Estimation of Pseudo Magnetic Field for Isotropic/Anisotropic Dirac Cones

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arXiv:1707.08601

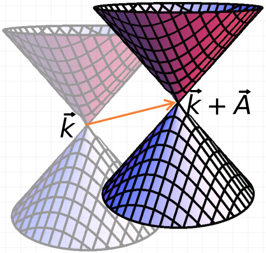
Motivation & Background

Landau levels without an external magnetic field.

Essence

Dirac cones shift
as gauge field

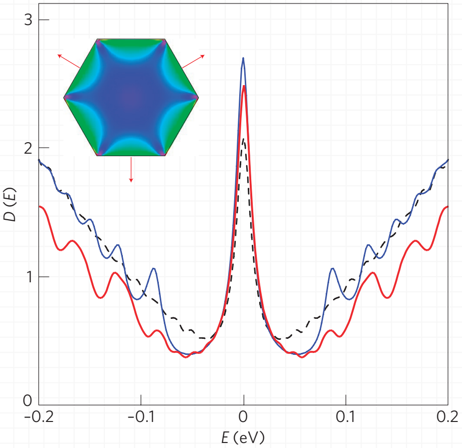
Any system with Dirac cones!

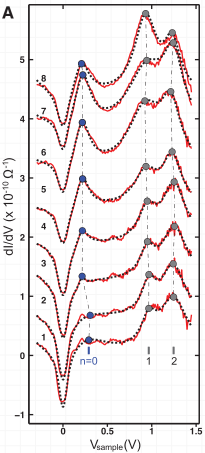


Even for a system inert to magnetic field: charge neutral particles, photons, phonons...

Example: Graphene under Strain

†Theory: F. Guinea *et al.*, Nat. Phys. **6**, 30 (2010). Exp.: N. Levy *et al.*, Science **329**, 544 (2010).

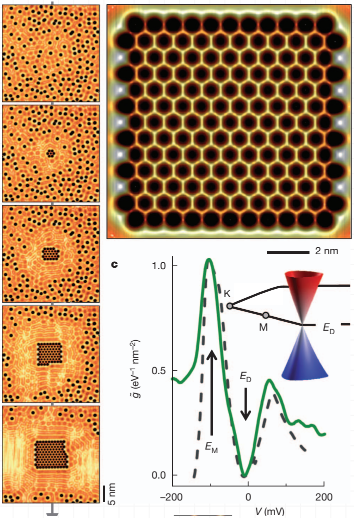


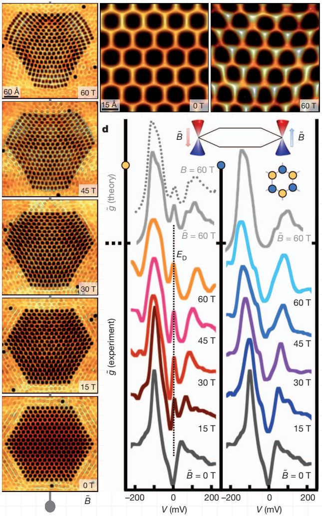


Example: Artifitial System

K. K. Gomes *et al.*, Nature **483**, 306 (2012).

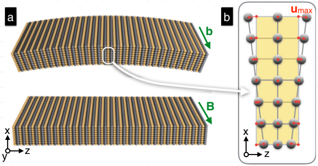
2D electrons on Cu surface with arranged molecule deposition

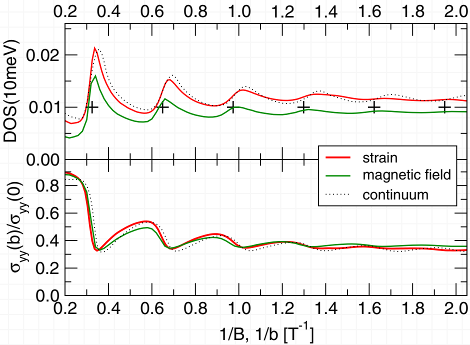




Quantum Oscillation

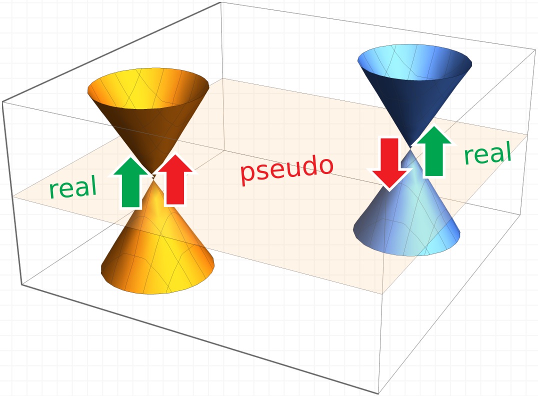
Strained 3D Weyl semimetal





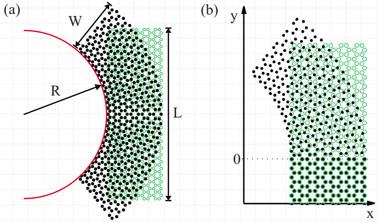
T. Liu, D. I. Pikulin, and M. Franz, Phys. Rev. B **95**, 041201 (2017).

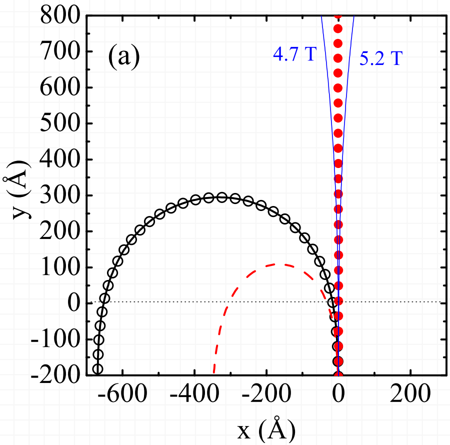
Valley Imbalance



Valley Imbalance

Valley dependent Lorentz force in strained graphene

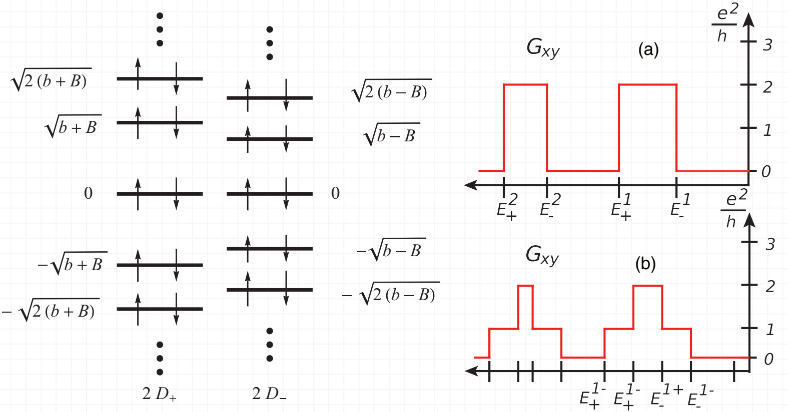




A. Chaves *et al.*, Phys. Rev. B **82**, 205430 (2010).

Valley Imbalance

Landau level splitting in strained graphene



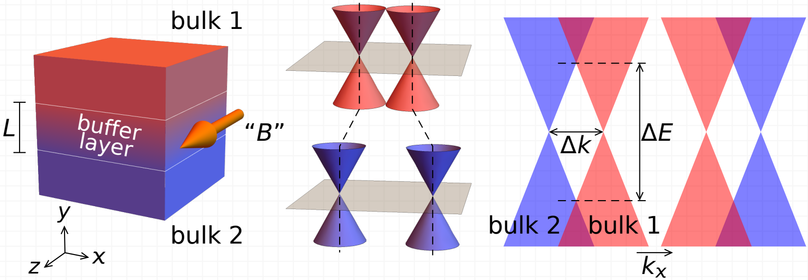
B. Roy, Z.-X. Hu, and K. Yang, Phys. Rev. B **87**, 121408 (2013).

Topic

1. Simple setup for pseudo magnetic field generation
   - not necessary strain
2. Concise formula to estimate pseudo magnetic field
   - Counting number of “observable” Landau levels
   - Effects of anisotropy of Dirac cones
3. Application to an exsisting material
   - 3D Dirac cones in an antiperovskite family

Setup

“Simplest” configuration



Important Parameters

- L: thickness of the buffer layer
- Δk: size of the Dirac cone shift

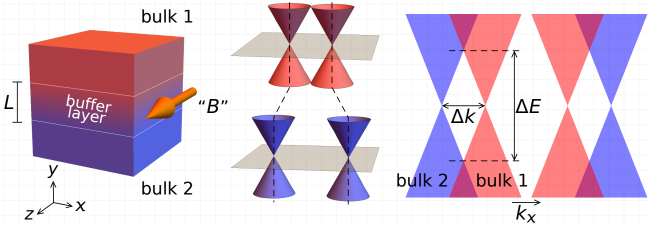
See also, A. G. Grushin *et al.*, Phys. Rev. X **6**, 041046 (2016). C. Brendel *et al.*, Proc. Natl. Acad. Sci. USA **114**, 3390 (2017). H. Abbaszadeh *et al.*, arXiv:1610.06406.

Formulation

$$H^{(\pm)}_{\vec{k}} = \hbar v(\vec{k} \pm \vec{k}_0) \cdot \vec{\sigma} \longleftrightarrow H^{(\pm)} = \hbar v(-i\vec{\nabla} \pm \vec{k}_0(y)) \cdot \vec{\sigma}$$

$$\vec{A}^{(\pm)} = \mp \frac{\hbar}{e}\vec{k}_0(y), \quad |\vec{B}| = |\vec{\nabla} \times \vec{A}| \sim \frac{\hbar}{e}\frac{\Delta k}{L} = \frac{h}{ea^2}\frac{R}{N}$$

$$\Delta k = \frac{2\pi R}{a}, \quad L = Na$$



Formulation

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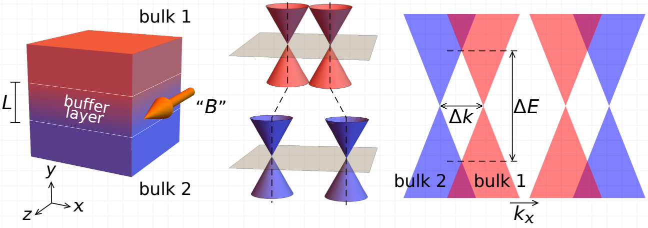
R: Dirac cone shift, N: buffer thickness



Formulation

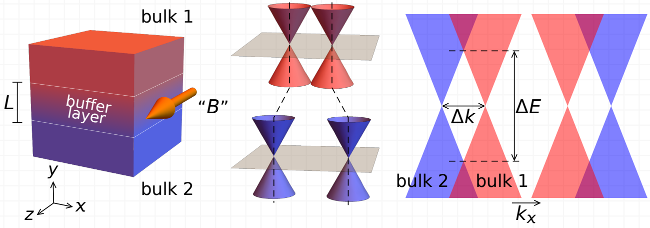
R: Dirac cone shift, N: buffer thickness

- typical case

$$a \sim 5\text{Å} \quad \to \quad \boxed{|\vec{B}| \sim 1.6 \times 10^4 \times \frac{R}{N}\ [\mathrm{T}]}$$

- observable Landau levels

$$E_n = \sqrt{\frac{4\pi v^2 \hbar^2 R |n|}{N a^2}} < \frac{\hbar v \Delta k}{2} \quad \to \quad \boxed{|n| < \frac{\pi}{4} N R}$$



Toy Model

$$H_{\vec{k}} = [1 + \delta + 2(\cos k_x + \cos k_y)]\sigma_z + 2\alpha \sin k_y \sigma_y$$

$$\Downarrow$$

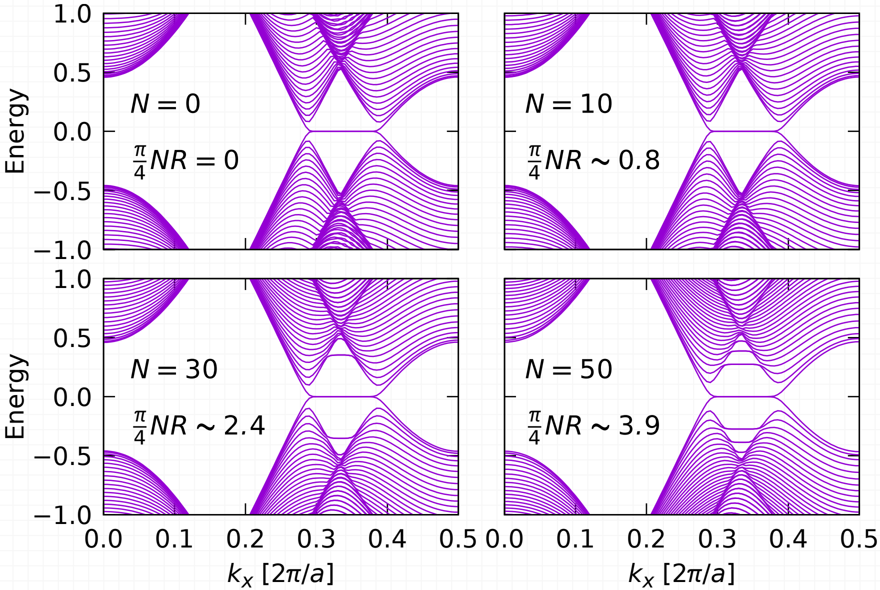
$$H_{\vec{k}} \sim -\sqrt{3}[(\tilde{k}_x - \tilde{\delta})\sigma_z + \tilde{\alpha} k_y \sigma_y]$$

$$\tilde{k}_x = k_x - \frac{2\pi}{3}, \quad \tilde{\delta} = \frac{\delta}{\sqrt{3}}, \quad \tilde{\alpha} = \frac{2\alpha}{\sqrt{3}}$$

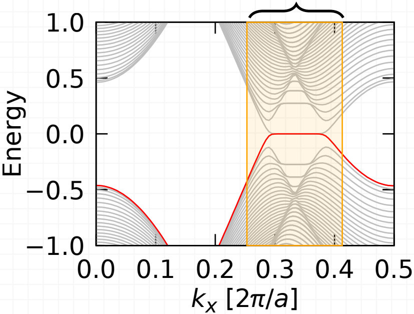
$$\tilde{\delta} \longleftrightarrow A_x \quad \& \quad \tilde{\alpha} \longleftrightarrow v_y/v_x$$

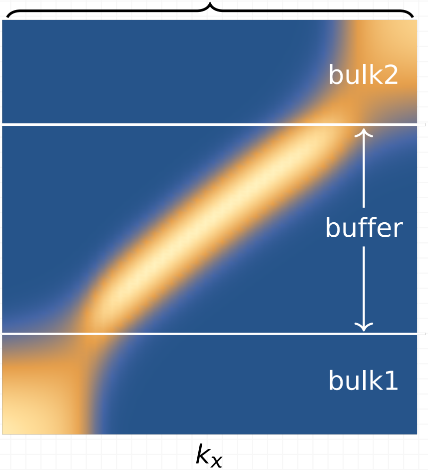
Results

R: Dirac cone shift, *N*: buffer thickness

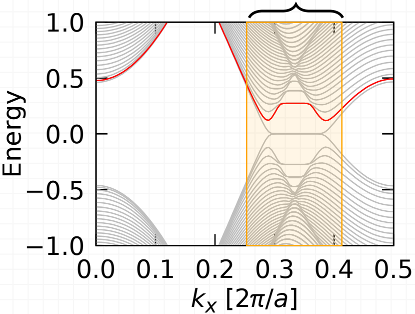


Discussion


1.0
0.5
0.0
−0.5
−1.0
Energy
0.0
0.1
0.2
0.3
0.4
0.5
k_x [2π/a]


bulk2
buffer
bulk1
k_x

Discussion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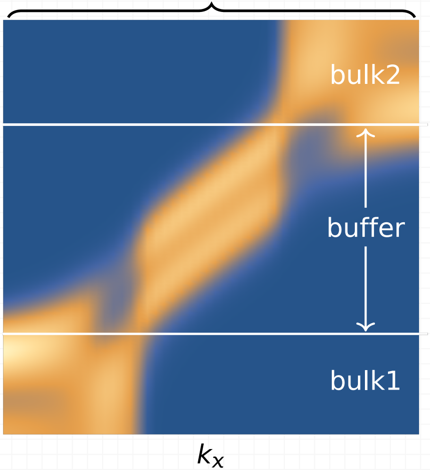
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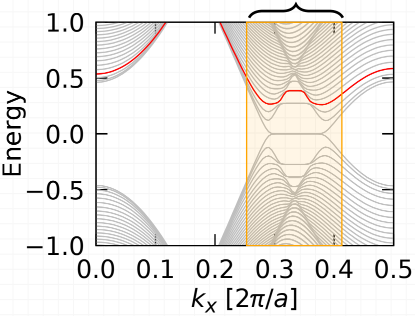

1.0
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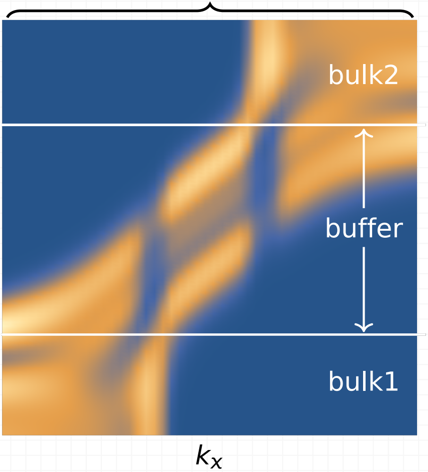
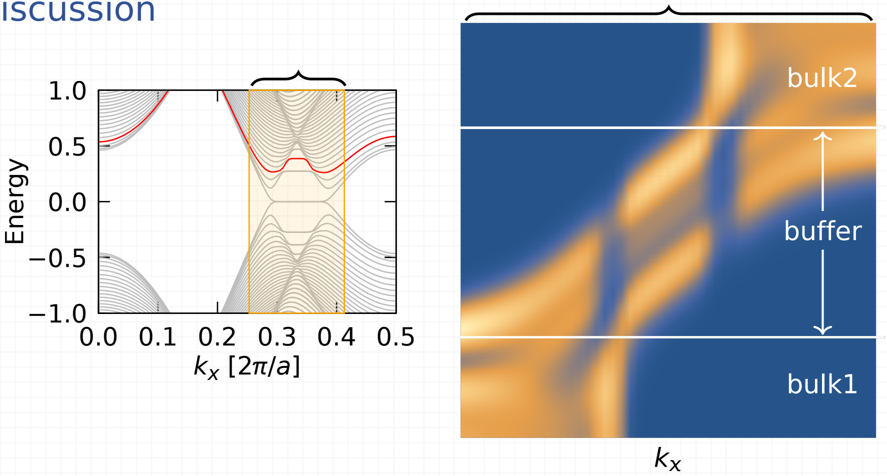


bulk2
buffer
bulk1
k_x

Discussion



wave function tail hits the boundary → no longer Landau level

- extension of the wave function $\sim \sqrt{n} l_B \propto \sqrt{nN/R}$
- extension < thickness → $n < NR$

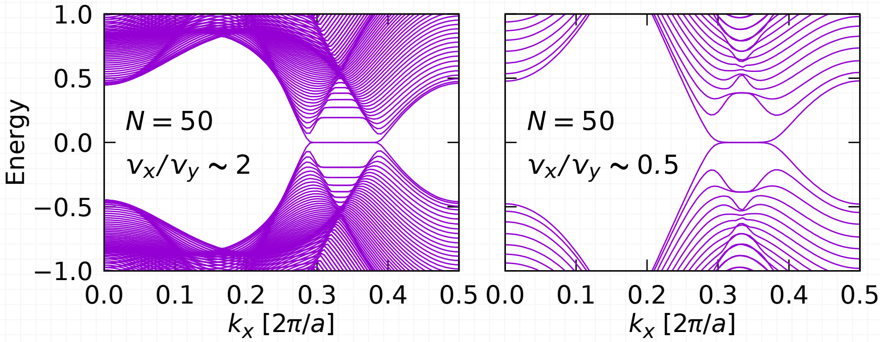
Anisotropy

R: Dirac cone shift, N: buffer thickness

$$\Delta E = \hbar v_x \Delta k$$

$$E_n = \sqrt{\frac{4\pi v_x v_y \hbar^2 R|n|}{Na^2}}$$

$$|n| < \frac{\pi}{4}\frac{v_x}{v_y} NR$$

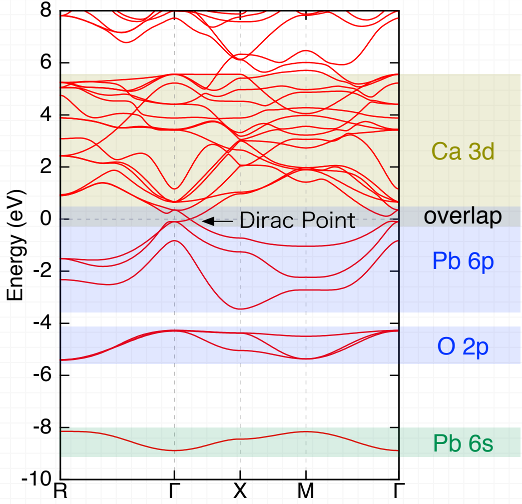


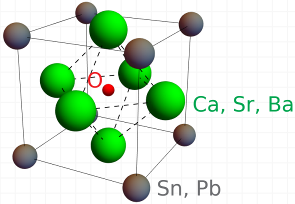
Anisotropy is advantageous for observing the LL structure!

Materials

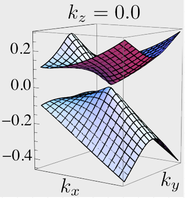
TK and M. Ogata, J. Phys. Soc. Jpn. **80**, 083704 (2011).

- Antiperovskite A_3EO (A=Ca,Sr,Ba and E=Sn,Pb) family





3D Dirac cones (with tiny mass) by d-p overlap!

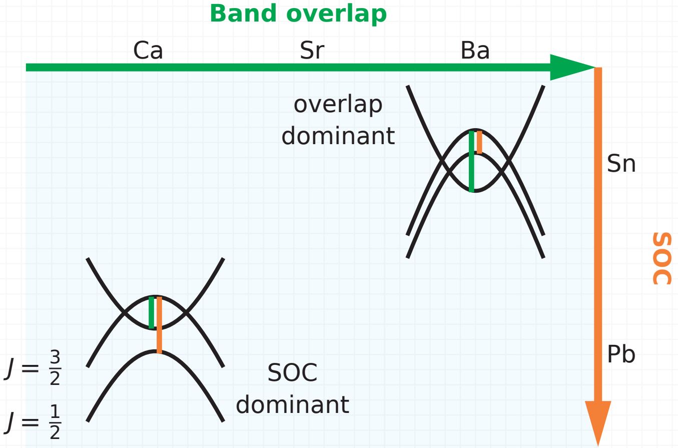


3D linear dispersion

;

Materials

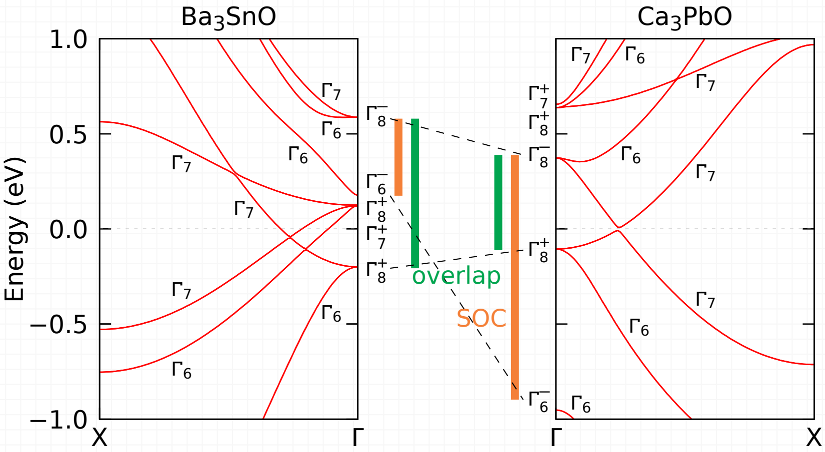
TK and M. Ogata, arXiv:1705.08934, to appear in PRMaterials.



(Potentially) tunable!

Materials

- Ba_3SnO (band inversion dominant) vs Ca_3PbO (SOC dominant)



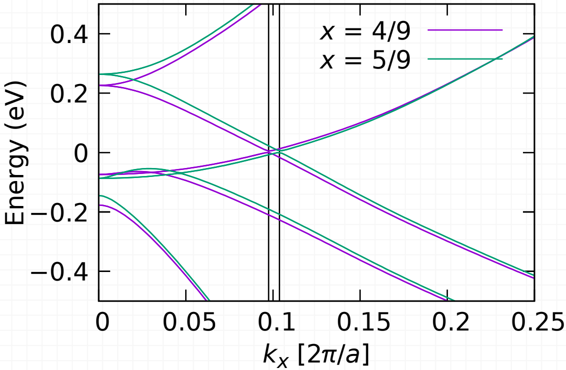
Strategy

- Inducing Dirac cone shift by modulating chemical composition
  - $Ca_3SnO \longleftrightarrow Sr_3SnO$

- Estimating R instead of $|B_{\mathrm{pseudo}}|$, to avoid computational burden

(Quasi) Ab-Initio Estimation: Wannier Interpolation

1. Derive effective models for the two end materials Ca_3SnO and Sr_3SnO
2. Interpolate the parameters to obtain a model for $Ca_{3(1-x)}Sr_{3x}SnO$



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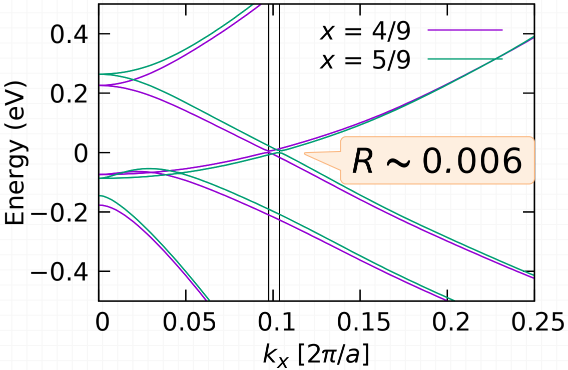
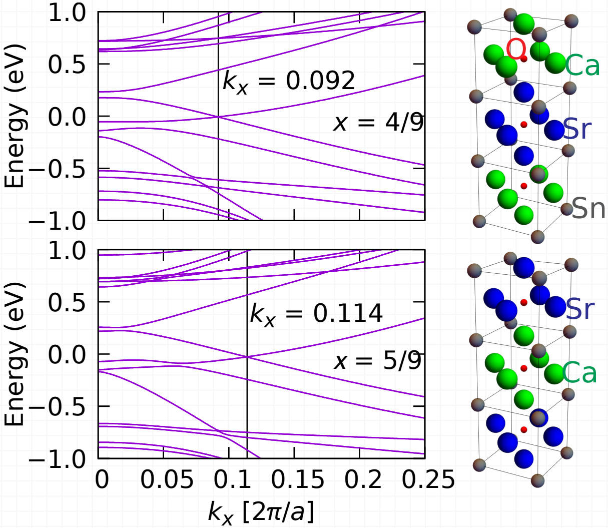


(Quasi) Ab-Initio Estimation

- heterostructure $Ca_{3(1-x)}Sr_{3x}SnO$, $a = (a_{x=0} + a_{x=1})/2$



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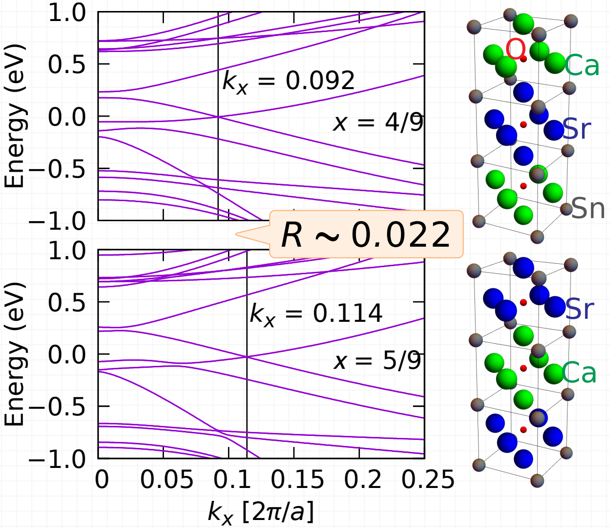

Fabrication of Films

- Sr_3PbO, molecular beam epitaxy, thickness 200nm-300nm
  D. Samal, H. Nakamura, and H. Takagi, APL Mater. **4**, 076101 (2016).

- Ca_3SnO, pulsed laser deposition
  M. Minohara *et al.*, arXiv:1710.03406.

Summary

TK, arXiv:1707.08601

- Concise formulae for the pseudo magnetic field & pseudo Landau levels

$$B \sim \frac{h}{ea^2}\frac{R}{N}, \quad |n| < \frac{\pi}{4}\frac{v_x}{v_y}NR$$

  - Anisotropic Dirac cones are better to observe LL structures.

- Estimation of R for an existing material

Perspective

- Interesting physical consequences!
  - eg. coexistence with a *real* magnetic field