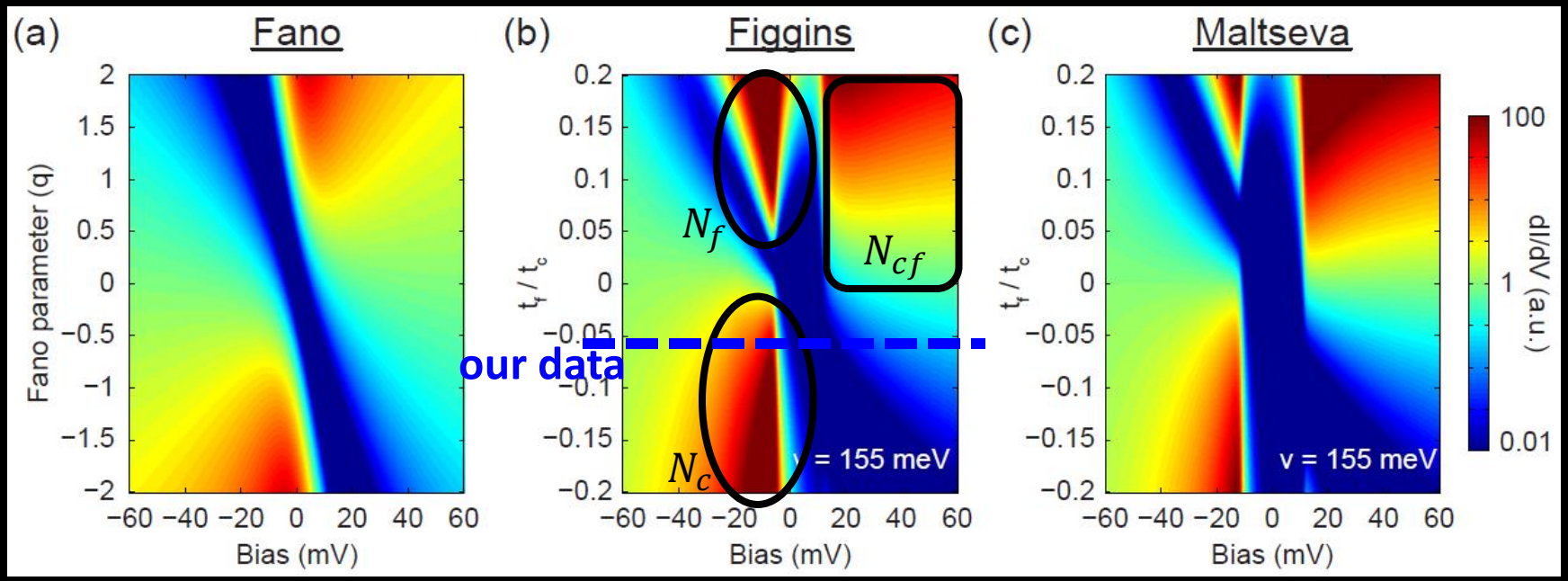


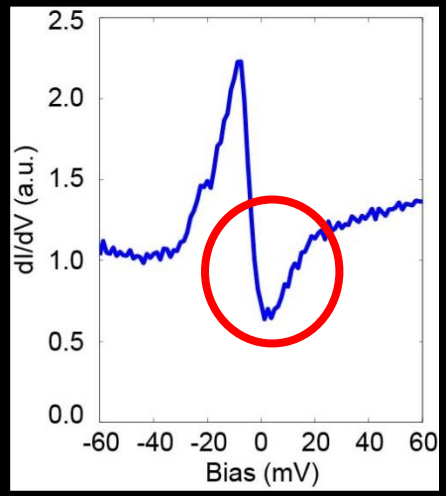
Hole-like conduction band



Tunneling ratio: t_f/t_c

$$\frac{dI}{dV} \propto N_c + \left(\frac{t_f}{t_c}\right)^2 N_f + 2\left(\frac{t_f}{t_c}\right) N_{cf}$$





All 3 models show $\mathrm{dI/dV} \approx 0$ in gap
(< 10% of background)

c.f. non-zero dI/dV in data

Comparison to ARPES

$^6H_{7/2}$ (meV)	$^6H_{5/2}$ (meV)	Δ (meV)	Spans E_F?	In-gap state?	2x1 ?	Reference
-200	-15 (X) to -20 (Γ)	~ 15	YES	-4 to -8 meV, weakly dispersing	yes (LEED)	Miyazaki, *PRB 86, 075105 (2012)*
-160	-20	~ 20	YES	2 dispersing bands	yes (folding)	Xu (H. Ding), *PRB 88, 121102 (2013)*
-150	-18	> 18	YES	2 dispersing bands, circular dichroism	yes (folding)	Jiang (D.L. Feng), *Nat Com 4, 3010 (2013)*
-150	-15	14	**NO**	-4 meV, non-dispersing	?	Neupane (Z. Hasan), *Nat Com 4, 2991 (2013)*
-170	**-40**	< 5 meV	**NO**	cannot resolve	no (LEED)	Frantzeskakis (Golden), *PRX 3, 041024 (2013)*
-150	-20			$\sim E_F$, ~ -2 eV dispersing	no (LEED)	Zhu (Damascelli), *PRL 111, 216402 (2013)*
-150	-18				?	Suga, *JPSJ 83, 014705 (2014)*

f band energies

→ partial 2x1 surface gives the -8 meV state:
this is the f band itself, not an "in-gap" state!!

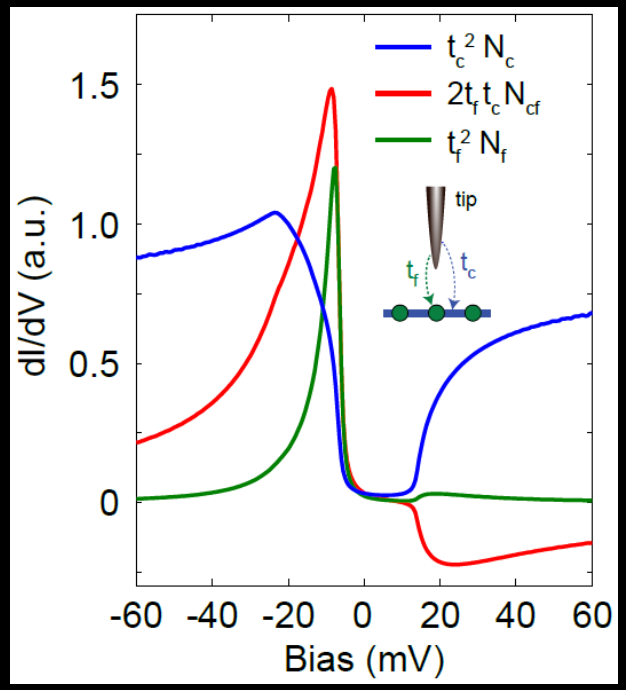
→ complete 1x1 surface causes band-bending, looks like Kondo metal?

SmB_6 conclusions

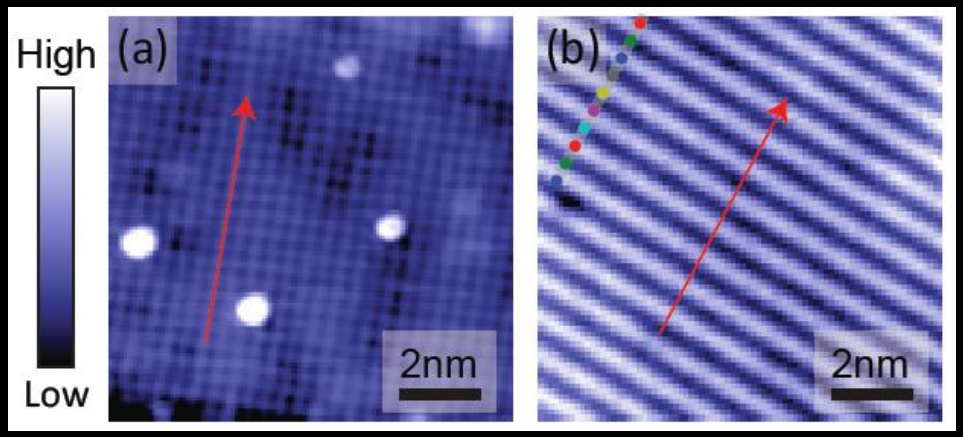
1. Band bending on varying surface morphologies

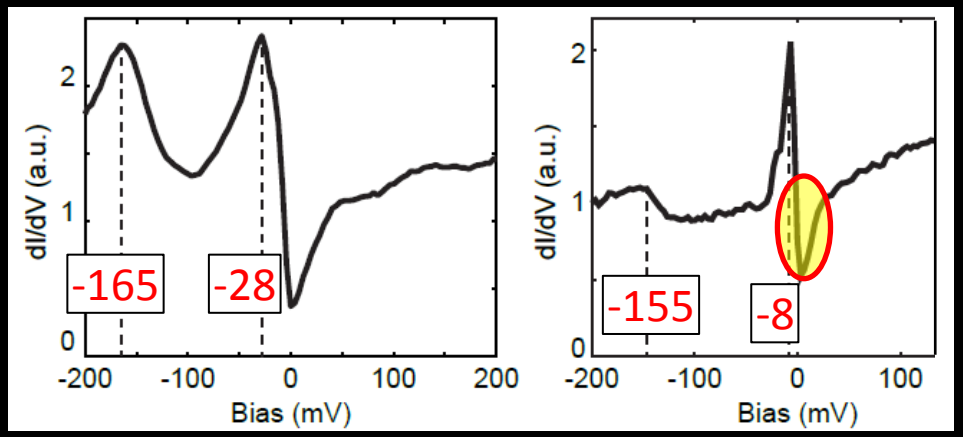
Need to decompose dI/dV into DOS & interference

2. Hybridization gap spans E_F → Kondo insulator



Sm 1 x 1 Sm 2 x 1





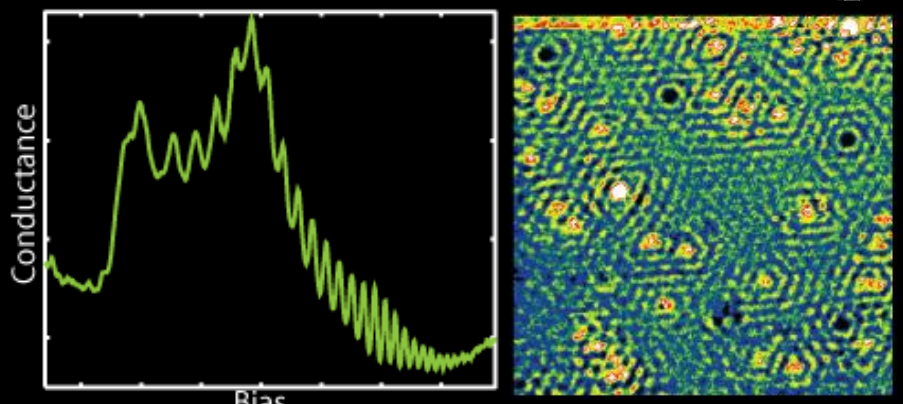
3. Residual 'in-gap' spectral weight

Next step: QPI to look for Dirac cone

arxiv:1308.1085

Conclusions

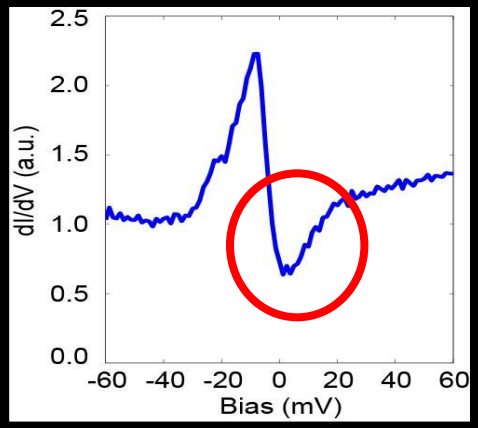
- Nanoscale Band Structure
  - Quasiparticle Interference
  - Landau Quantization
  - → Reconciled!!



arxiv:1311.1758

- Topological surface states in Sb:
  - mean free path → $\ell = 65$ nm
  - spin-orbit coupling → $v_0 = 0.51$ eV·Å
  - g-factor → $g = 12.8$

- SmB_6: Topological Kondo **Insulator**?
  - Hybridization gap spans E_F → Kondo insulator
  - In-gap spectral weight → topological surface state?



arxiv:1308.1085