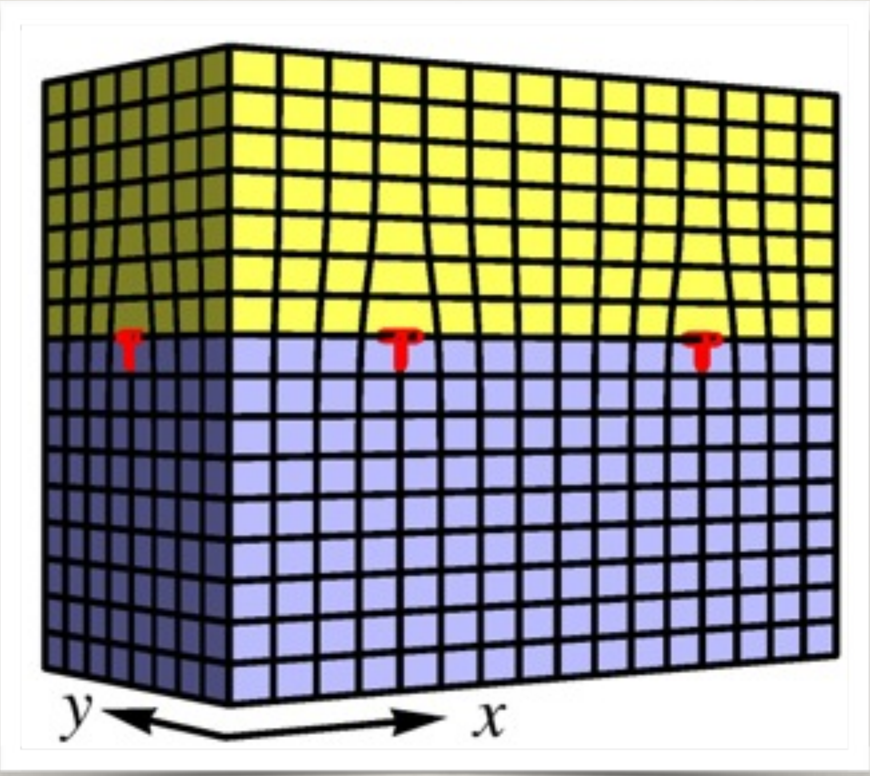
KITP, July 2015

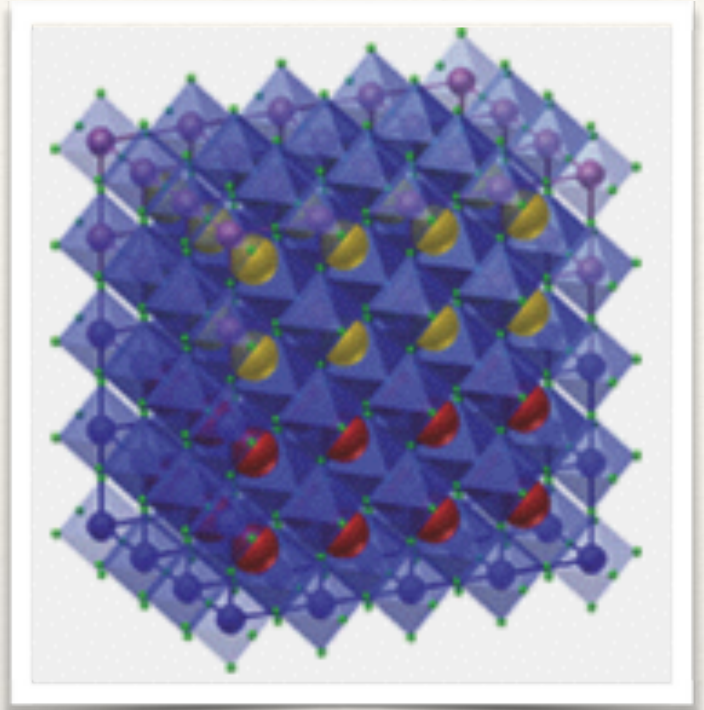
Strain-induced Partially Flat Band, Helical Snake States, and Interface Superconductivity in Topological Crystalline Insulators

Evelyn Tang
Liang Fu

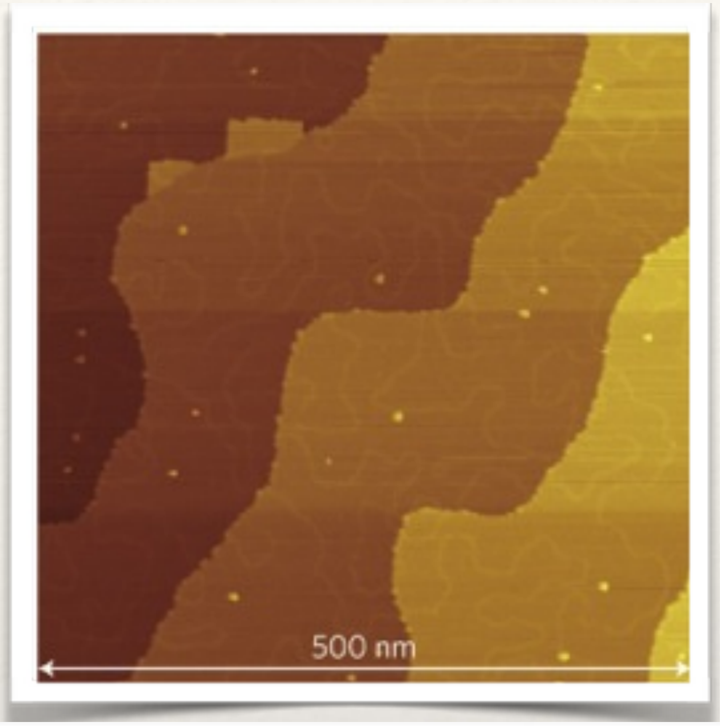
Nature Physics **10**, 964-969 (2014)



Interface superconductivity

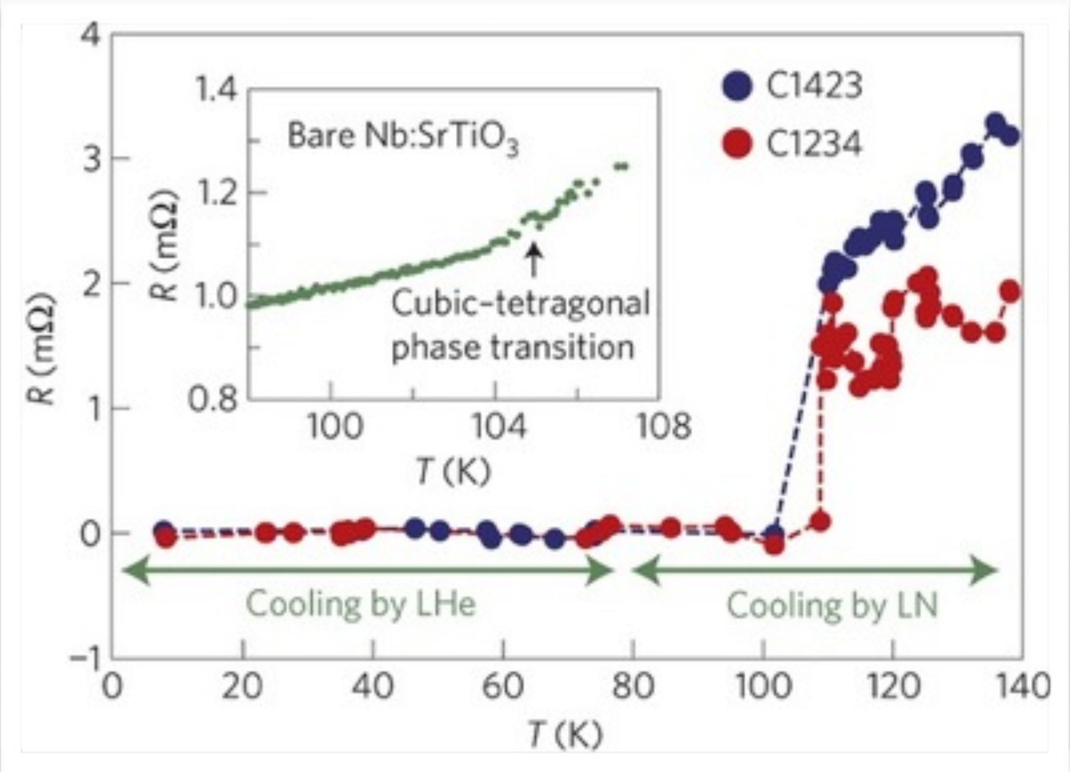


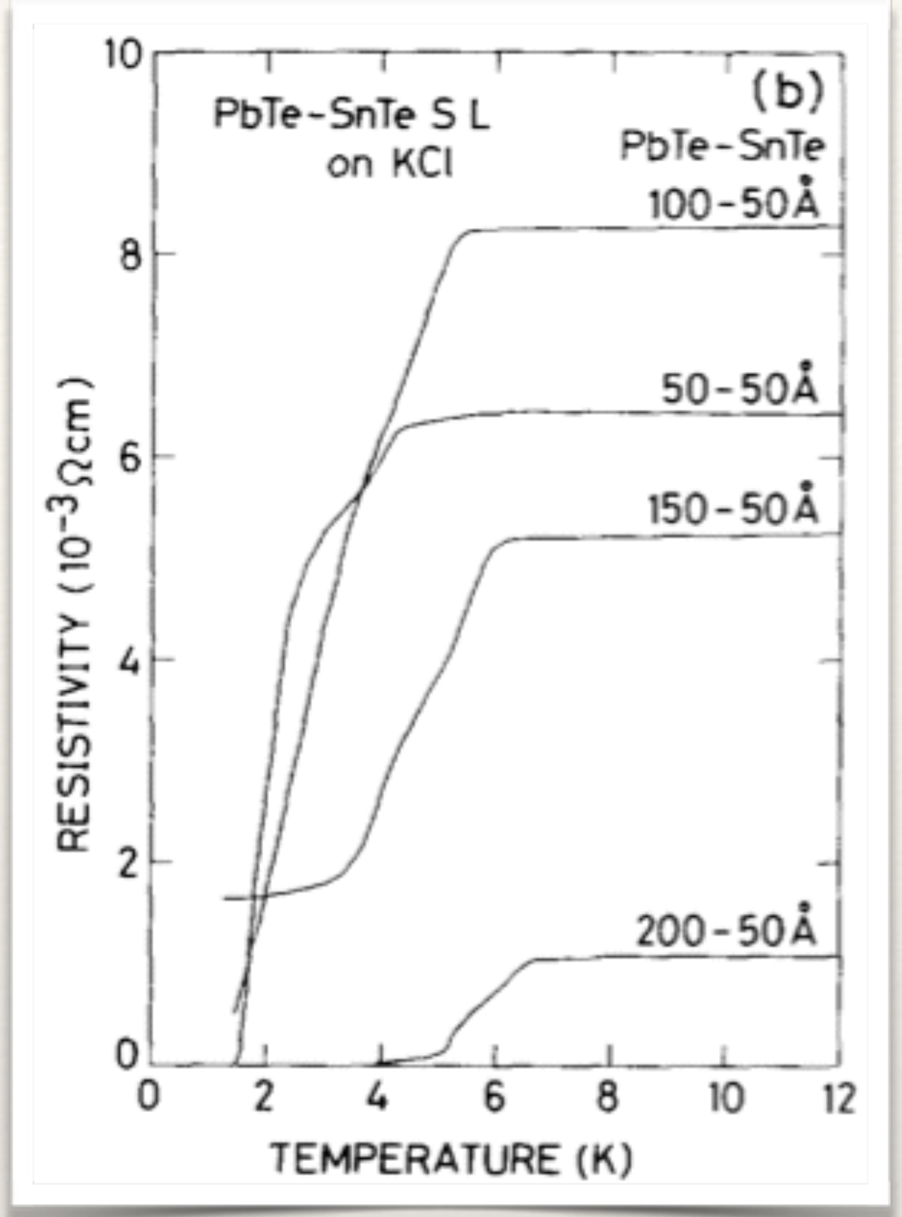
LAO/ STO
Hwang group,
Nature 2004
$T_c \sim 0.5K$

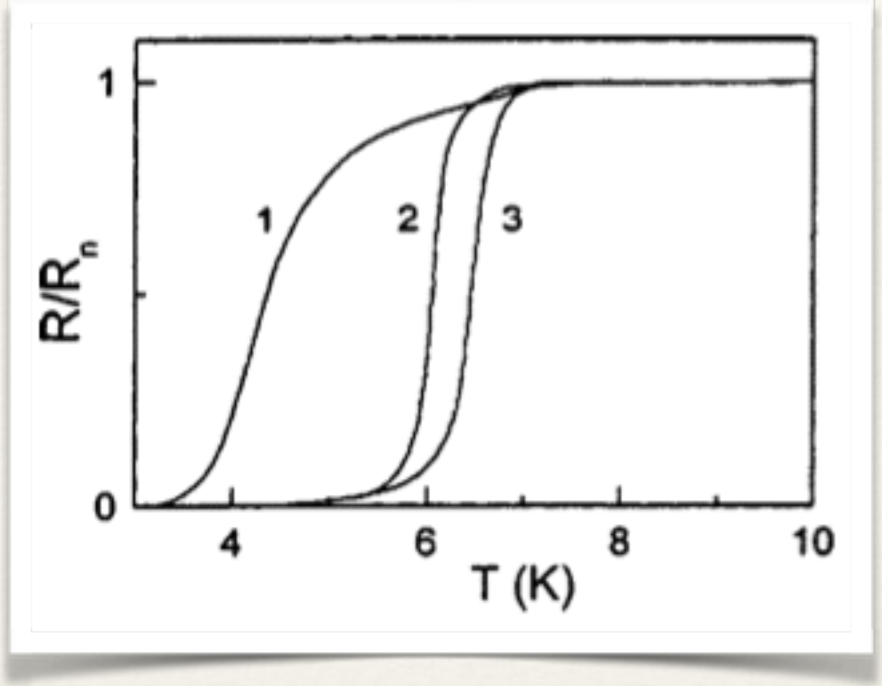


1-layer FeSe/ STO
Liu-Xue-Jia group,
Nat. Materials 2014
$T_c > 100K$

- Interface exhibits superconductivity (or much higher T_c) than constituent materials







PbS/PbSe; PbTe/PbSe; PbS/YbS bilayers
N.Y. Fogel et al., PRB 2002

PbTe/SnTe superlattice
K. Murase et al., Surf. Sci 1986

Older experiments

Single films non-superconducting; multilayers T_c~6K

Why superconductivity at the interface?
What is the origin or mechanism?

Outline

A. Our theoretical model

   1. IV-VI semiconductors ➤ Topological crystalline insulators

   2. Strain + Dirac fermions ➤ Pseudo-magnetic field

   3. Landau-levels ➤ Large DOS ➤ Non-BCS superconductivity

B. Comparison with experiments / Our predictions

C. Discussion and outlook

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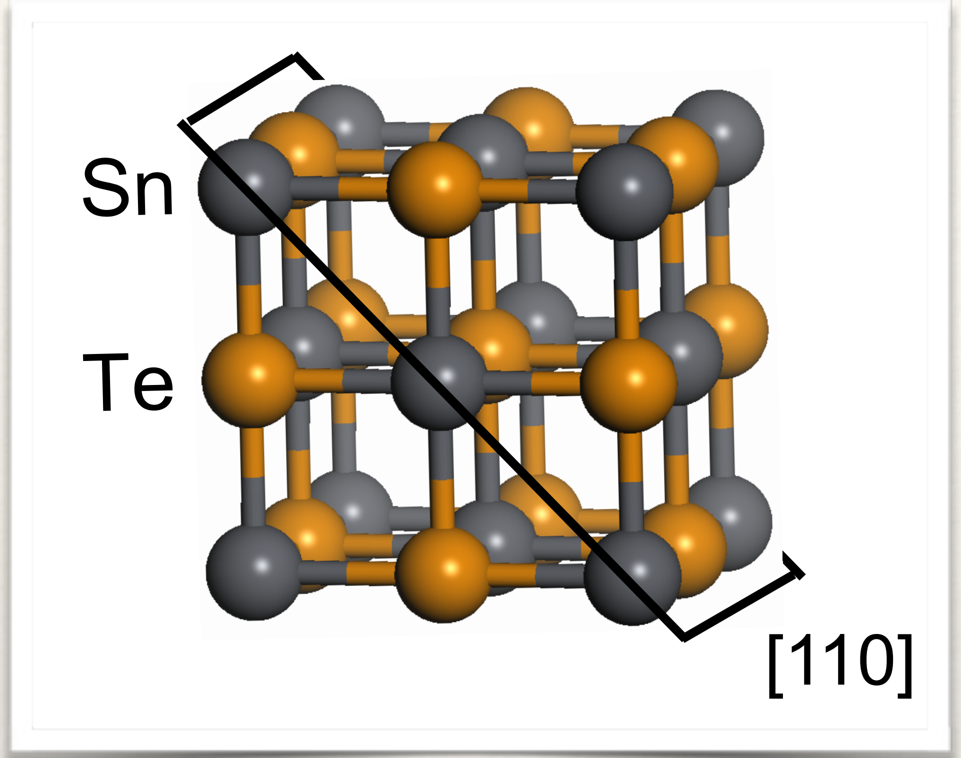
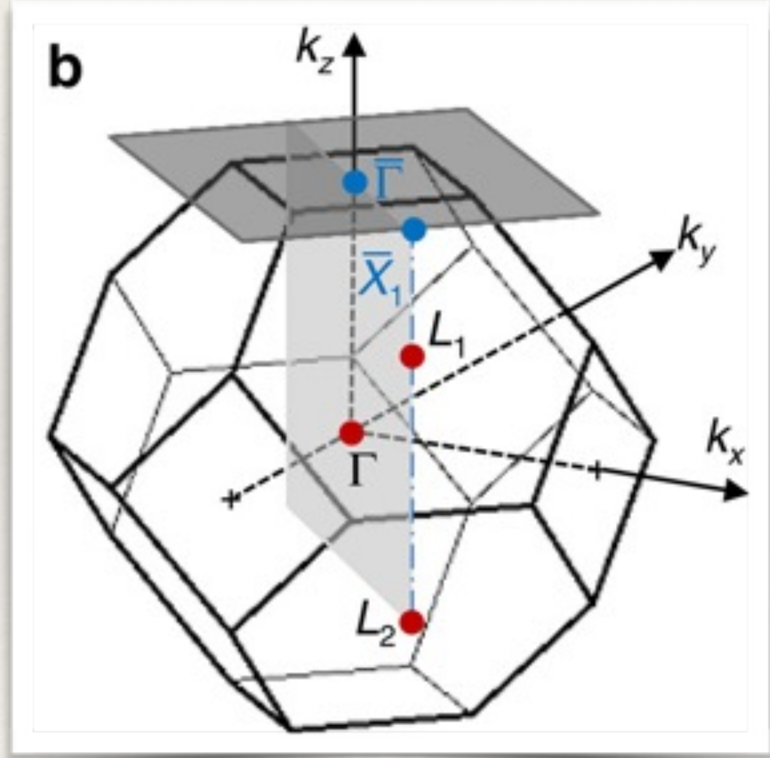
IV-VI semiconductors



Rocksalt FCC structure
Mirror symmetry

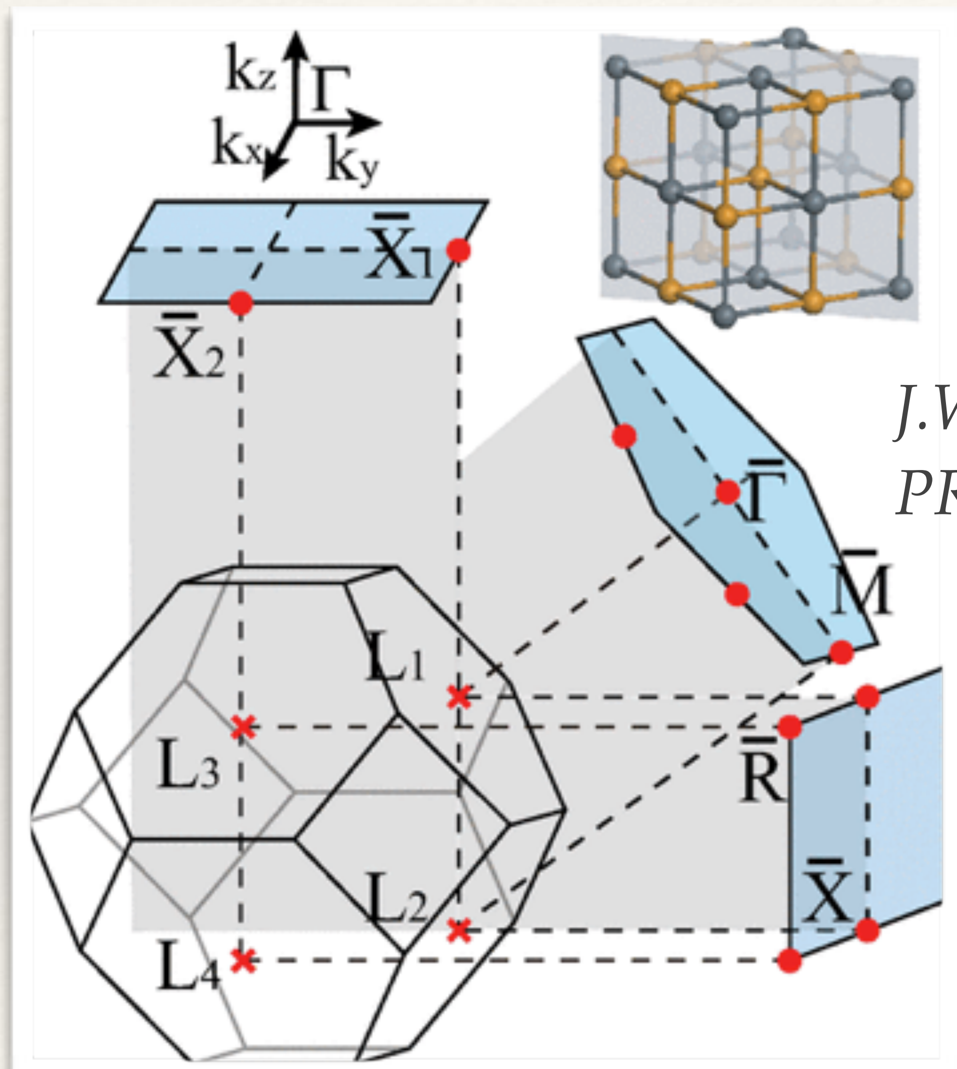
T.H. Hsieh et al., Nature Comm. 2013



- Chalcogenide material class e.g. SnTe, PbSe
- Alloying, pressure or strain: Band inversion
- Topological crystalline insulator (TCI) phase
  - Protected by mirror symmetry and U(1) charge conservation

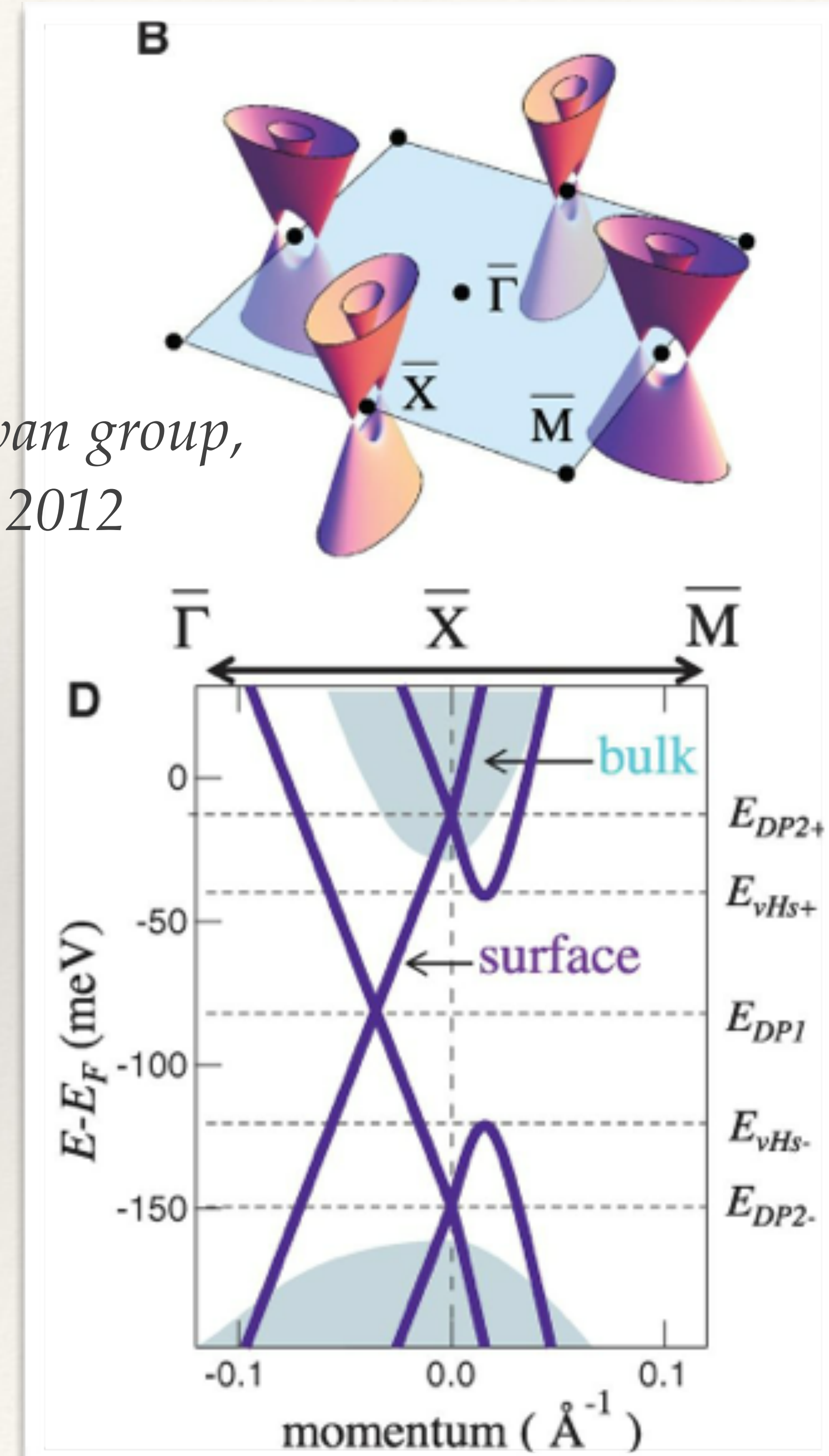
Surface states of the TCI

- Low-energy surface states in the (111), (110) and (001) directions



J.W. Liu et al., PRB 2013

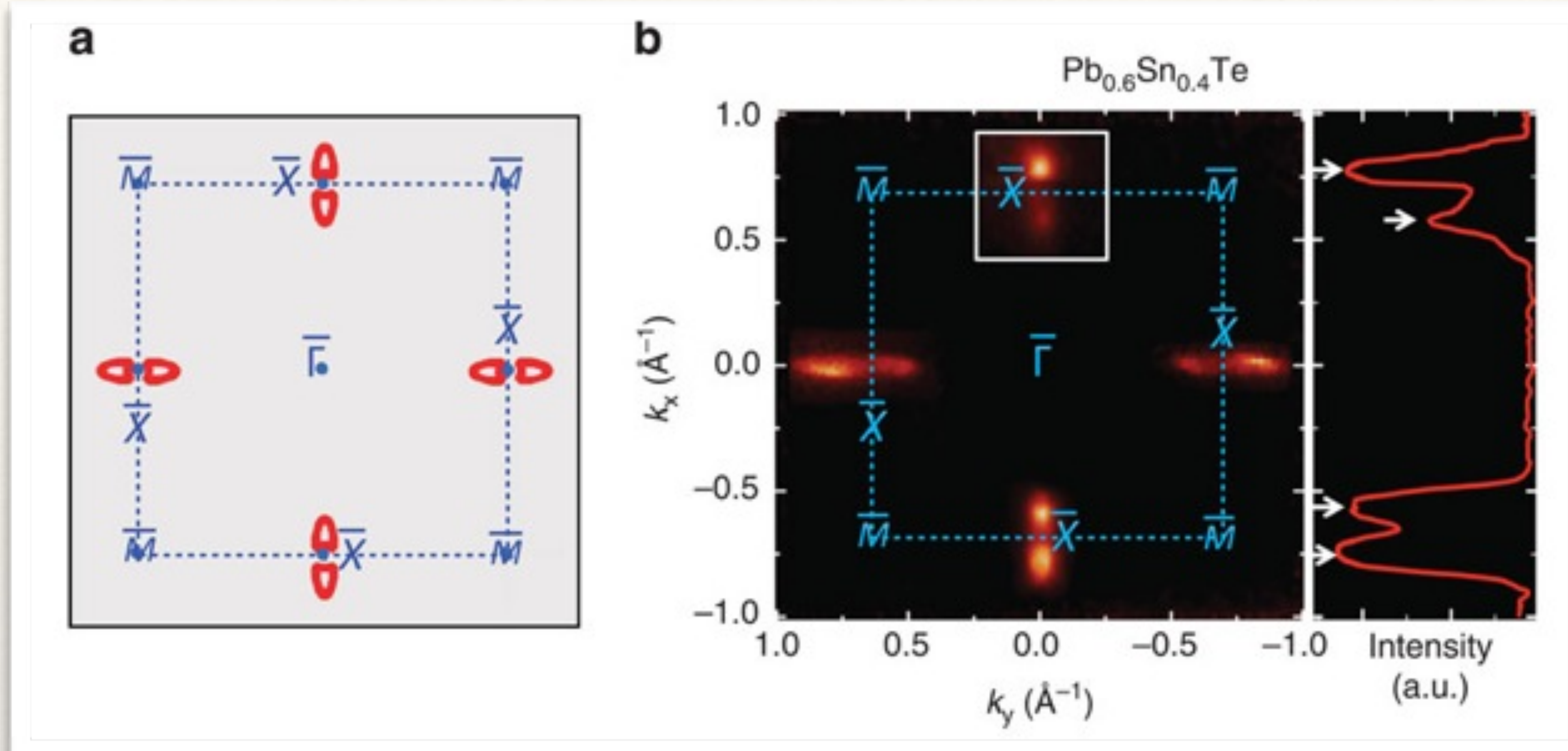
Madhavan group, Science 2012



- Dirac fermions described by *k.p* theory

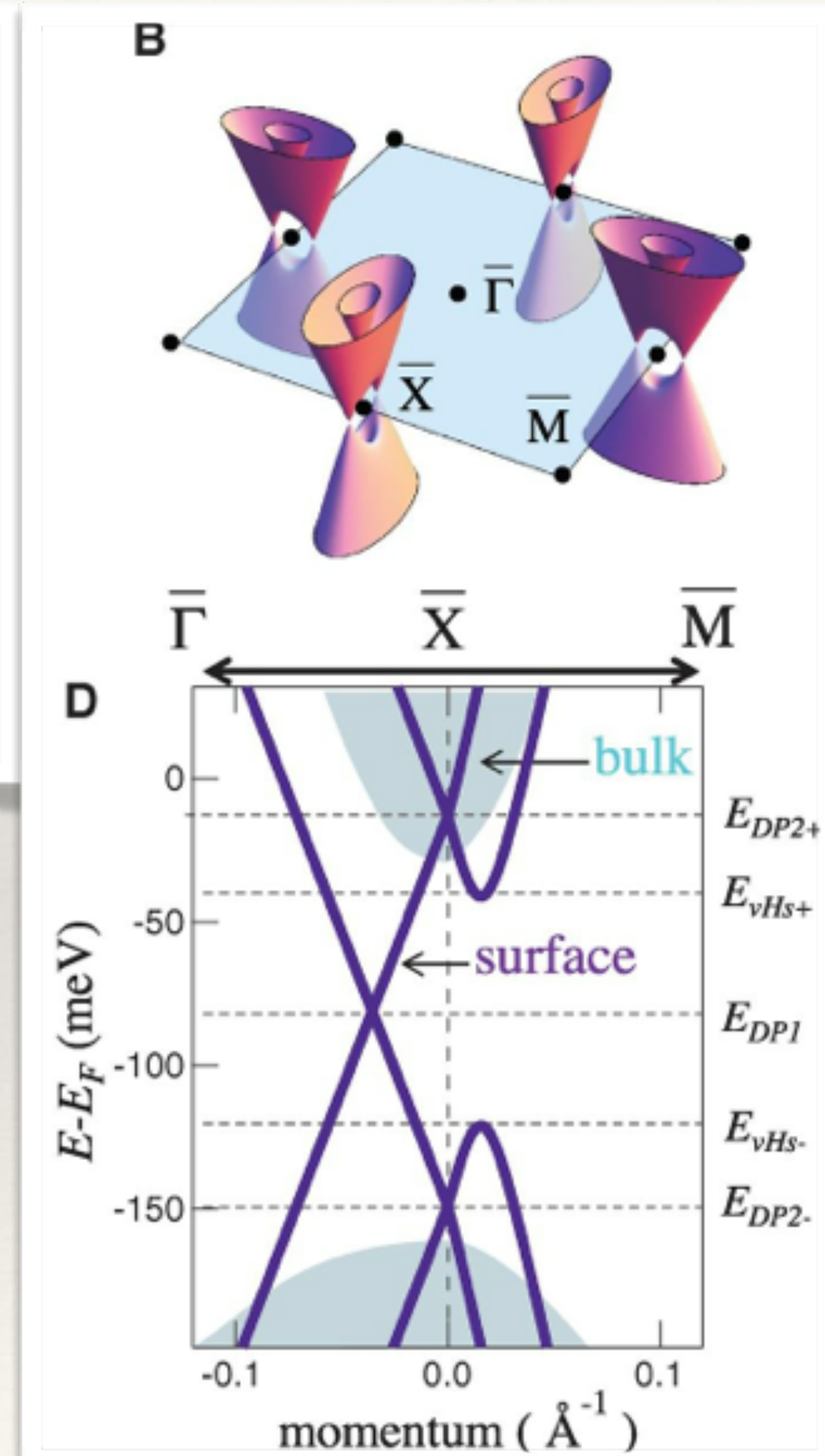
$$H_{\bar{X}_1}(\vec{k}) = v_1 k_1 s_y - v_2 k_2 s_x + m\tau_x + \delta s_x \tau_y$$

Surface states in the (001) direction



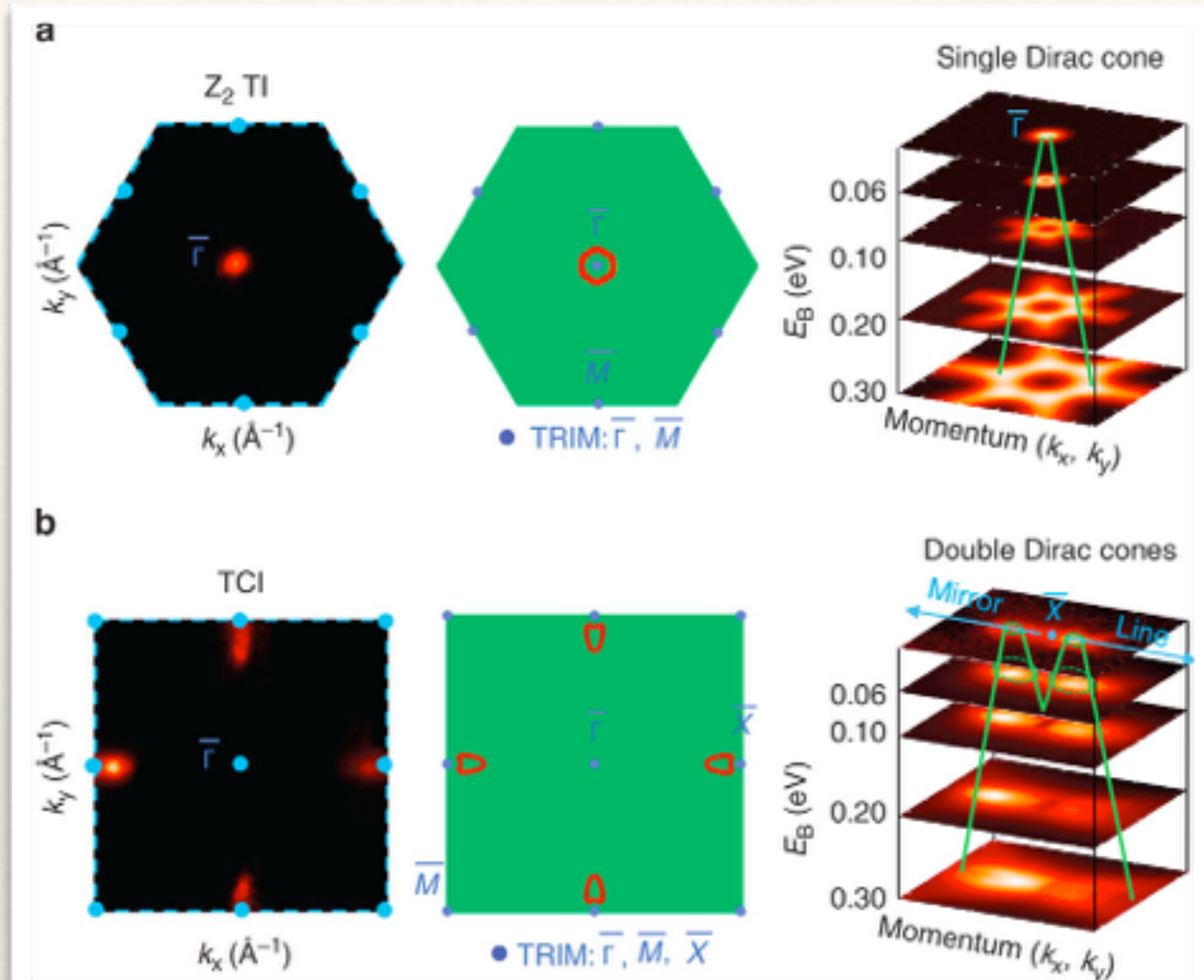
ARPES: *Hasan group, Nature Comm. 2012*

- Two pairs of Dirac cones
- Lie along two orthogonal mirror axes
- Related by four-fold rotation symmetry



STM: *Madhavan group, Science 2012*

Properties under time-reversal

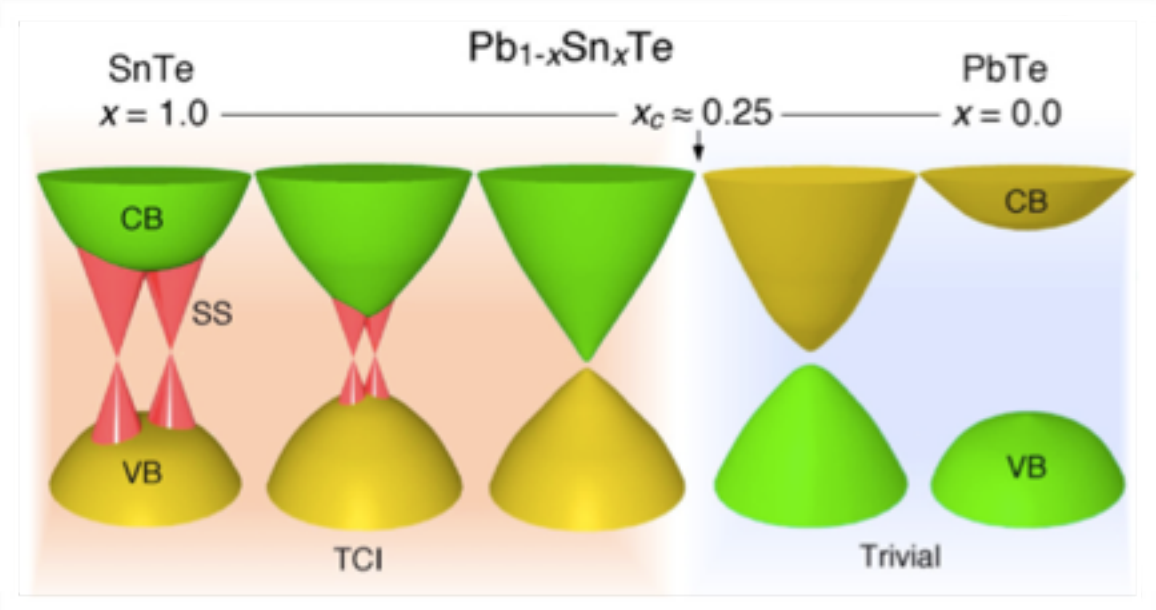


- Qualitatively different features
- Topological insulator (TI): Dirac points at time-reversal invariant momenta (TRIM)
- Its own time-reversed partner

ARPES: *Hasan group, Nature Comm. 2012*

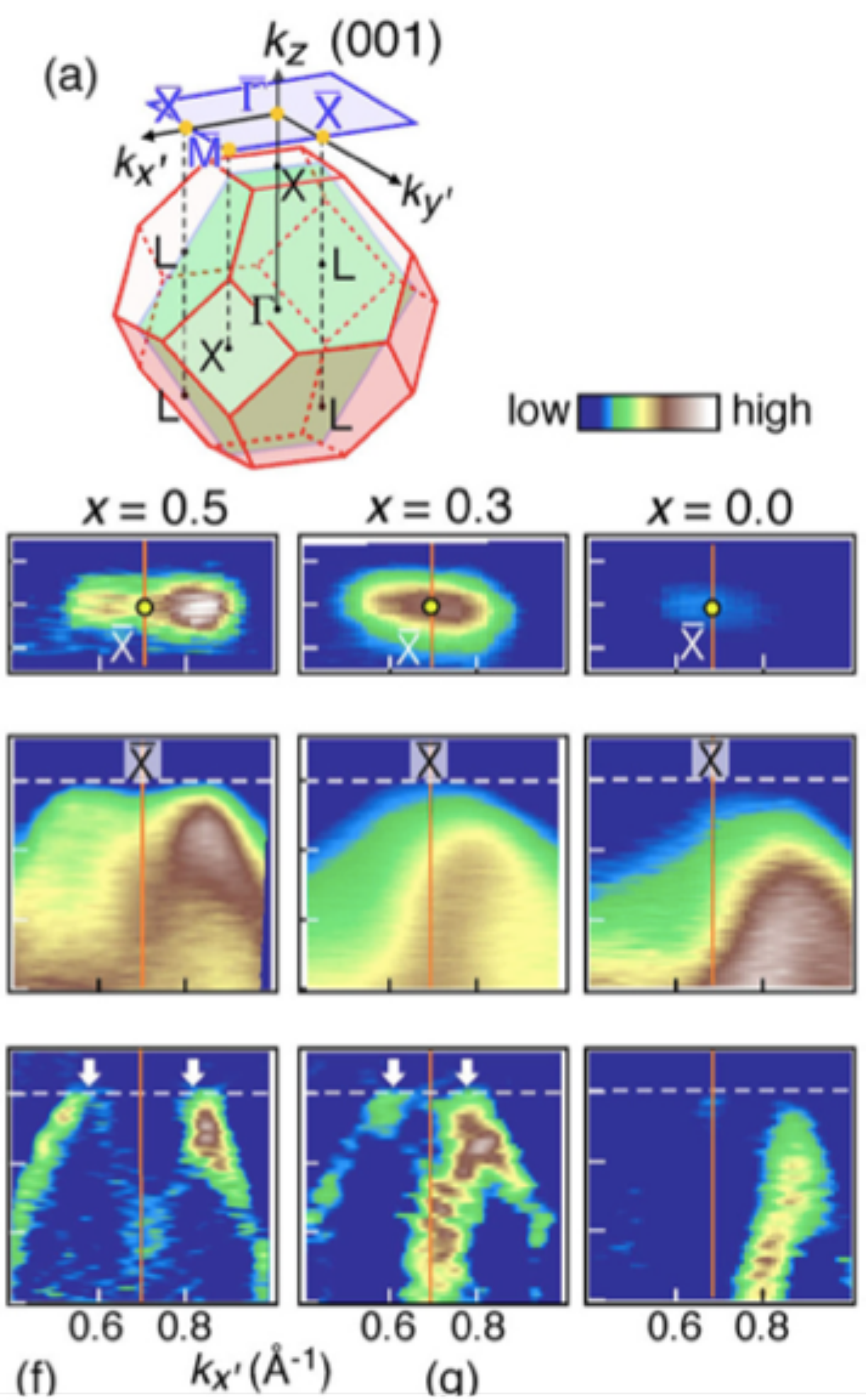
- TCI: Dirac points occur in pairs as time-reversed partners
- Couple oppositely to strain-induced pseudo gauge-field
- Unlike Dirac points in a regular TI which cannot couple to strain

Shifting of Dirac cones in $Pb_{1-x}Sn_xTe$



- In TCI phase, pair of Dirac points seen
- With changing alloy composition, they move towards zone center
- Similar effect from strain
  - *Serbyn & Fu, PRB 2014*

Ando group PRB 2013



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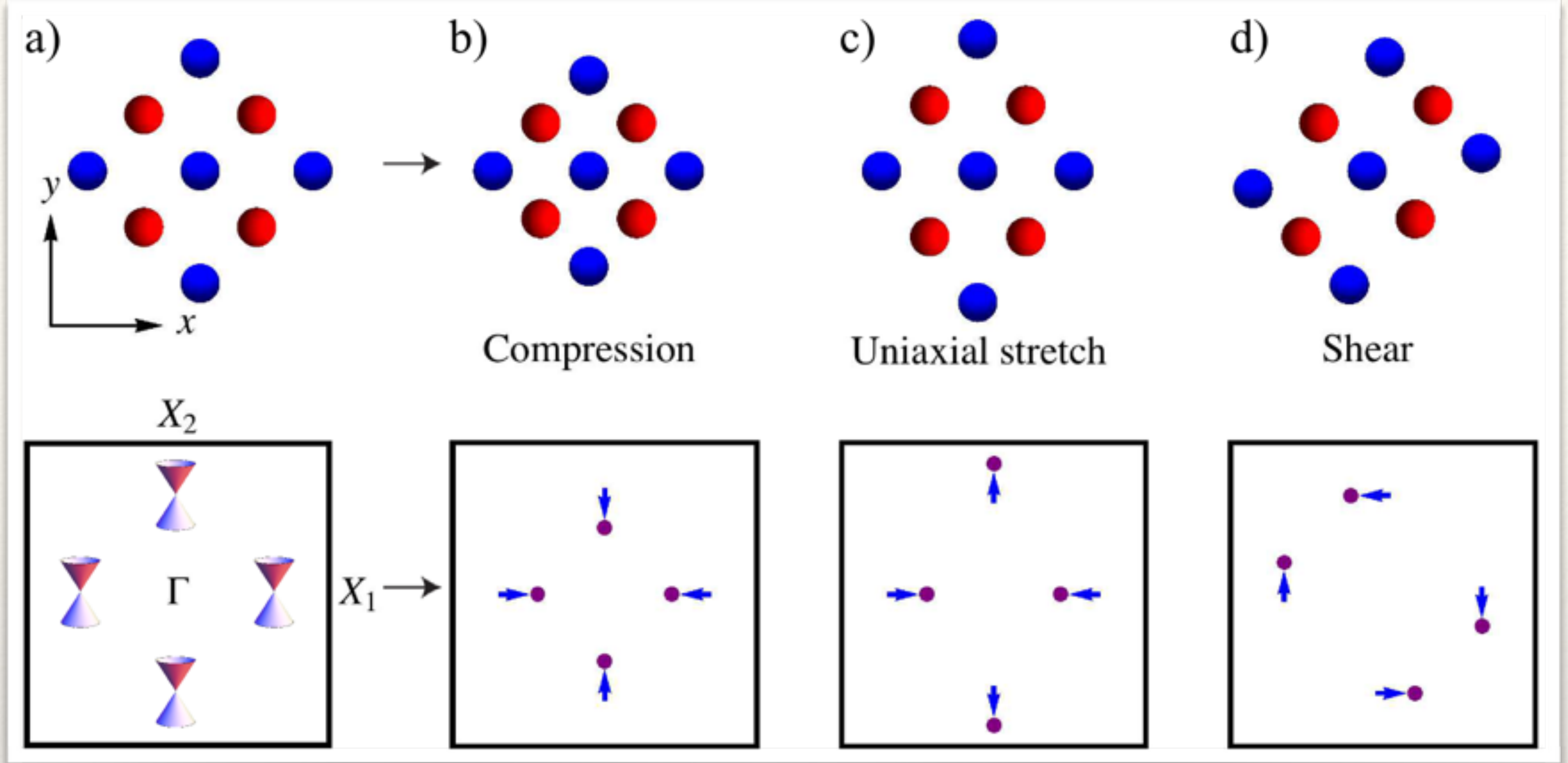


Three independent types of strain; resulting shift in BZ

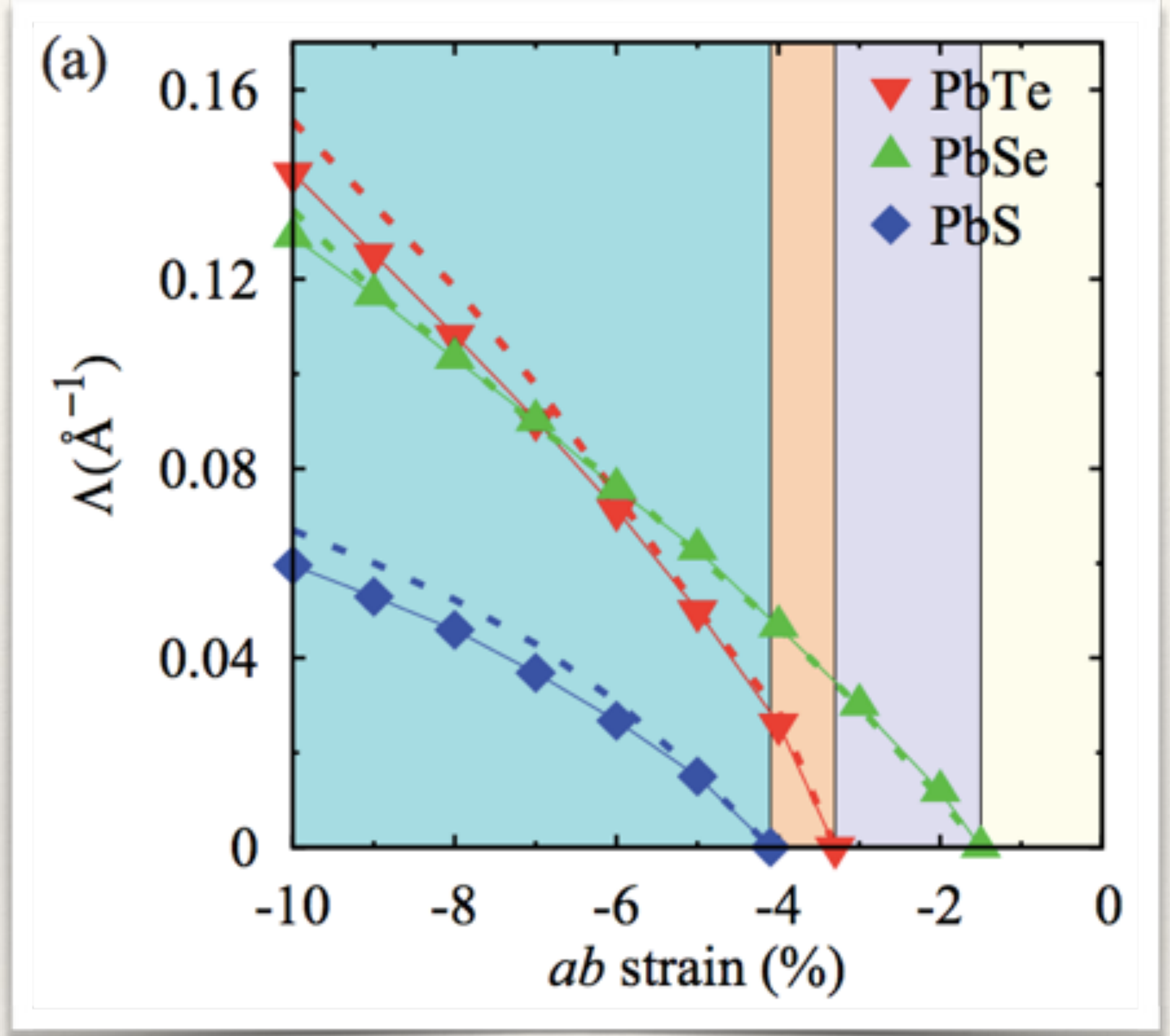
Strain in a TCI

The strain field $u_{ij} \equiv (\partial_j u_i + \partial_i u_j)/2$ (where $\mathbf{u}$ is the displacement field) is

- Compression/dilation: $u_{xx} + u_{yy}$
- Uniaxial stretch: $u_{xx} - u_{yy}$
- Shear: $u_{xy} + u_{yx}$

Ab-initio calculations

- Isotropic strain pushes certain materials into a TCI
- In TCI phase, compressing the lattice shifts surface Dirac points
- Extract how strongly strain couples to Dirac point shifts, e.g. for PbTe, $\alpha_1 = 2.2 \mathring{A}^{-1}$



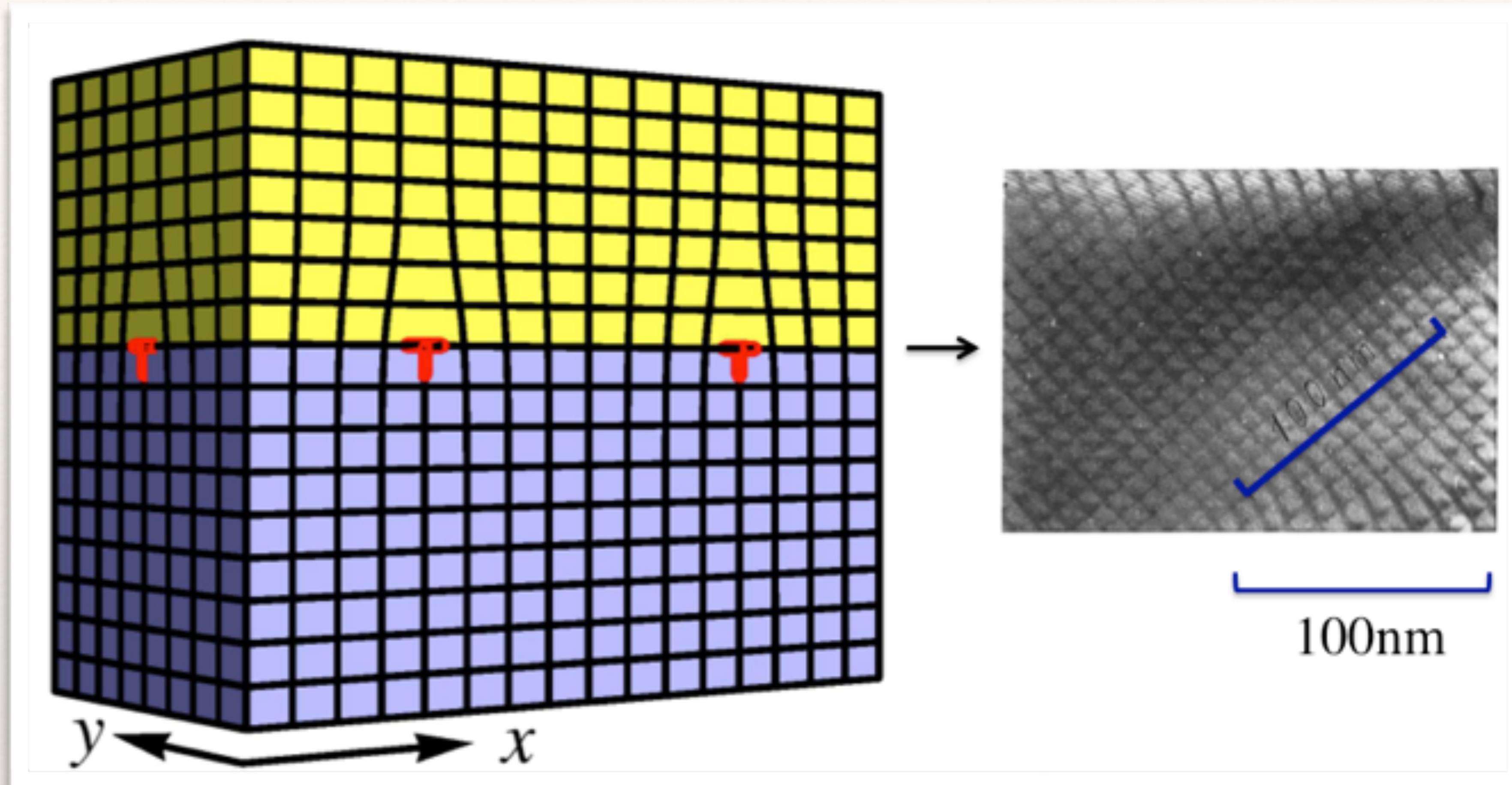
P. Barone et al., Phys. Status Solidi 2013

Pseudo gauge-field for Dirac fermions

- Linear shift of momentum: similar to minimal coupling $\vec{k} \to \vec{k} + \vec{A}$
  - Allows identification with a gauge-field
  - Nonrelativistic fermions instead also give terms of $\vec{k} \cdot \vec{A}$
- Exact form depends on lattice symmetries
  - Graphene has one coupling constant, *J.L. Mañes PRB 2007*
  - TCIs have three independent coupling constants
  - For the Dirac fermion at valley $\mathbf{K}_j$, the strain-induced vector potential $\mathbf{A}_j \equiv \mathbf{K}'_j - \mathbf{K}_j$ is to lowest order

$$\mathbf{A}_j = (A_j^x, A_j^y); \qquad \begin{aligned} \mathbf{A}_1 &= (\alpha_1 u_{xx} + \alpha_2 u_{yy},\ \alpha_3 u_{xy}), \\ \mathbf{A}_2 &= (\alpha_3 u_{xy},\ \alpha_1 u_{yy} + \alpha_2 u_{xx}). \end{aligned}$$

Strain profile in a TCI bilayer

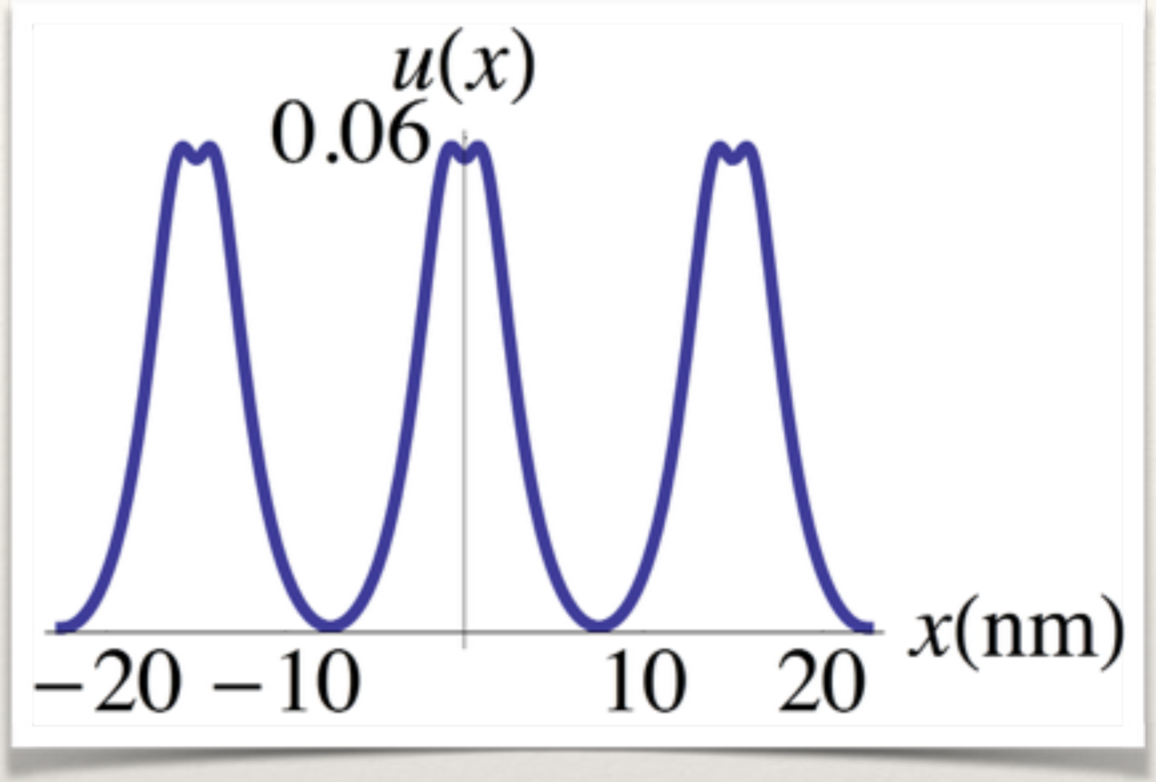


TEM image of the square misfit dislocation grid, which forms at the interface of PbTe/PbSe (lattice spacing is 0.64nm)

N.Y. Fogel et al., PRB 2002

- Lattice mismatch between two materials of 3-10%
- Spontaneous formation of misfit edge dislocations
- Regular two-dimensional dislocation array along the mirror axes

Spatially-varying strain field



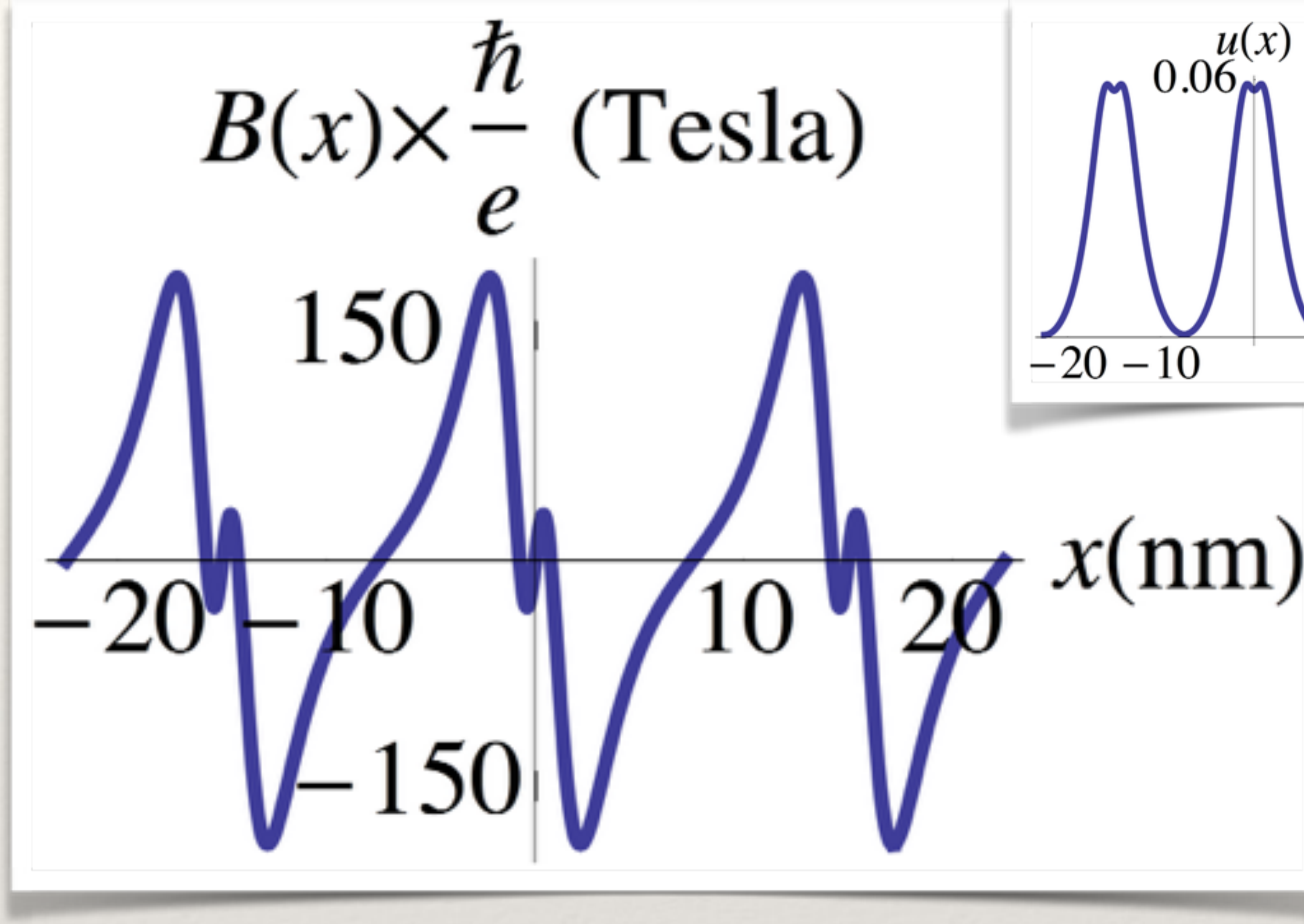
Plotted using representative parameters: array period 15nm, Poisson ratio for PbTe of 0.26, lattice constant 0.64nm

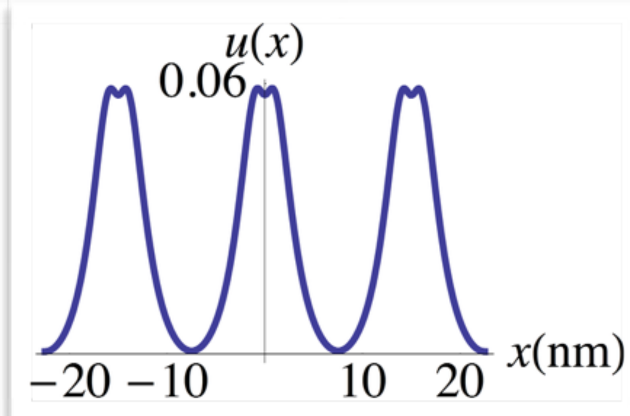
$$u_{xx}(x) = \sum_N u^0_{xx}(x - N\lambda),$$

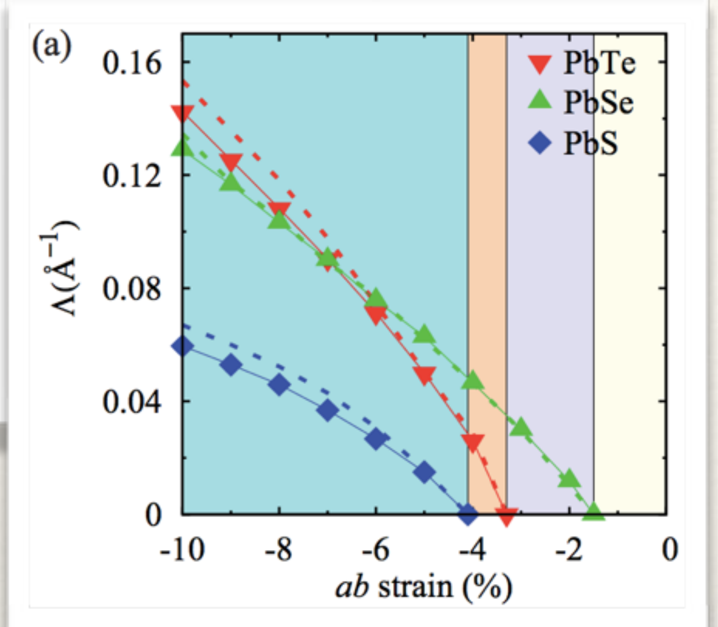
$$u^0_{xx}(x) = \frac{bz}{2\pi(1-\nu)} \frac{(3x^2+z^2)}{(x^2+z^2)^2}.$$

- Total strain field is sum of contributions from each dislocation
- Field for single dislocation given by classical strain theory
- Similar behavior along other mirror axis obtained by rotation

Periodically-alternating B-field





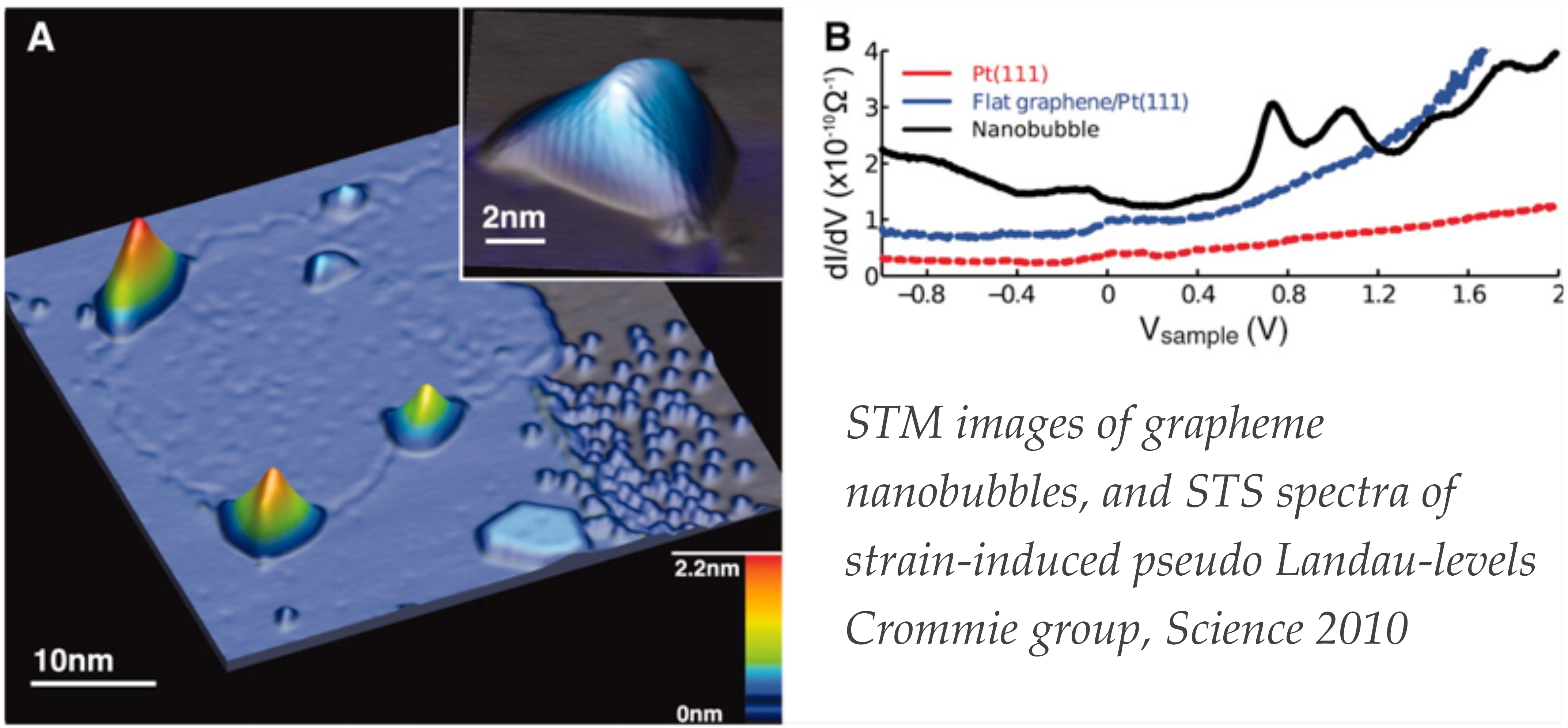


Strain coupling from ab-initio

$$B_2(x) = \nabla \times \mathbf{A}_2^T(x)$$

- Maximum pseudo-magnetic field is ~180 Tesla
- Spatially-varying strain necessary to produce non-zero B-field
- Periodically-alternating field that averages to zero

Macroscopic array vs. nanobubbles



STM images of grapheme nanobubbles, and STS spectra of strain-induced pseudo Landau-levels Crommie group, Science 2010

- Pseudo magnetic-fields seen in localized graphene nanobubbles
- Dislocation array covers macroscopic regions altering electronic properties globally
- A periodic field is easier to achieve than a uniform field (which has infinite gauge potential at boundary)

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Pseudo Landau-levels

- When the field varies on scales larger than the magnetic length, we expect the formation of local Landau levels

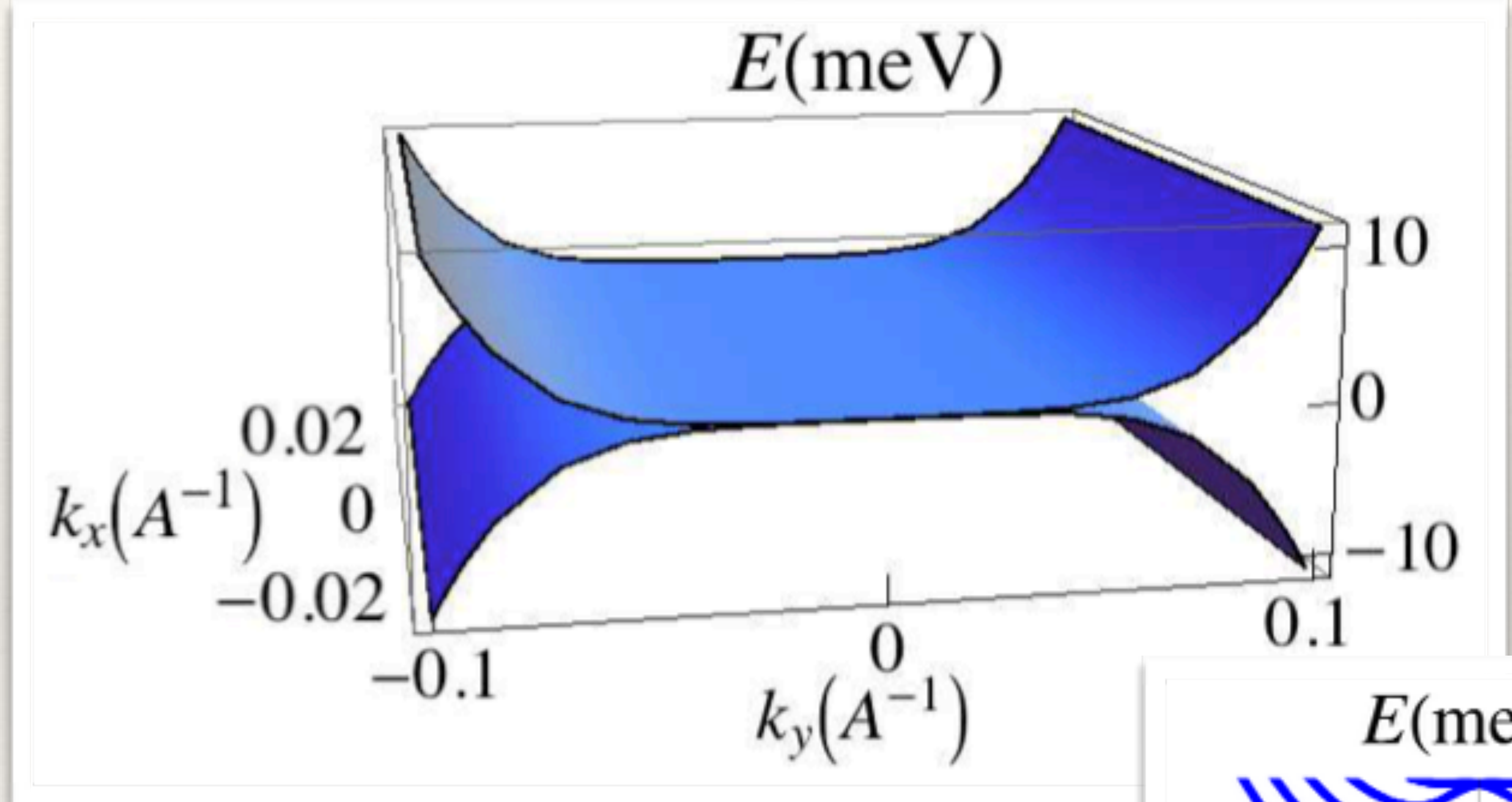
- Energy level spacing depends on local field strength
  - $E_n(x) = \mathrm{sgn}(n)\sqrt{2nv_xv_y|B(x)|}.$

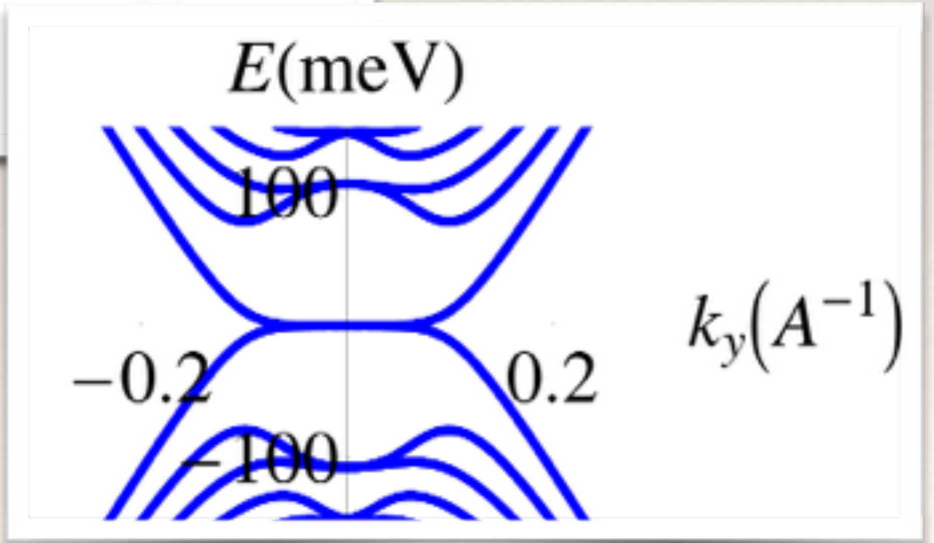
- *n=0* Landau level has *E=0* regardless of field strength
  - Extensive degeneracy at zero energy

Flat bands at low momenta

- Approximate periodic field with first Fourier component

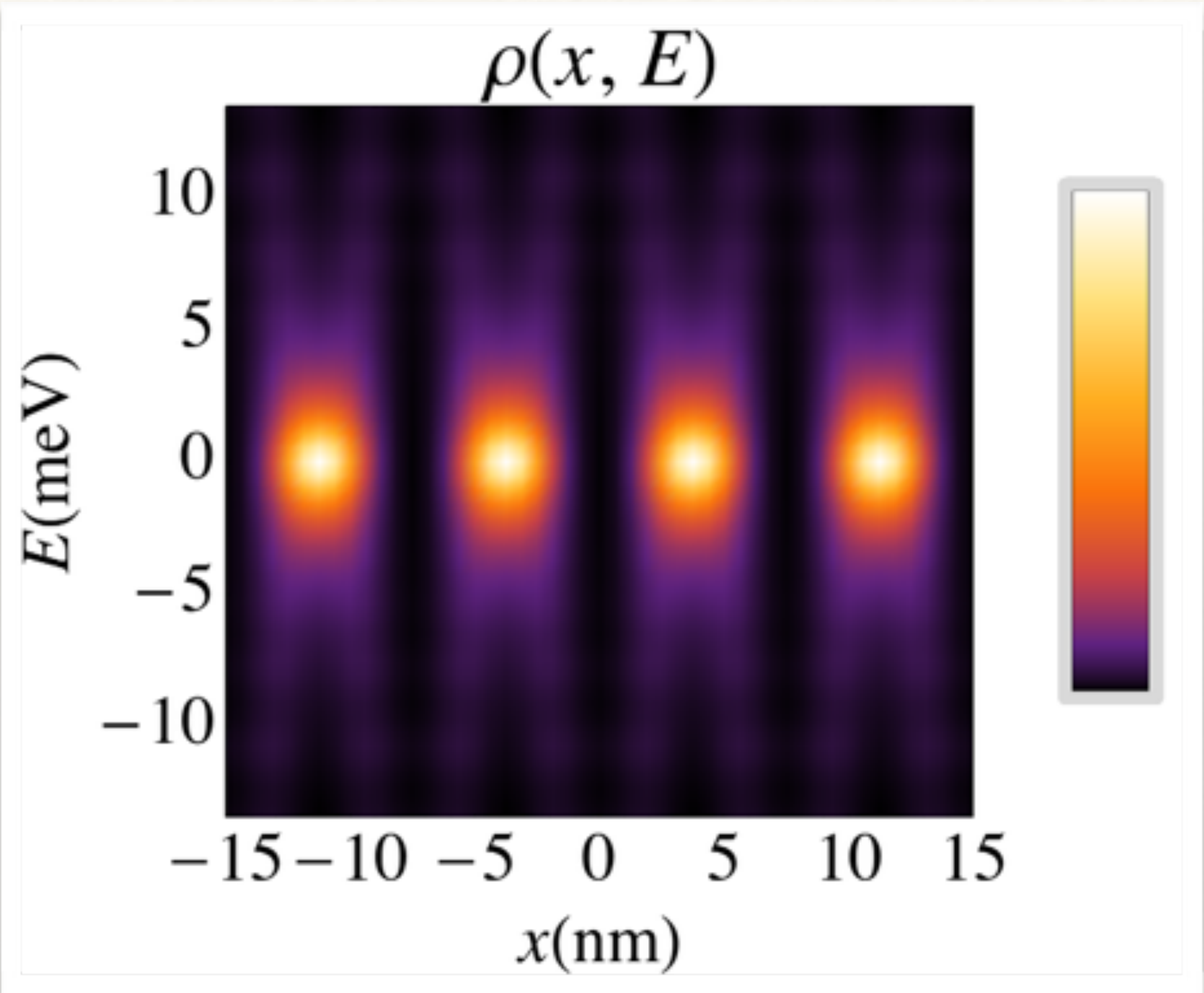
$$H = -iv_x \partial_x s_y - v_y(k_y - A_y(x))s_x, \quad A_y(x) = A_0 \cos(2\pi x/\lambda)$$



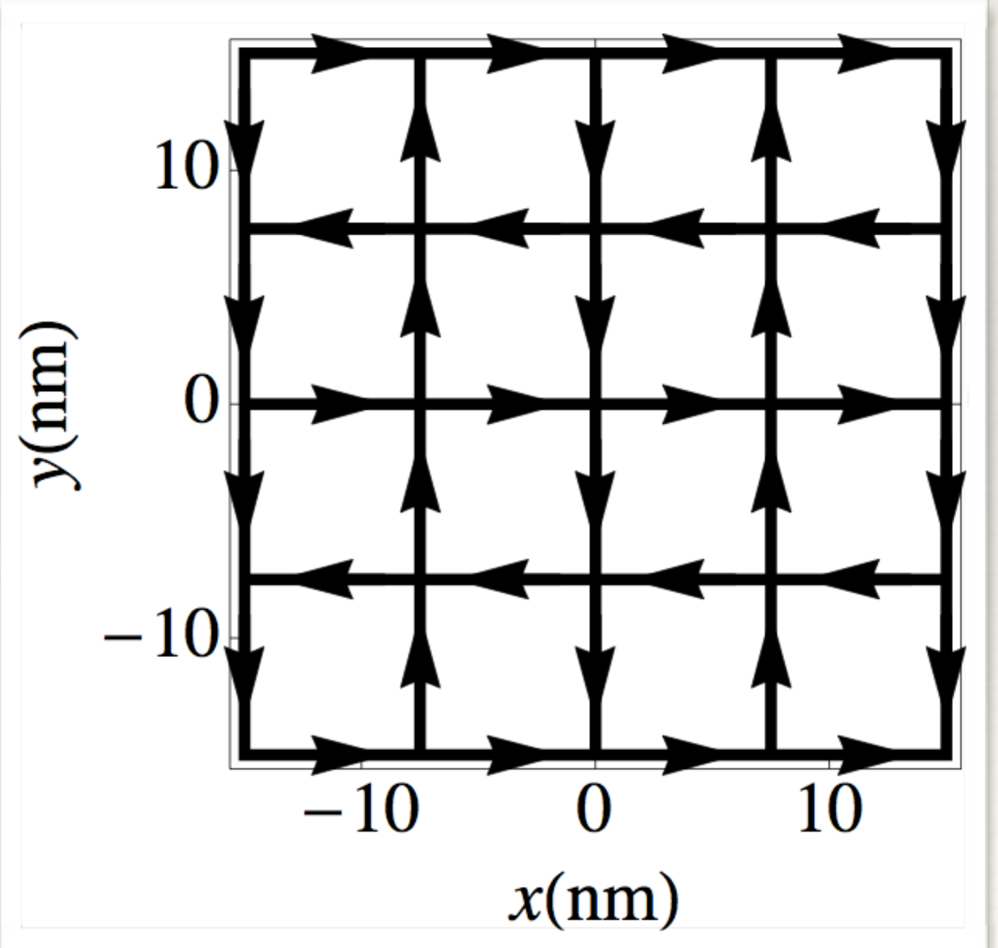


- Two flat bands corresponding to positive and negative regions of pseudo B-field respectively

Large DOS and snake states



- Large DOS at *E=0* from flat bands
- Dispersive states at transition regions: chiral snake states
  - $\sigma_{xy} = \mathrm{sgn}(\mu B)\frac{1}{2}\frac{e^2}{h}$



- Another time-reversed copy from opposite valley
  - Jointly give helical snake states

Flat bands drive instabilities

- Large density of states enhance interaction effects and can favor superconductivity
- Carrier density in the flat band ~ 10^{12}cm^{-2}
  - Expect Fermi energy there
- Solving the BCS mean-field gap equation gives

$$k_B T_c \sim \Delta_0 \rightarrow \begin{cases} \hbar\omega_D \exp(-1/VD(E_F)) & \text{Fermi surface} \\ V n_{FB} & \text{flat band} \end{cases}$$

  - *Khodel & Shaginyan, JETP Lett 1990; Kopnin, Heikkila & Volovik, PRB 2011*

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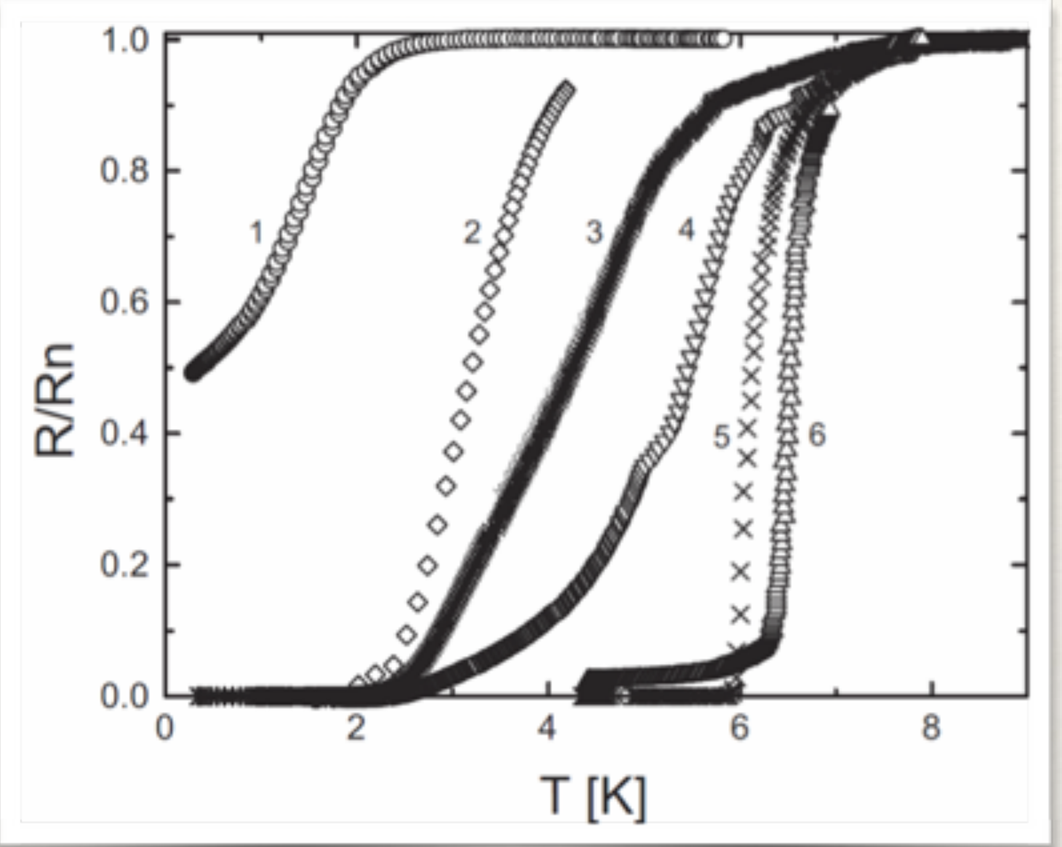
Experimental features

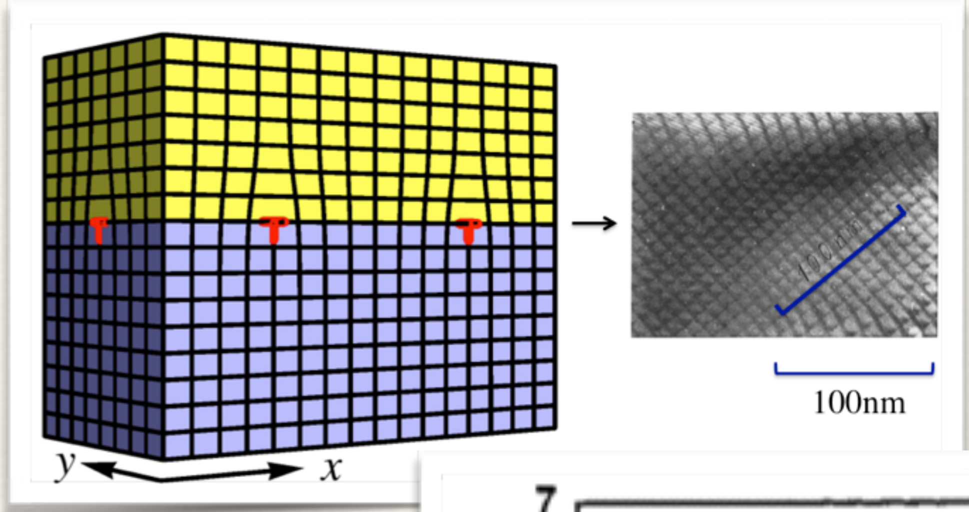
- Superconductivity measured in several IV-VI multilayers, T_c is 2.5-6.4K
  - Individual constituents non-superconducting above 0.2K
- Superconductivity is two-dimensional
  - Anisotropy of upper critical field
- In narrow-gap semiconductors ($E_g < 0.3$eV)
  - Wide-gap semiconductors do not superconduct above 1.5K



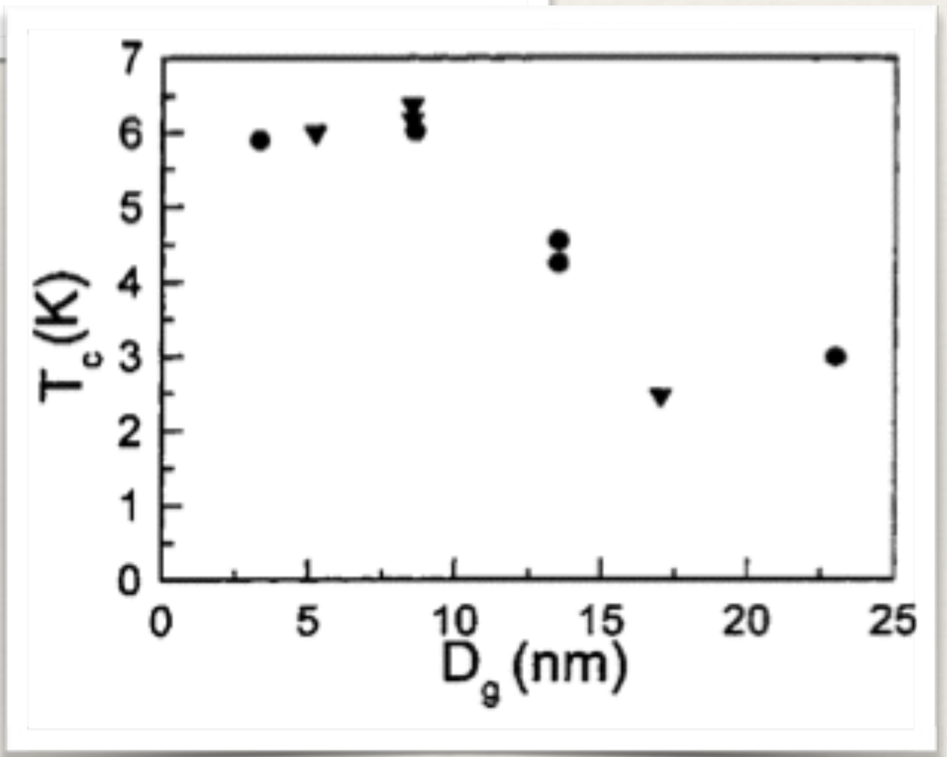
Six PbTe/PbS bilayers (different thicknesses)

N.Y. Fogel et al., PRB 2006

Dependence on dislocation array



- Samples without a regular dislocation array show only partial superconducting transitions



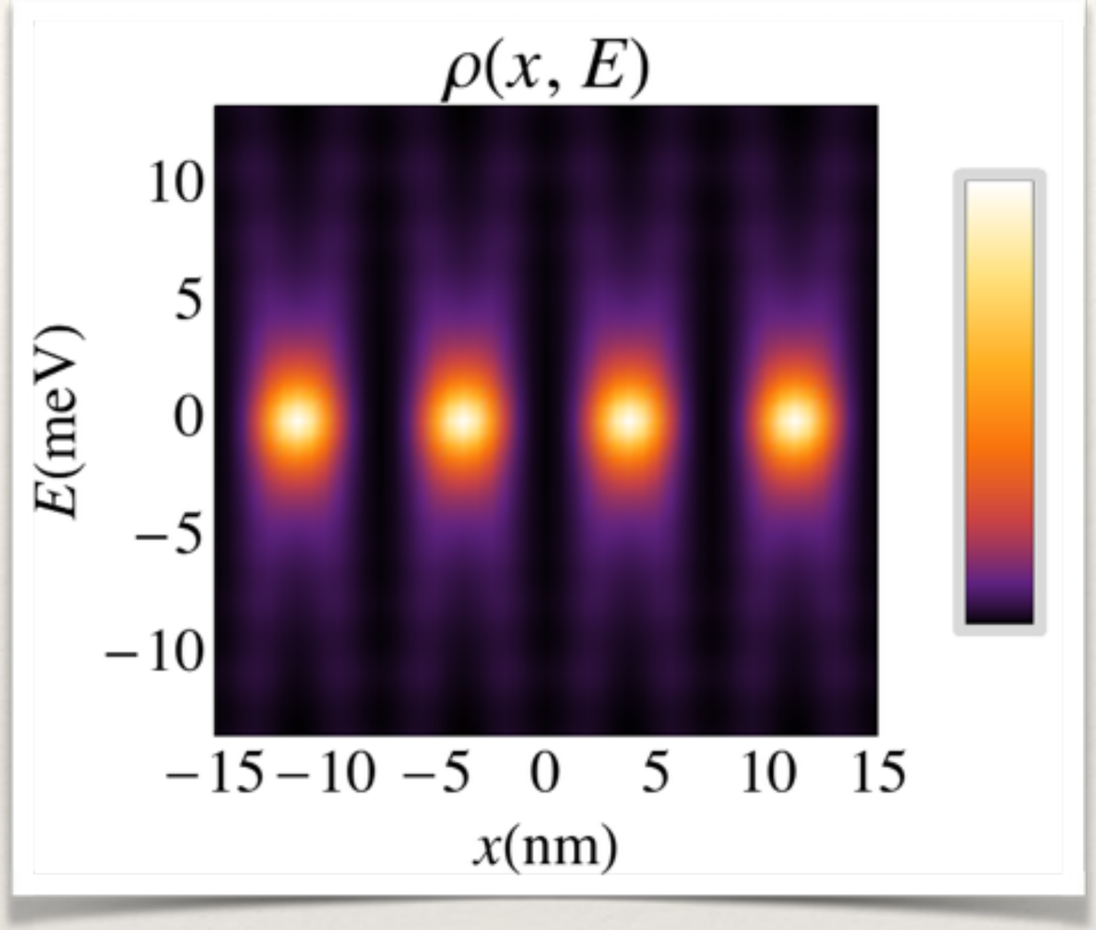
- In superconducting samples, T_c increases from 3K to 6K as array period D_g decreases from 23nm to 10nm

N.Y. Fogel et al., PRB 2002

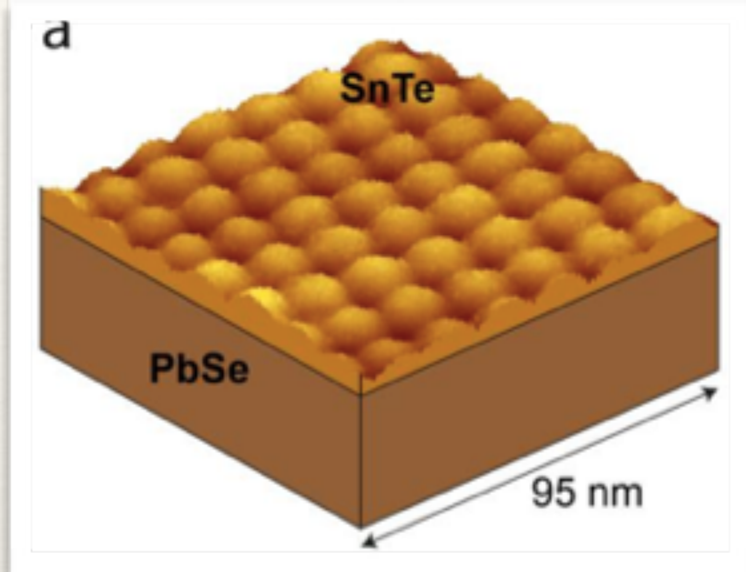
- Consistent with T_c depending parametrically on the flat band degeneracy — non-BCS dependence

Predictions from our theory

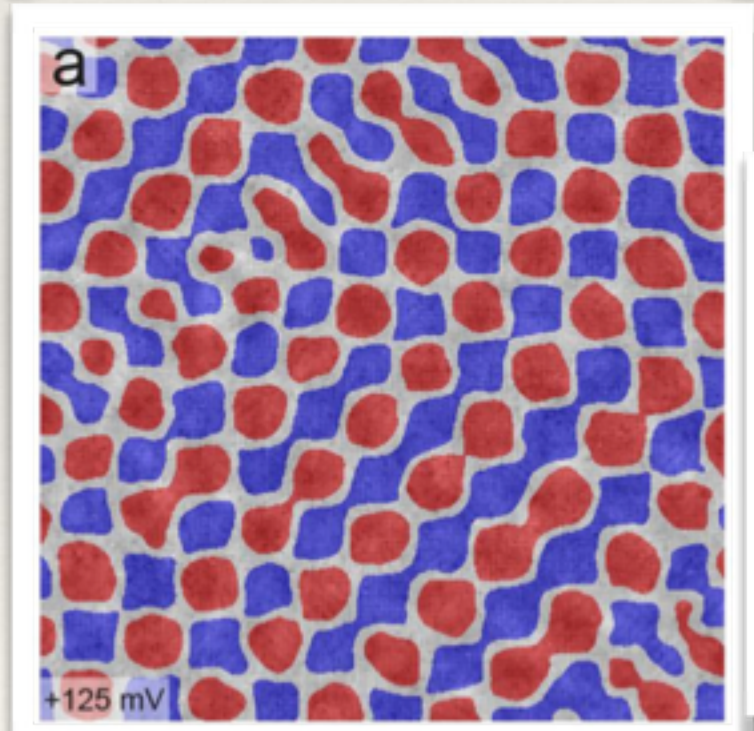
- Unique DOS spectrum from tunneling conductance measurements
- Drop in T_c when gating out of flat band
- De Haas-van Alphen measurements should reflect periodicity of superlattice

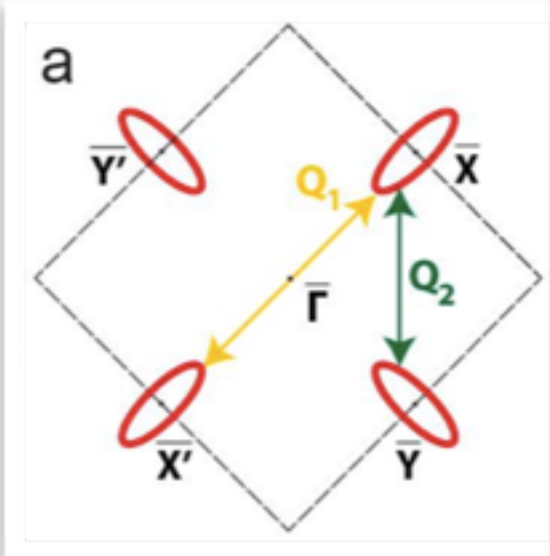


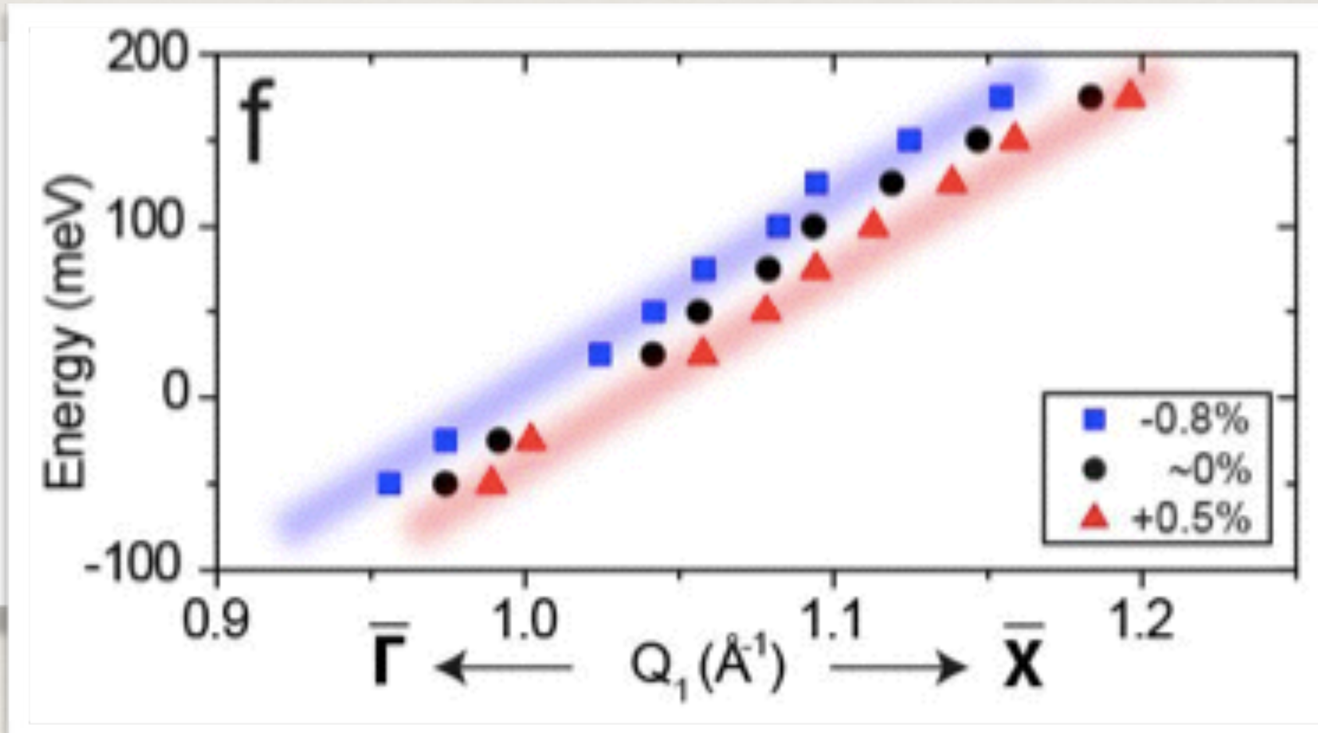
STM measures Dirac point shifts



- SnTe thin film grown on PbSe substrate
- Local atomic measurements map strain: tensile (red) and compressive (blue)
- QPI measures wavevector Q_1: dispersions are offset in momentum — agrees with theory







Madhavan group, arXiv 2015

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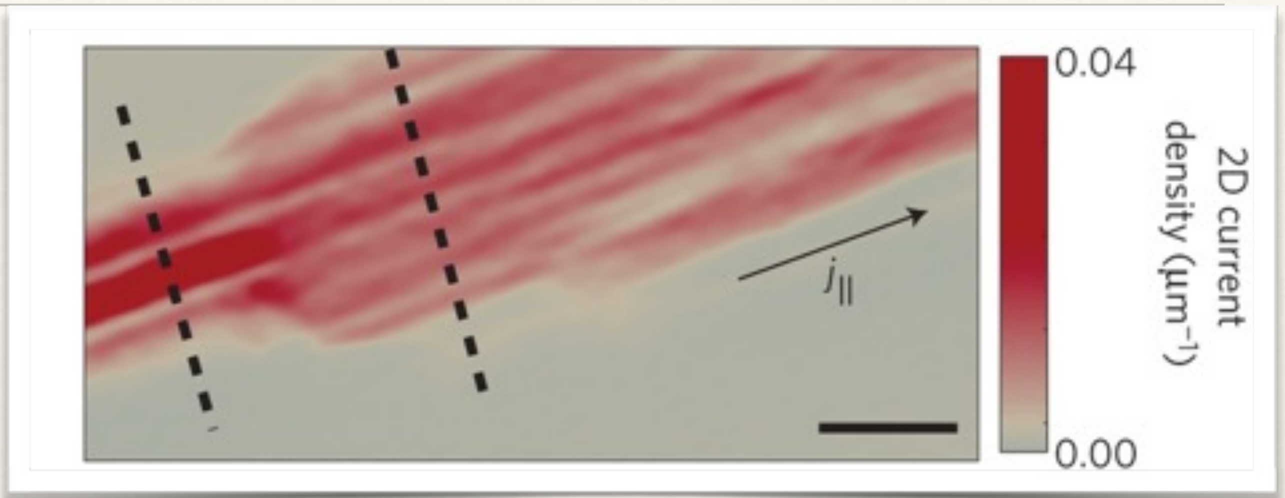
- Theoretical model for strain-induced helical flat bands and interface superconductivity in TCIs
  - Demonstrates role of topological electronic states
  - Opens realistic route to strain-induced flat bands
  - Can account for previously unexplained experimental features (e.g. dependence on dislocation array and its relation to T_c)

Further work



Moler group, Nature Mat. 2013

- Open questions
  - Role of interactions?
  - Analytical description?
- Connection to interface superconductivity in other systems?
  - Conductance channels in STO related to structural distortions
  - Strain effects seem important
- Usefulness of flat bands
  - New states with repulsive interactions? E.g. FQHE
  - Possible route towards higher T_c by strain engineering

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Thank you!

Coloumb repulsion in a flat band?

- Typically, the electron repulsion is renormalized by the electron bandwidth *W*, so phonon-mediated attraction can dominate.

$$k_B T_c = 1.14\epsilon_D \exp\left(-\frac{1}{\lambda - \mu^*}\right) \quad \text{where} \quad \mu^* = \frac{\mu}{1 + \mu \ln(W/\epsilon_D)}$$

- In a flat band (no bandwidth), how does this happen?

- Revisit Anderson-Morel calculation, using a peak in density of states at very narrow bandwidth (less than phonon energy):

$$k_B T_c = 1.14\Gamma_{FB} \left(\frac{\epsilon_D}{\Gamma_{FB}}\right)^{\frac{1}{\alpha}} \exp\left(-\frac{1}{\alpha(\lambda - \mu^*)}\right)$$