Topological Insulators and Thermoelectric Effects

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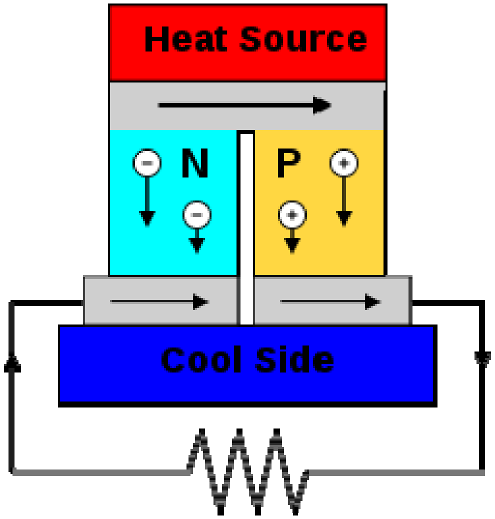
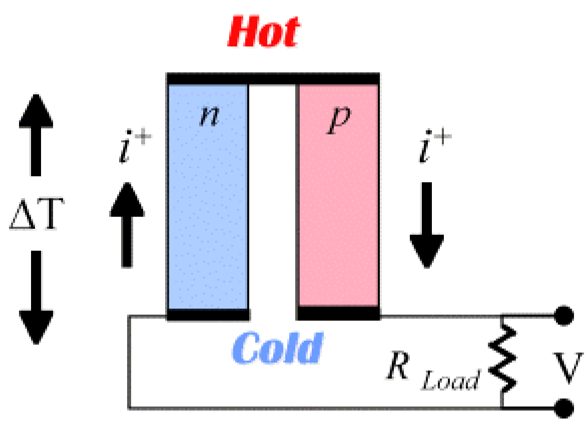
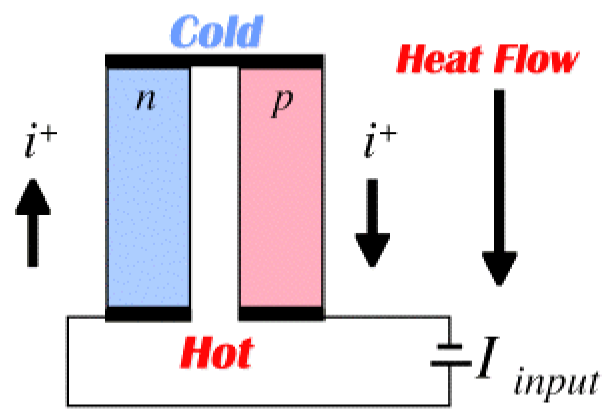


Thermoelectric (TE) effects

Interconversion of heat and electricity





Seebeck: power generation   **Peltier**: cooling

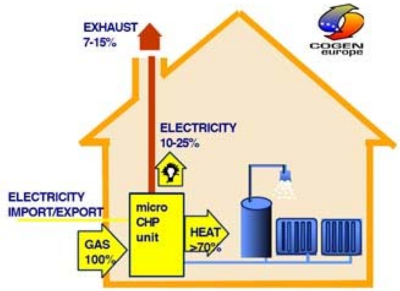
Key advantages

- ❖No moving parts, silent and reliable
- ❖Scalable (power from mW to MW)

TE applications

Mars Rover

Heat-Electricity Cogeneration



Thermally-
Controlled
Car Seat

IR Night Vision

Portable Refrigerator

Waste Heat Recovery

Wide applications but low efficiency!

TE figure of merit (zT)

$$zT = \frac{\sigma S^2 T}{\kappa_e + \kappa_l}$$

Electrical conductivity

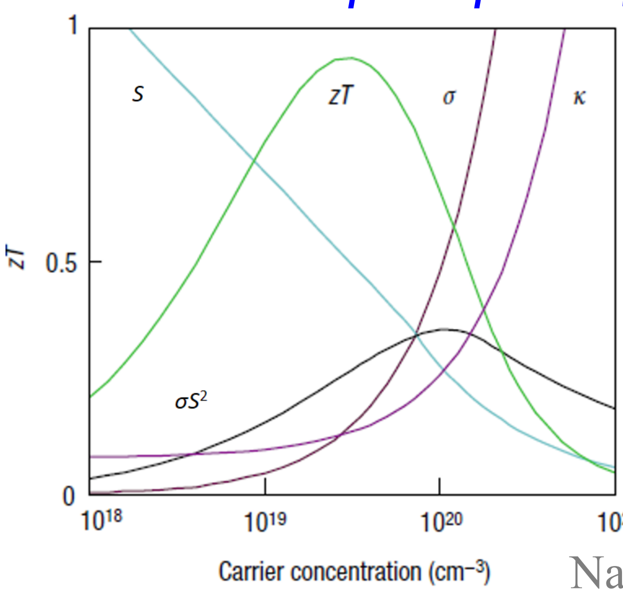
Thermopower

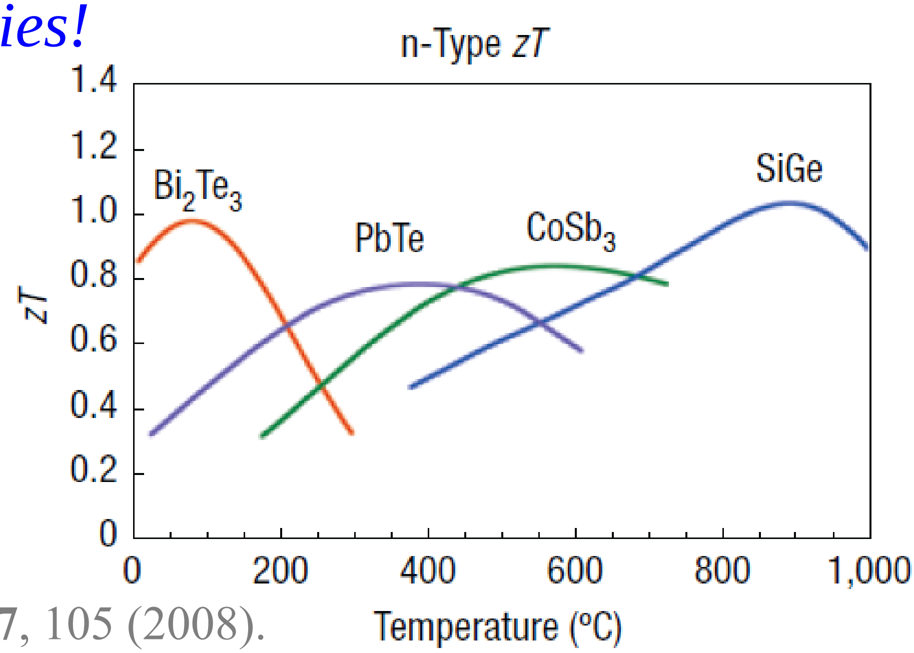
Thermal conductivity

Efficiency of a TE generator:

$$\eta = \frac{\Delta T}{T}\frac{\sqrt{1+\overline{ZT}}-1}{\sqrt{1+\overline{ZT}}+1}$$

A combination of conflicting quantities!





Nature Mater. **7**, 105 (2008).

Improving zT is a grand challenge in material science!

New materials prompt TE developments

Early stage (1820~1830)
Metal: $zT<<1$ (thermocouple only)

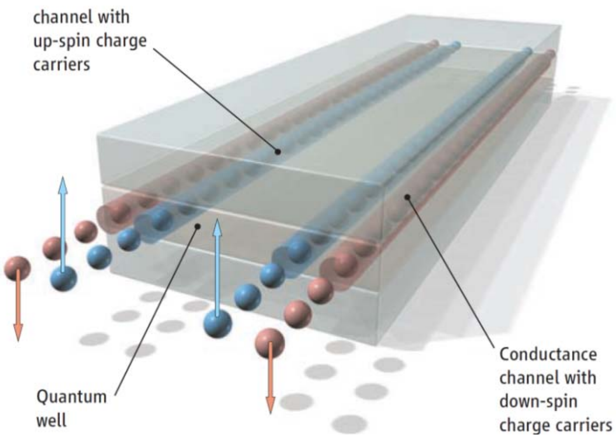
Mature period (1950~1960)
Semiconductor: $zT\sim1$
(power generation and cooling)

Revival (1990~present)
Nano-material: $1 < zT < 3$

New development:
Topological insulator: $zT > 3$?

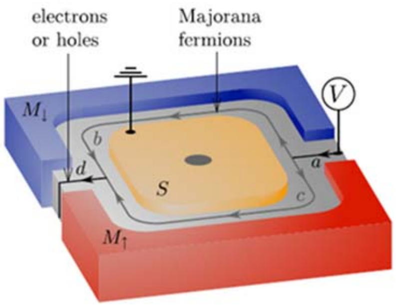
Topological insulators (TIs)

Unusual surface/edge states

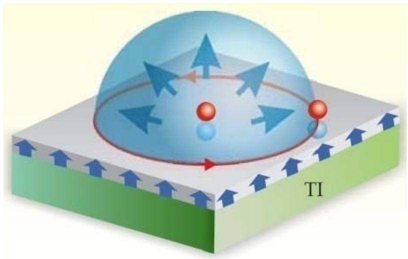


M. König, *et al*. Science **318**, 5851 (2007).

Majorana fermions

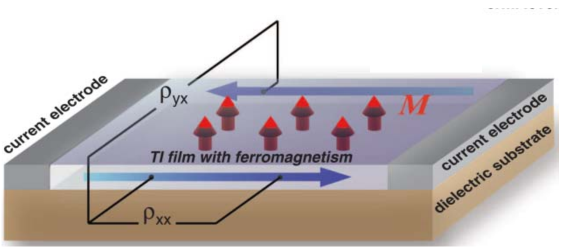


Magnetic monopole



X. Qi, *et al*. Science **323**, 5918 (2009).

Quantum anomalous Hall effect



C. Chang, *et al*. Science **340**, 6129 (2013).

Many TIs are excellent TE materials!

Material examples:

Bi_xSb_{1-x}

Bi_2Te_3, Bi_2Se_3, Sb_2Te_3,

Bi_2Te_2Se, Bi_2Te_2S, $Tl(Bi,Sb)(Te,Se,S)_2$, $Ge_1Bi_4Te_7$, $Ge_2Bi_2Te_5$,

$Ge_1Bi_2Te_4$, $PbBi_2Se_4$, $Pb_1Sb_2Te_4$, $ZrTe_5$, $HfTe_5$,

ternary Heusler compounds, filled skutterudites, ……

Material traits	TI	TE
Heavy elements	Strong SOC	Low thermal conductivity
Narrow band gap	Band inversion	Large power factor (σS^2)

- **How to use the novel TI states for TE?**
- **Are there any fundamentally new features in TI?**

Definition of *zT*

Typical definition

$$zT = \frac{\sigma S^2 T}{\kappa}$$

- σ: **Electrical conductivity**
- S: **Thermopower**
- κ: **Thermal conductivity**

Inexplicit assumption:

zT is an intrinsic material property, independent of geometry size.

Not true for TIs!

The definition of *zT* has to be changed in TI

Bulk & boundary states: ***different geometry dependence***

Typical definition

$$zT = \frac{\sigma S^2 T}{\kappa}$$

Electrical conductivity

Thermopower

Thermal conductivity

General definition

$$zT = \frac{G S^2 T}{K}$$

Electrical conductance

Thermopower

Thermal conductance

The general definition is required to describe TI!

YX *et al.* PRL 112, 226801 (2014).

Relation between the two definitions

General definition

$$zT = \frac{GS^2T}{K}$$

$\Rightarrow$

Typical definition

$$zT = \frac{\sigma S^2T}{\kappa}$$

Equivalent conditions:

(1) Ohm's scaling law: $G \propto A/L$

Fourier's scaling law: $K \propto A/L$

$\Rightarrow$ $\frac{G}{K} = \frac{\sigma}{\kappa}$

(2) S is size independent.

Geometry size: length L and area A

***zT* then will be independent of geometry size.**

zT is size-dependent in TI!

Two mechanisms induce size dependence of *zT*:

(1) Ohm's or Fourier's scaling laws fail.

(2) S depends on the geometric size.

Both mechanisms take effect in TI!

Boundary/bulk: "1"/ " 2".

$A\downarrow$

$G_1/G_2\uparrow$

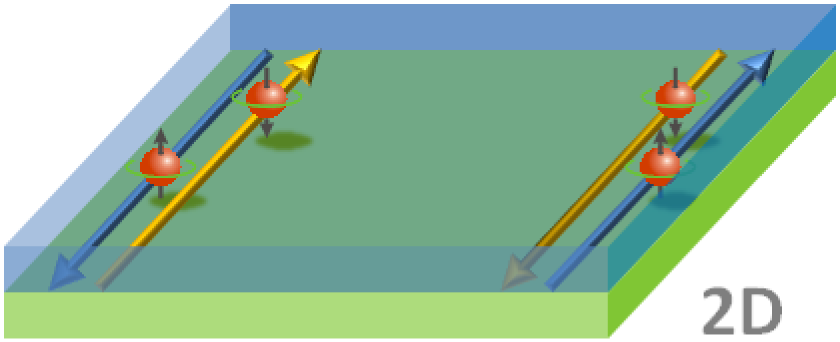
$L\uparrow$

$$S=\frac{G_1S_1+G_2S_2}{G_1+G_2}$$

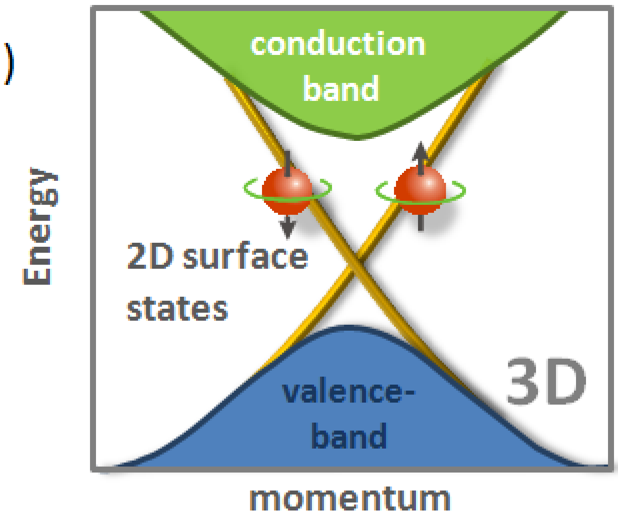
Improve *zT* by optimizing geometry!

2D and 3D TIs

a)



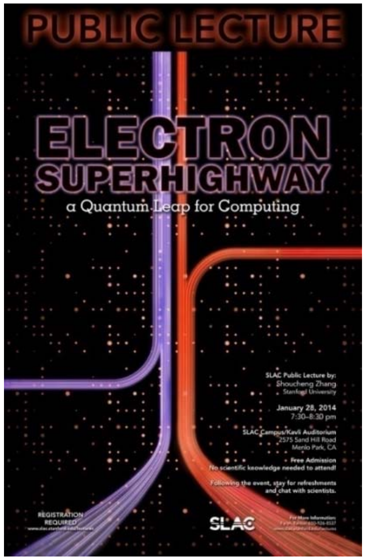
b)

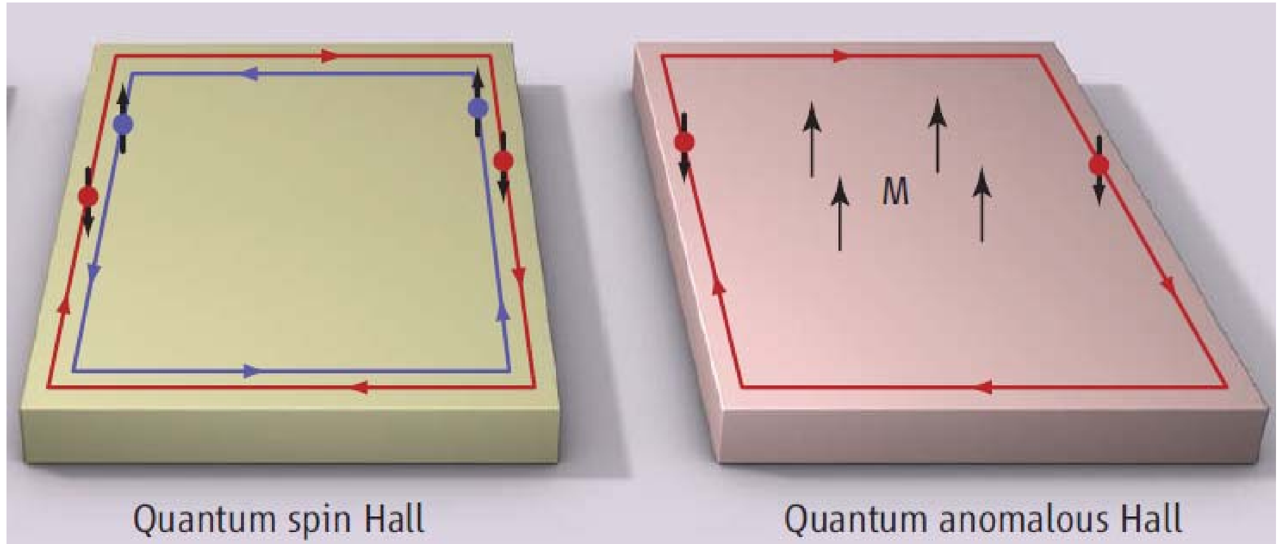


Spin-momentum locked (helical) boundary states:

- Backscattering is forbidden.
- Scatterings at $\theta \neq 180°$ are allowed in 3D TIs!

Electron conduction without dissipation





QSH Science **340**, 153 (2013). **QAH**

Low power consumption
little heat generation

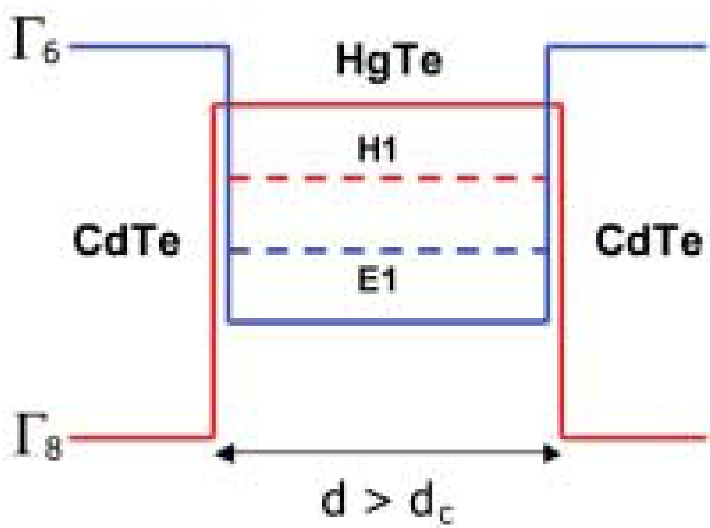
Dissipationless edge channels

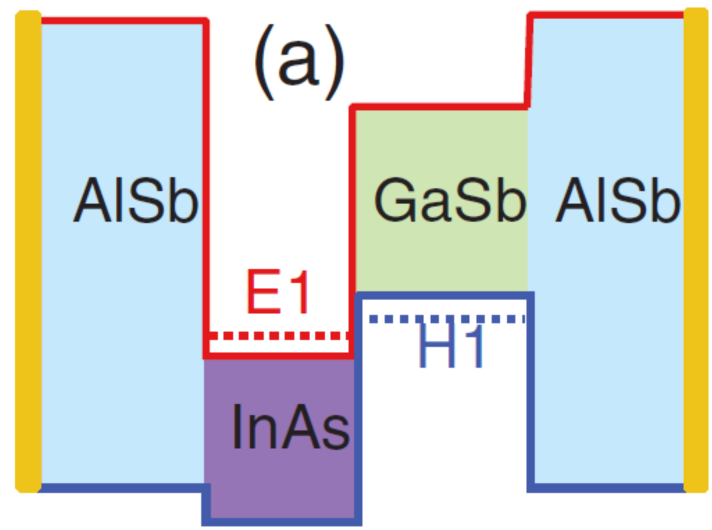
The QAH effect (our theoretical works):

Magnetic TI Cr-doped $Bi_2(Se,Te)_3$ — **PRL 111, 136801 (2013).**
Ferromagnetic CdO/EuO quantum well — **PRL 112, 096804 (2014).**
Magnetic doped p-n junction quantum well — **PRL 112, 216803 (2014).**

Search for large-gap QSH insulators (2D TIs)

Typical 2D TIs: quantum wells



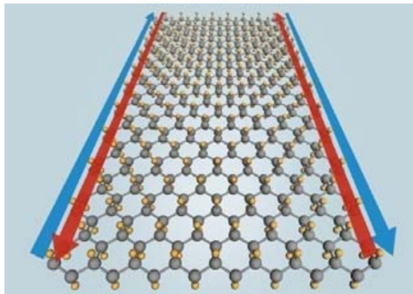


B. A. Bernevig, *et al*. Science **314**, 1757 (2006).
M. Koenig, *et al*. Science 318, 766 (2007).
C. Liu, *et al*. Phys. Rev. Lett. **100**, 236601(2008).
I. Knez, *et al*. Phys. Rev. Lett. **107**, 136603 (2011).

Low working temperature (<10 K) due to the small band gap!

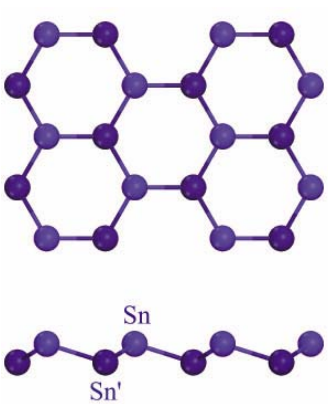
A new material class of "stanene"

Sn: "stannum"

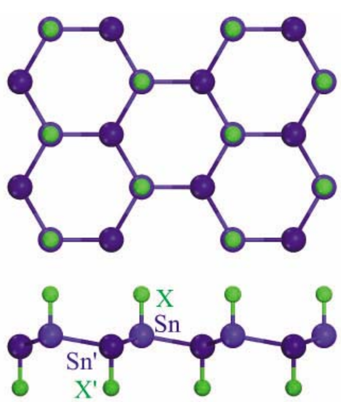


Room-temperature QSH effect

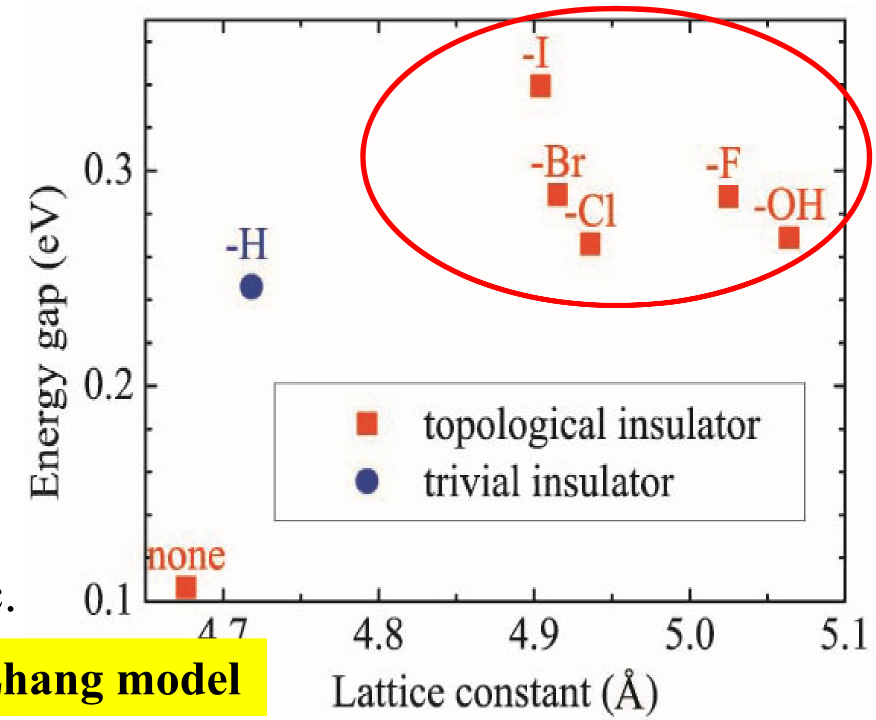
Stanene



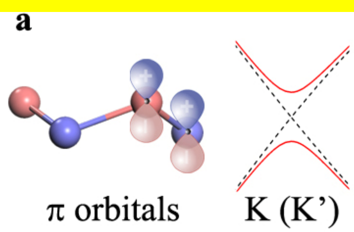
Decorated stanene



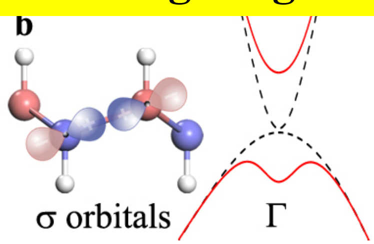
X=-F, -Cl, -Br, -I, -OH, etc.



Kane-Mele model



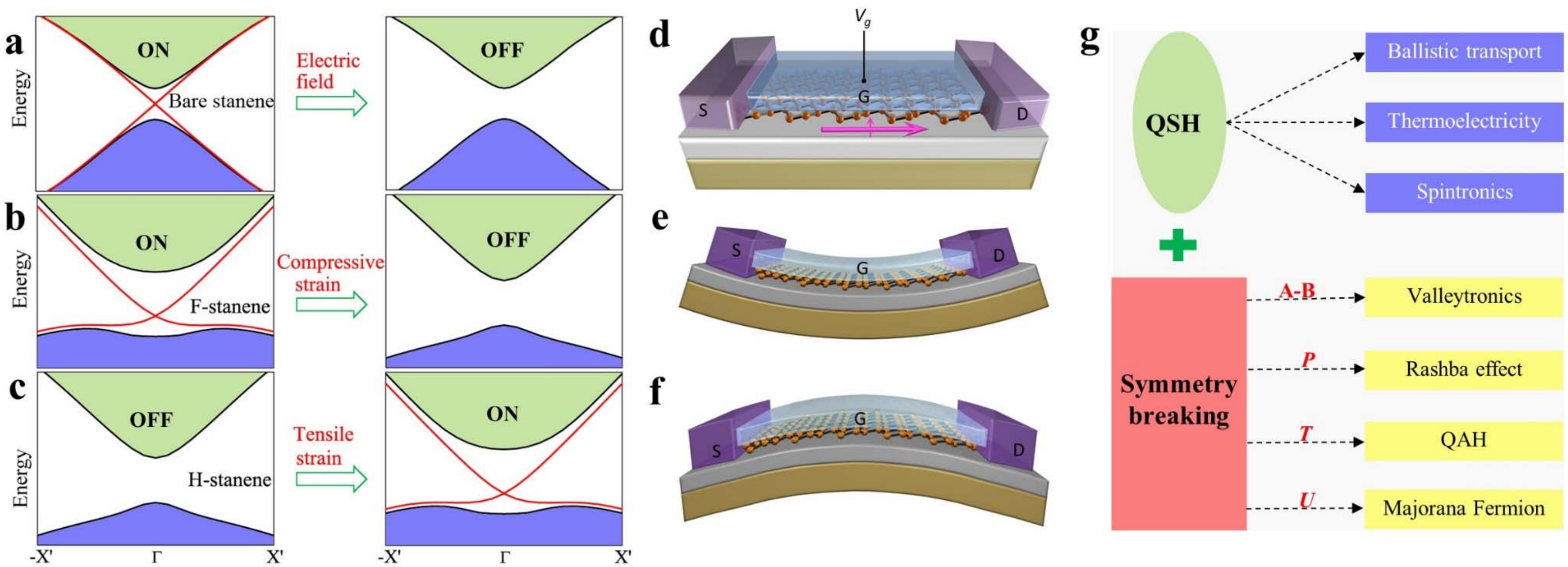
Bernevig-Hughes-Zhang model



YX *et al.* PRL 111, 136804 (2013).

Quantum TI-FET and piezotronic devices

Topological bit: **ON**/**OFF** (**with**/**without** the edge states)
Controlled by topological phase transition



Nature Mater. Invited Progress Article (under review).

Recent progresses of stanene research

Large-gap QSH[1]

Epitaxial growth of stanene[5,6]

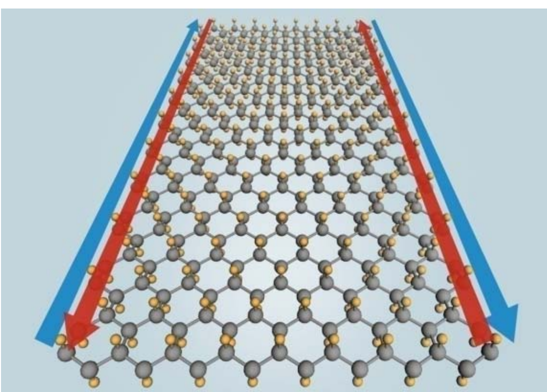
Enhanced thermoelectricity[2]

Large-gap QSH on substrate[7]

2013 2014 2015

Near-room-temperature QAH[4]

2D topological superconductivity[3]



[1] **YX** *et al*., PRL 111, 136804 (2013).
[2] **YX** *et al*., PRL 112, 226801 (2014).
[3] J. Wang, **YX**, *et al*., PRB 90, 054503 (2014).
[4] S.-C. Wu, *et al*., PRL 113, 256401 (2014).
[5] F. Zhu, W. Chen, **YX**, *et al*., Nature Mater. 14, 1020 (2015).
[6] J. Deng, **YX**, *et al*. (in preparation).
[7] **YX** *et al*., PRB 92, 081112(R) (2015).

nature materials

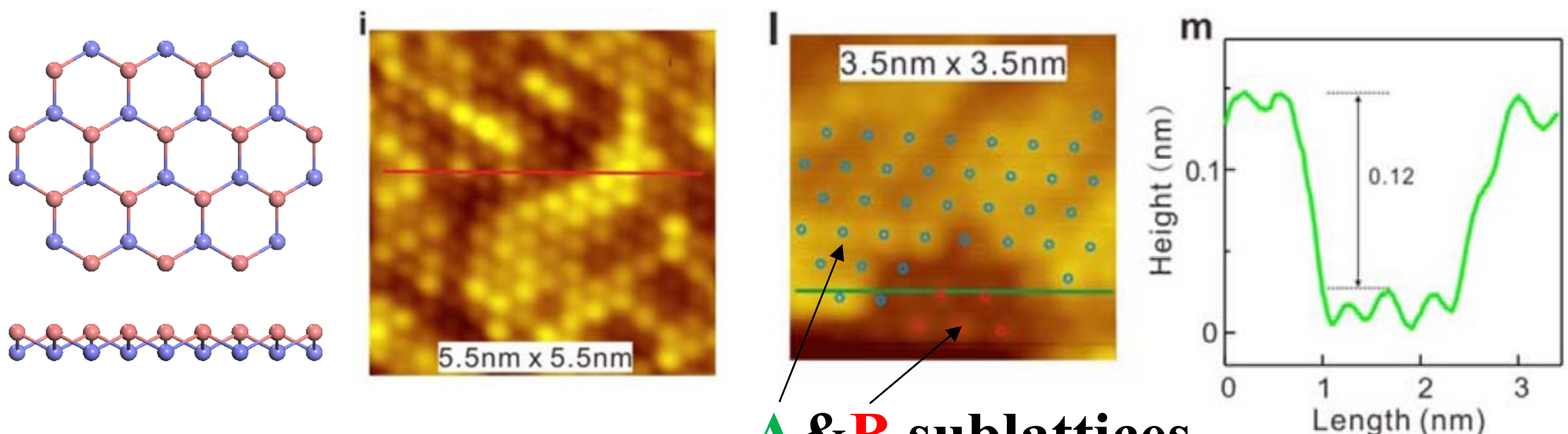
ARTICLES

PUBLISHED ONLINE: XX MONTH XXXX | DOI: 10.1038/NMAT4384

Epitaxial growth of two-dimensional stanene

Fengfeng Zhu[1†], Wei-jiong Chen[1†], Yong Xu[2,3,4†], Chun-lei Gao[1,5], Dan-dan Guan[1,5], Canhua Liu[1,5], Dong Qian[1,5★], Shou-Cheng Zhang[2,3,4] and Jin-feng Jia[1,5★]

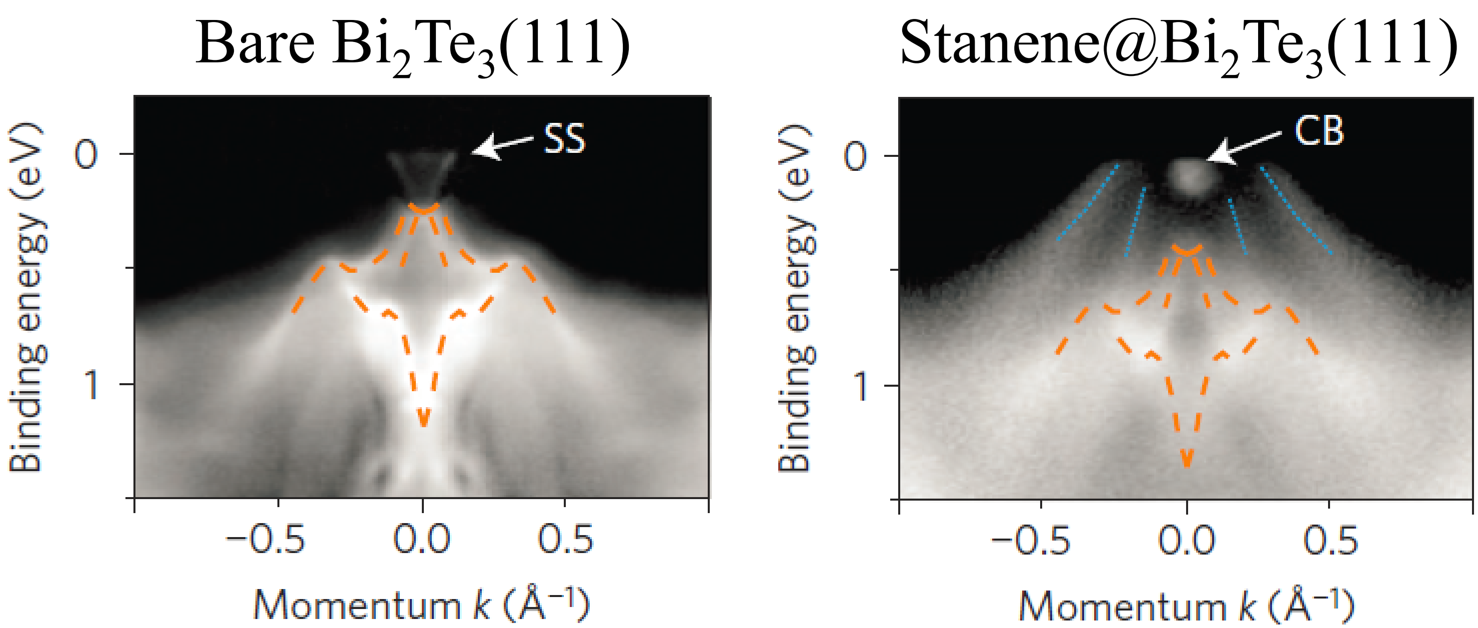
MBE growth of monlayer stanene@Bi_2Te_3(111)



A&B sublattices

Buckled honeycomb lattice (confirmed by STM).

ARPES: before and after the growth of stanene

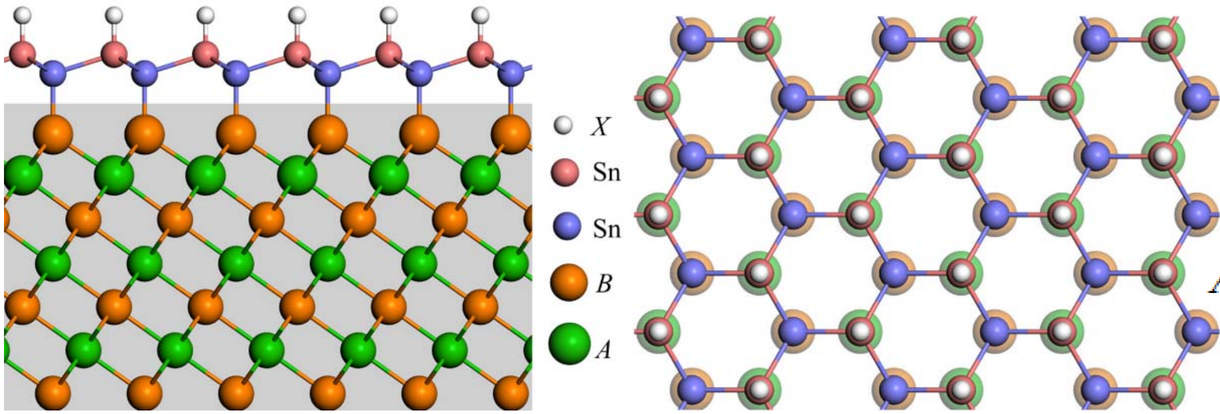


Two features (agree with DFT):

- Electron transfer from stanene to $Bi_2Te_3(111)$
- Two hole bands given by stanene

Stanene becomes metallic due to substrate effects!

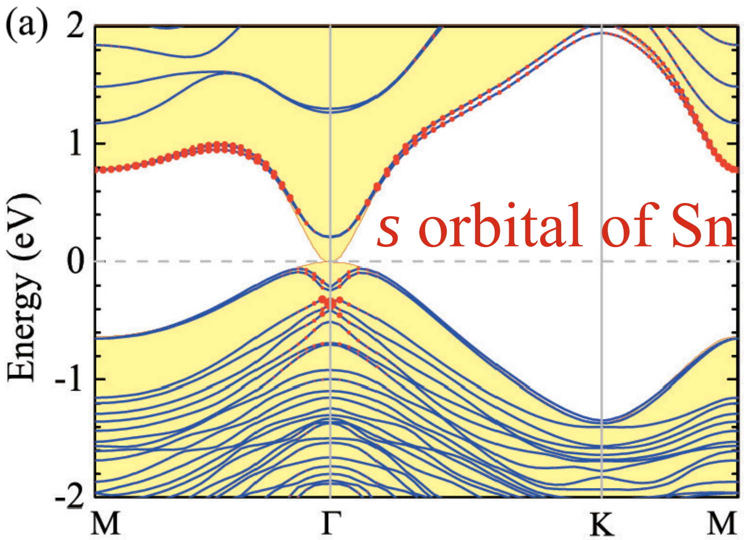
Large-gap QSH states in stanene grown on substrate



Stanene@*AB*(111)-*B*

A = Pb, Sr, Ba and B = Se, Te

Stanene@SrT*e*(111)-Te



QSH gap of stanene grown on substrates:

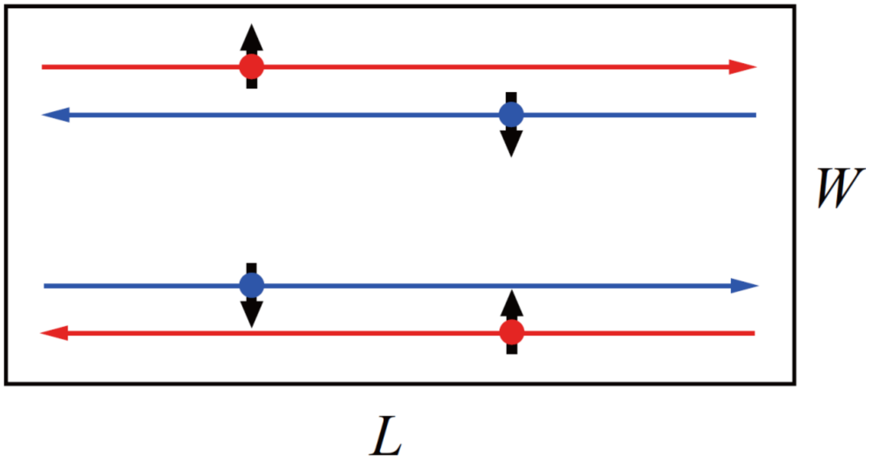
- SrTe: 0.26 eV
- PbTe: 0.09 eV
- BaSe: 0.24 eV
- BaTe: 0.30 eV

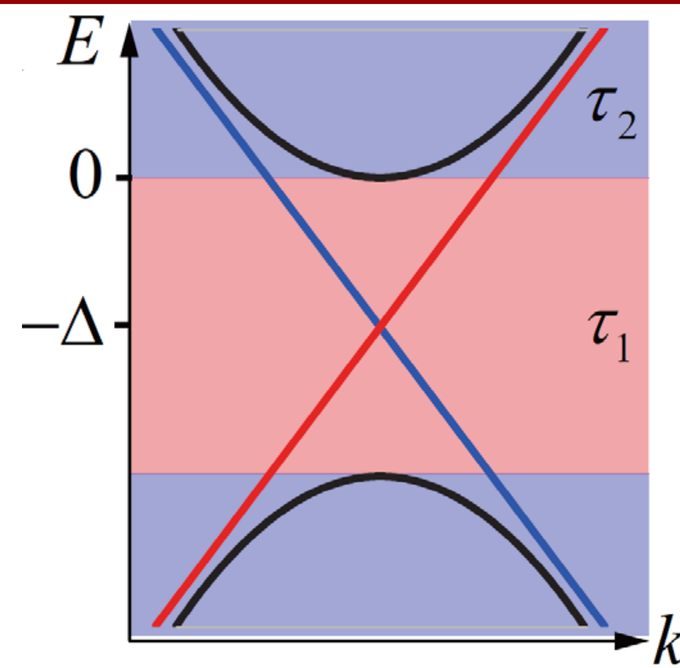
Awaiting for following experiments!

YX *et al.*, PRB 92, 081112(R) (2015).

Critical issue of using TI for TE

Two dimensional TI





Helical edge states:
favorable for electric conduction

Gapless band structure:
disadvantageous for Seebeck

Large S → Open a hybridization gap

P. Ghaemi, et al., PRL 105, 166603 (2010).

Large S → Better ways? (use intrinsic features of TI)

Two mechanisms to enhance *S*

Sommerfield expansion:

$$S = -\frac{\pi^2 k_B^2 T}{3e} \left. \frac{\partial \ln[\overline{T}(E)]}{\partial E} \right|_{E=E_F}$$

→ Transmission function

M. Paulsson and S. Datta, Phys. Rev. B 67, 241403 (2003).

Strong *E*-dependence in ⇐ **Large *S***

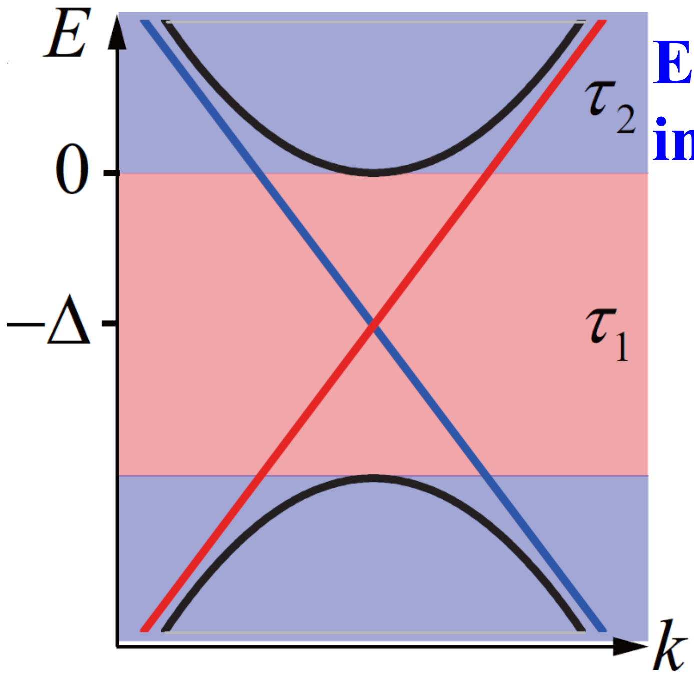
$$\overline{T}(E) \propto M(E)\tau(E)$$

Distribution of conduction modes $M(E)$
Scattering time $\tau(E)$

Open a band gap, introduce defect levels…

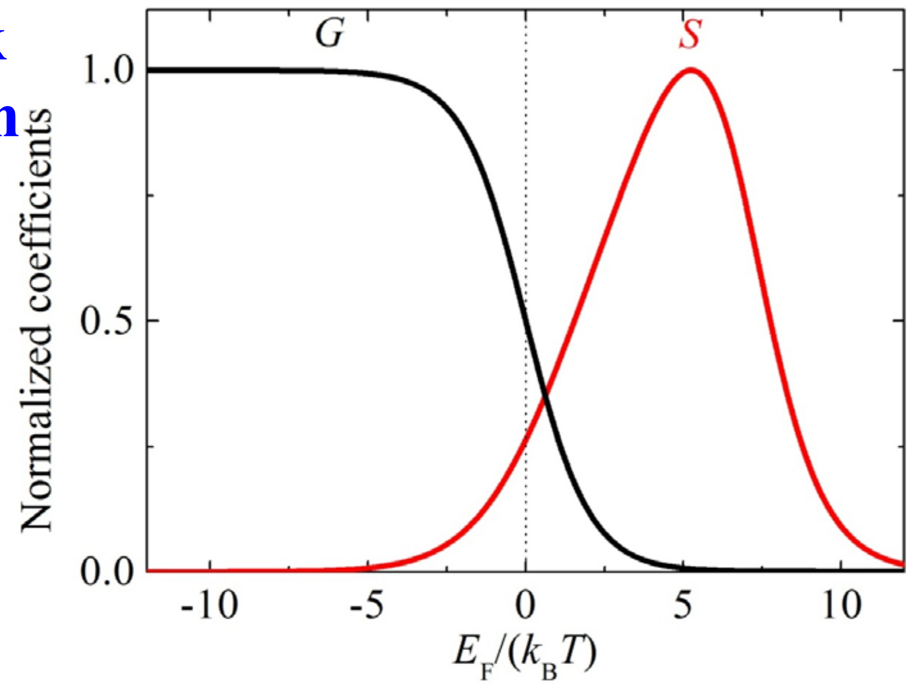
Usually neglected, but crucial for TIs.

The lifetime of TI edge states is strongly energy-dependent!



Dual scattering time (DST) model: $\tau_1 \gg \tau_2$

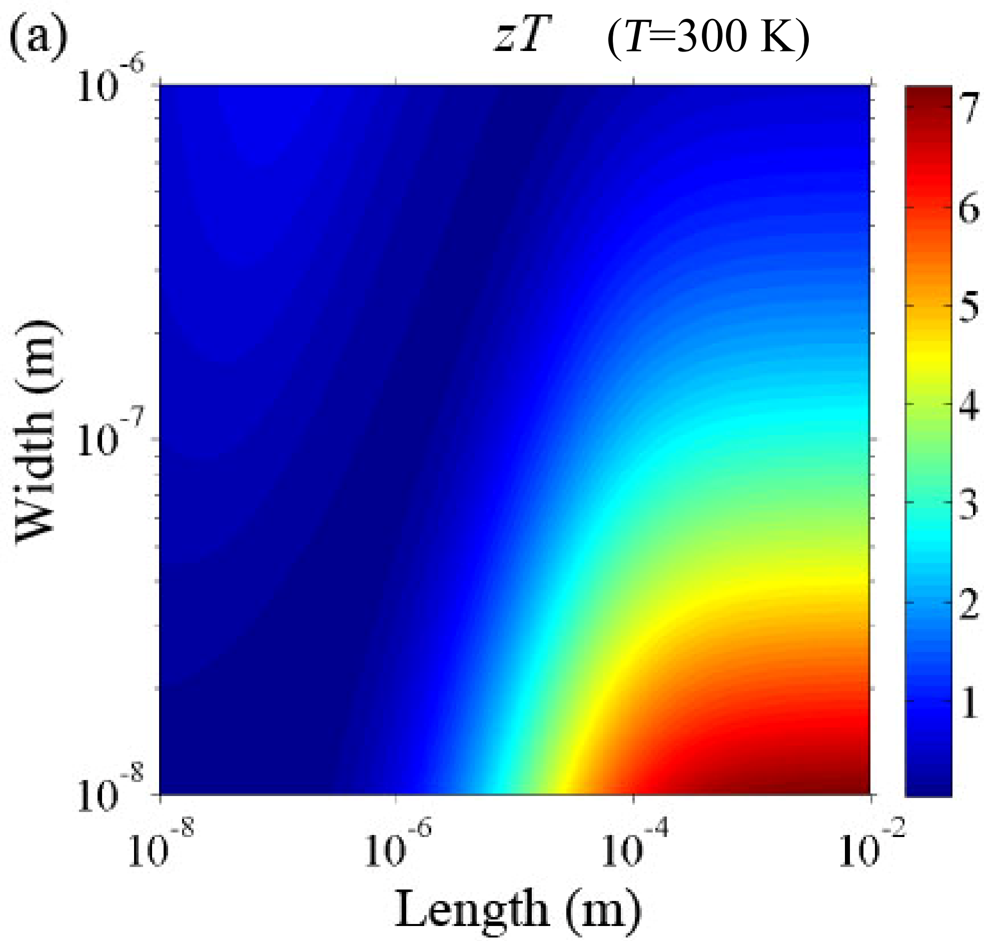
For edge states only



S_{max} = +450 μV/K (for $\tau_1/\tau_2 = 10^3$)

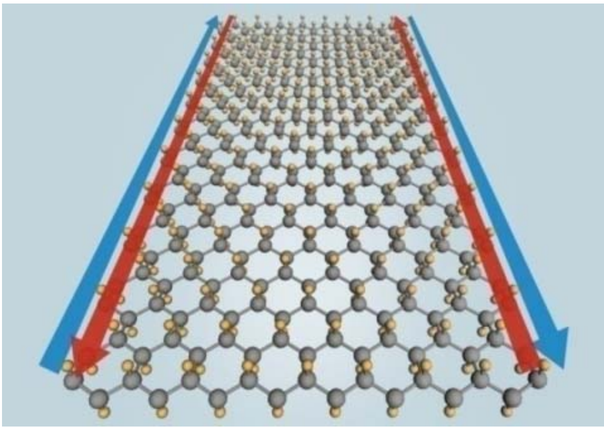
Large *S* (from gapless bands) with an unusual sign

Improve *zT* of TI by geometry optimization



Strong size dependence

Example study: stanene



Maximize edge contribution:
***zT* >3**

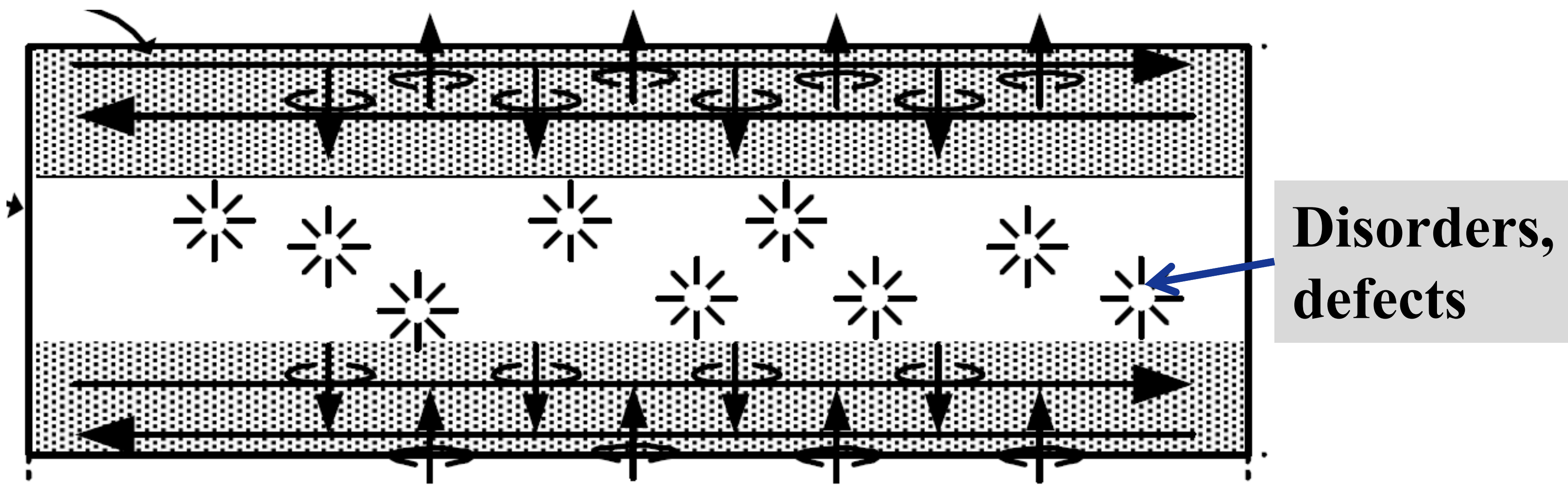
Simple and effective!

China, US patent applications

YX *et al*. PRL 112, 226801 (2014). (Editors' suggestion)

Why can *zT* be high in TIs?

Effective decoupling between electrons and phonons



"Electron-Crystal Phonon-Glass"

Main conclusions

Predictions for TIs: **YX** *et al.* PRL 112, 226801 (2014).

◆**Strong size dependence of** ***zT***

◆**Anomalous Seebeck effect (sign anomaly)**

Apply to other topological materials, including *topological crystalline insulators* and *quantum anomalous Hall insulators*.

Graphene-based TI: $zT \sim 3$ at $T \sim 40$ K

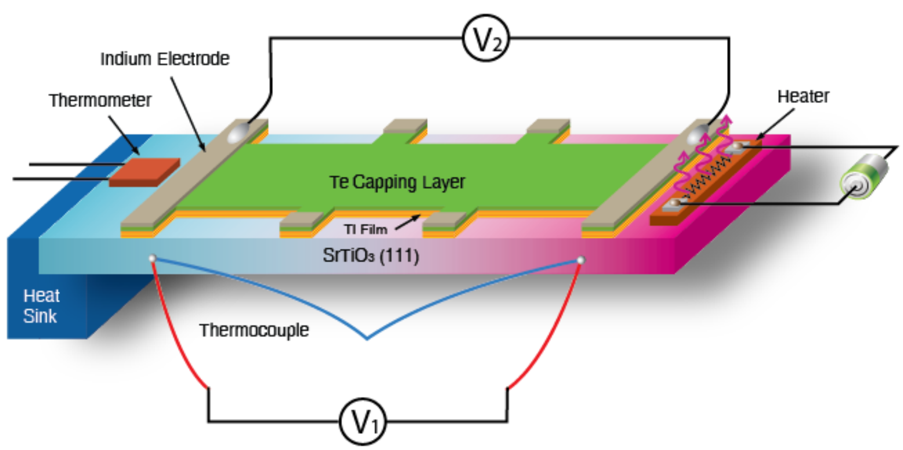
P.-H. Chang, *et al*. Nano Lett., **14**, 3779 (2014).

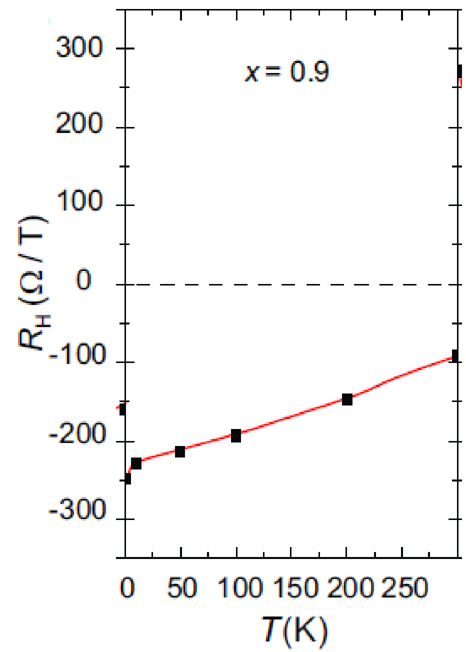
Await for experimental verification!

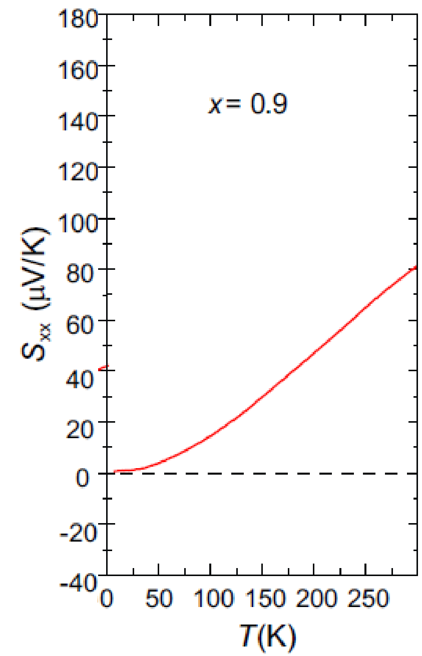
Sign anomaly of Seebeck and Hall coefficients

Our experiment: 5QL $(Bi_{1-x}Sb_x)_2Te_3$ (thin film of 3D TI)

In collaboration with Prof. Yayu Wang, Prof. Ke He and Prof. Qi-Kun Xue (Tsinghua).







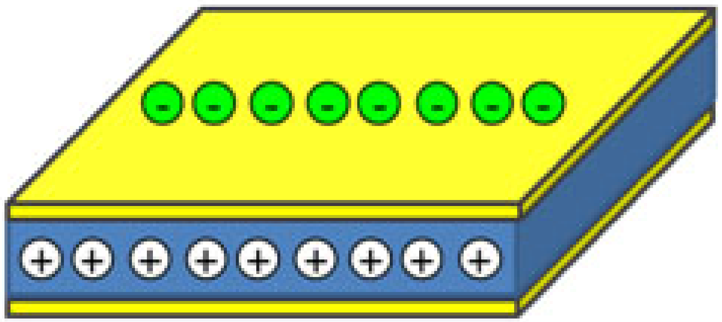
Electron-like Hall

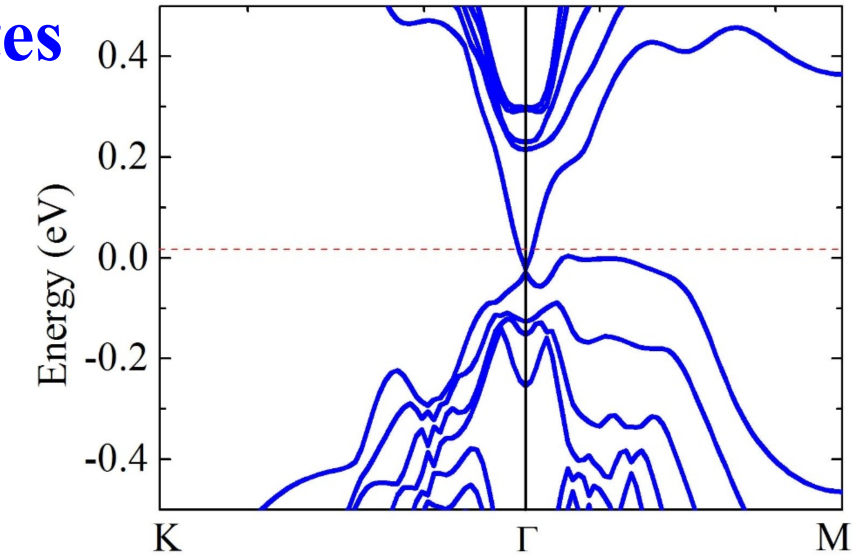
Hole-like Seebeck

J. Zhang, X. Feng, **YX** *et al*. PRB 91, 075431 (2015).

Bulk-to-surface transitions of Seebeck and Hall effects

ARPES: **N-type surface states and P-type bulk states**





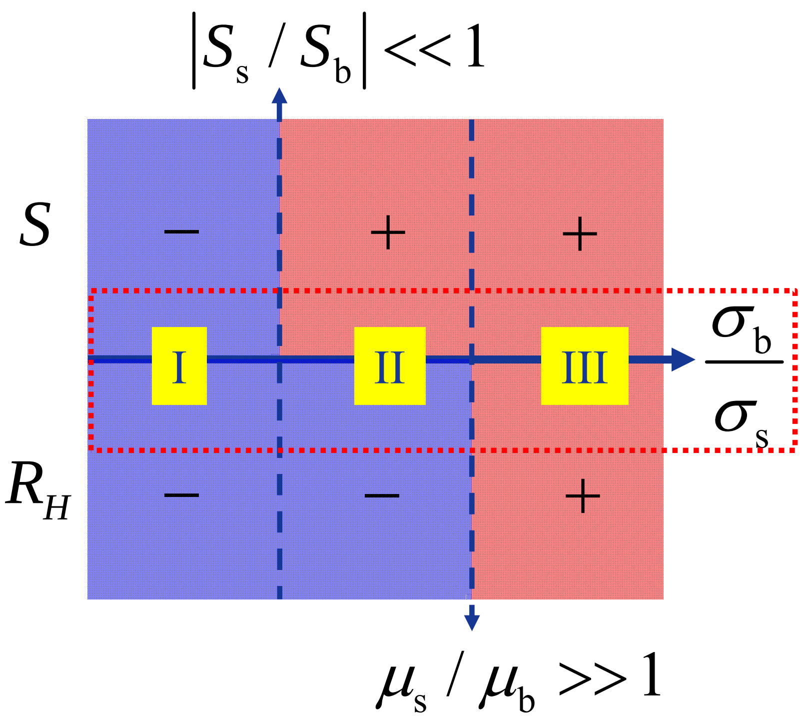
For $S_s < 0$ and $S_b > 0$,

$$S = \frac{-\sigma_s |S_s| + \sigma_b S_b}{\sigma_s + \sigma_b} = 0 \quad \Rightarrow \sigma_b / \sigma_s = |S_s / S_b| << 1$$

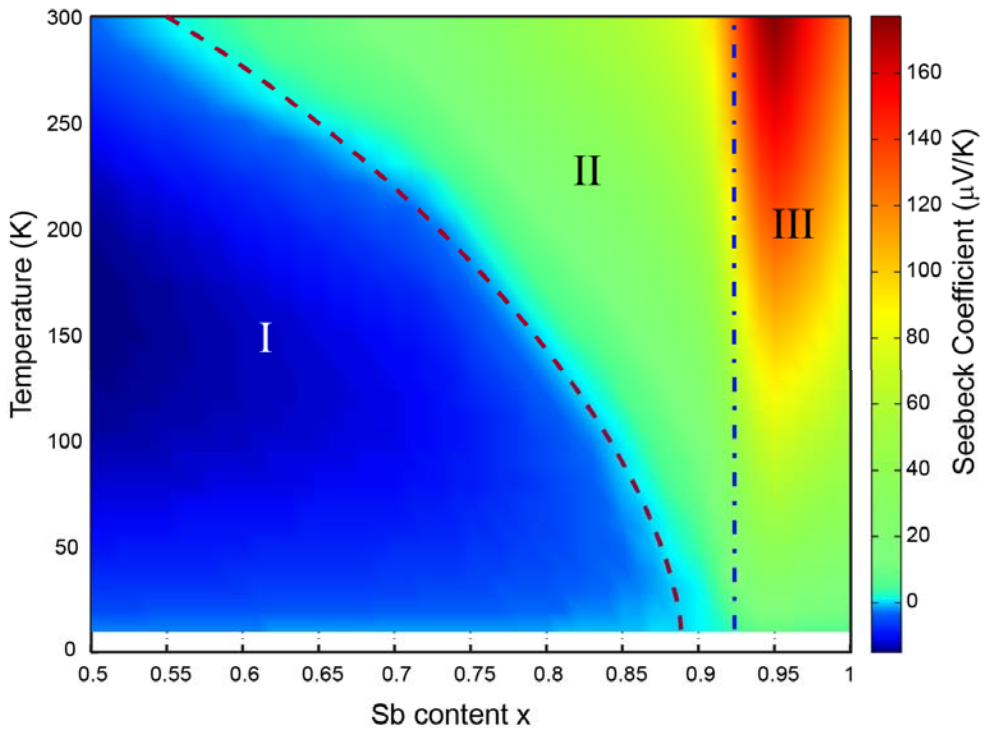
$$R_H = \frac{-\sigma_s \mu_s + \sigma_b \mu_b}{(\sigma_s + \sigma_b)^2} = 0 \Rightarrow \sigma_b / \sigma_s = \mu_s / \mu_b >> 1$$

Bulk-to-surface transition driven by tuning σ_b / σ_s

Bulk-to-surface transitions of Seebeck and Hall effects



Exp. data



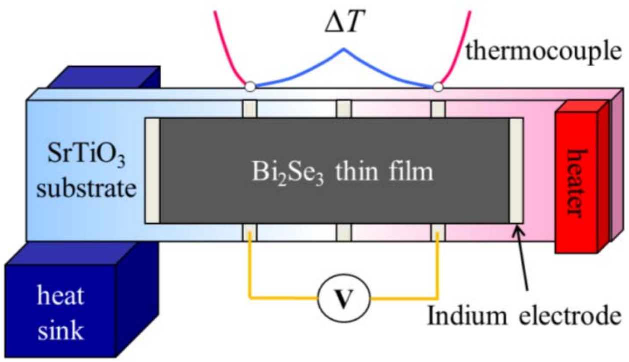
5QL $(Bi_{1-x}Sb_x)_2Te_3$

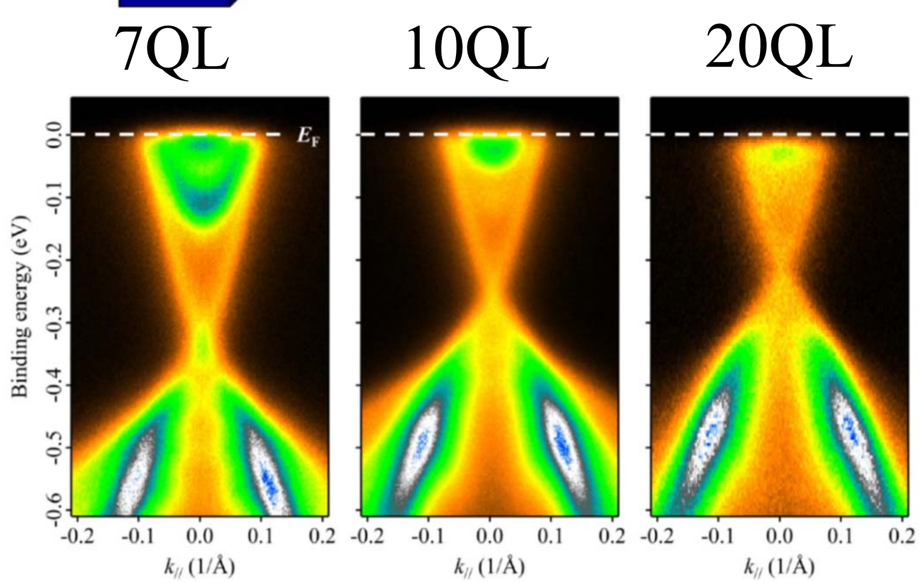
2D metallic surface states: **large μ and small *S*.**

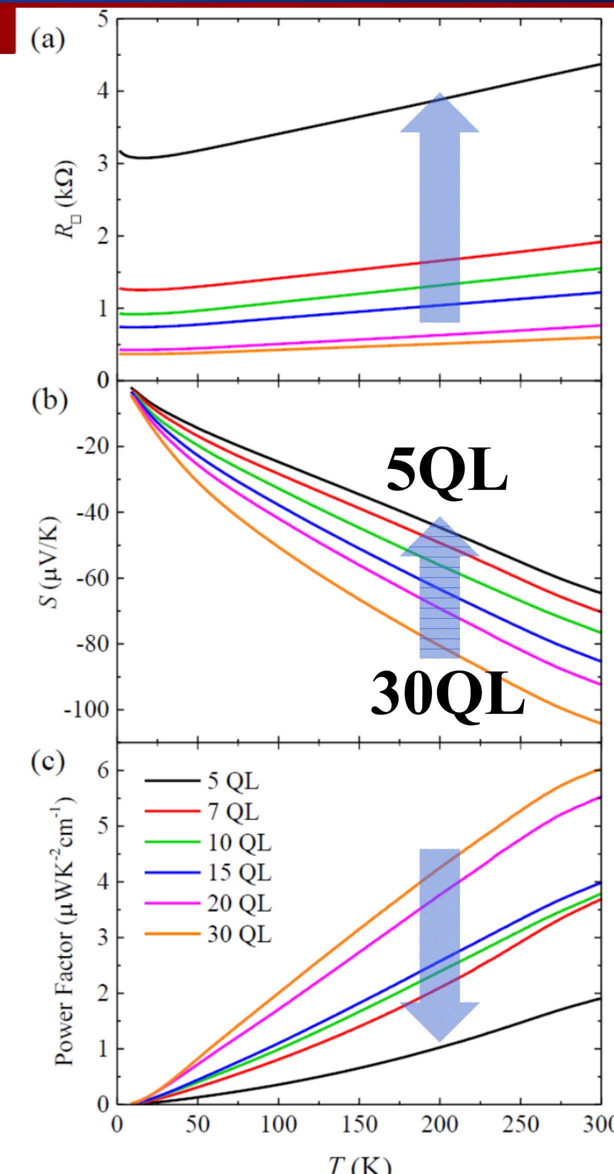
Very likely to reach region II (*S*>0, R_H<0)!

Strong Size effects in TI thin films

Exp. on 3D TI Bi_2Se_3 thin films

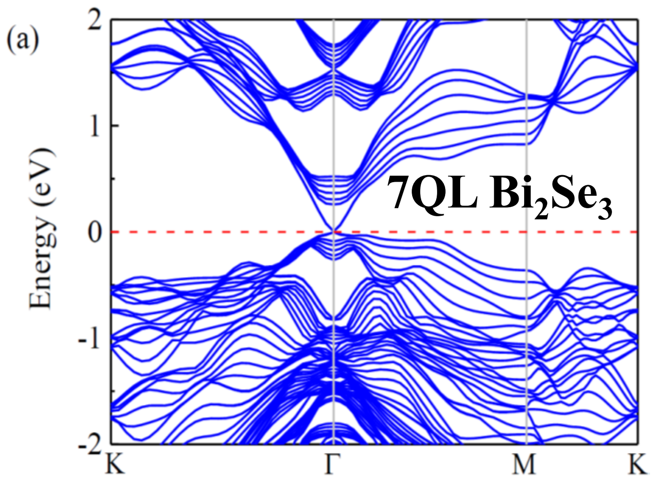






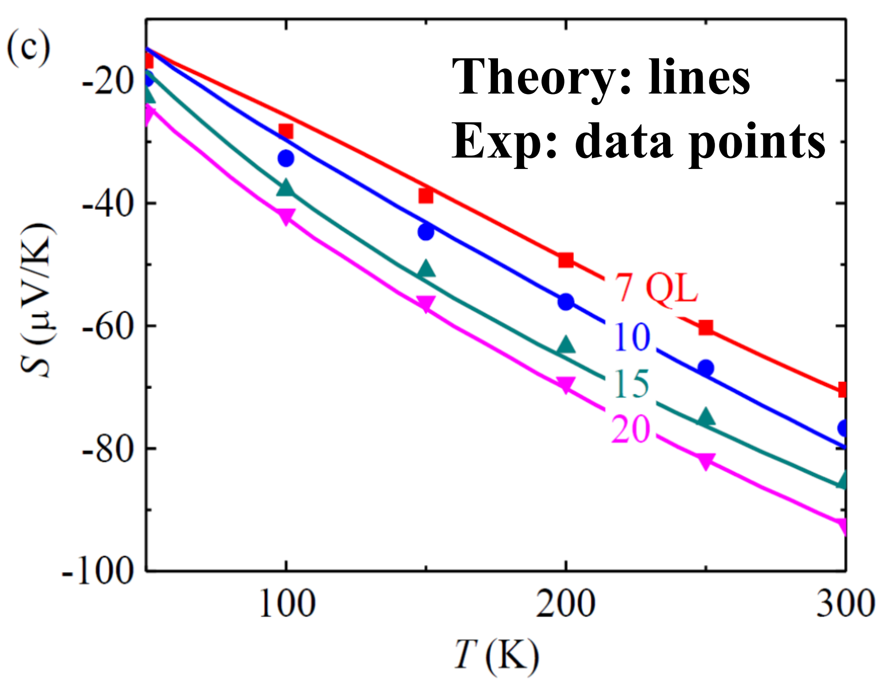
M. Guo, Z. Wang, **YX** *et al*. New J. Phys. 18, 015008 (2016).

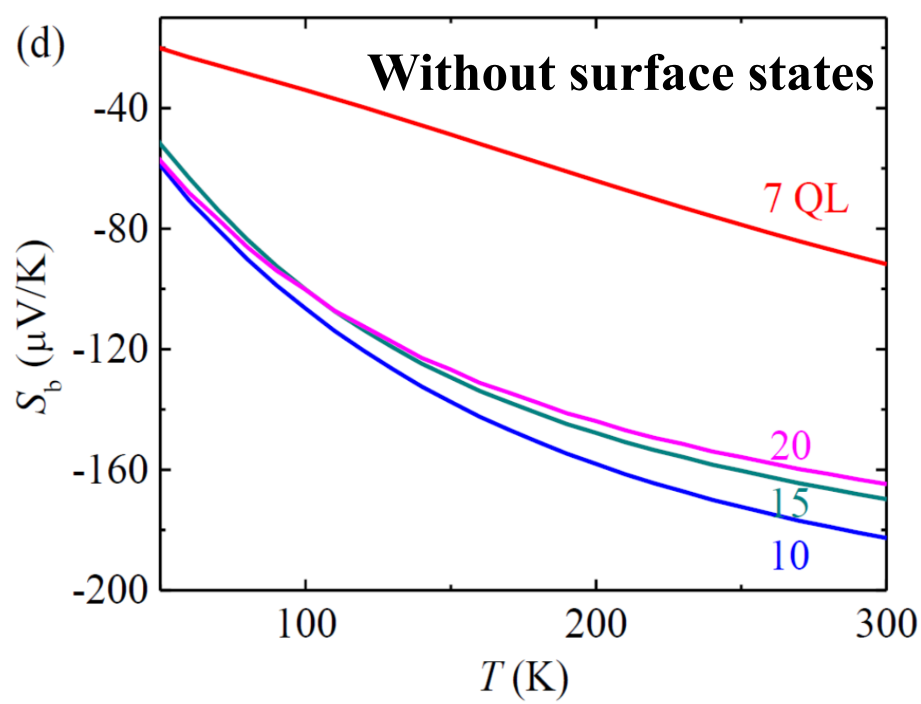
S is suppressed by the surface states



DFT & Landauer transport formalism.

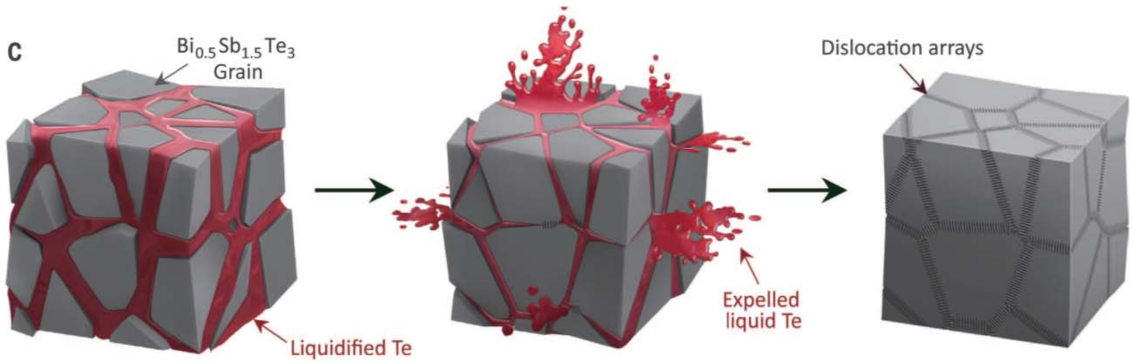
Use E_F determined by ARPES.





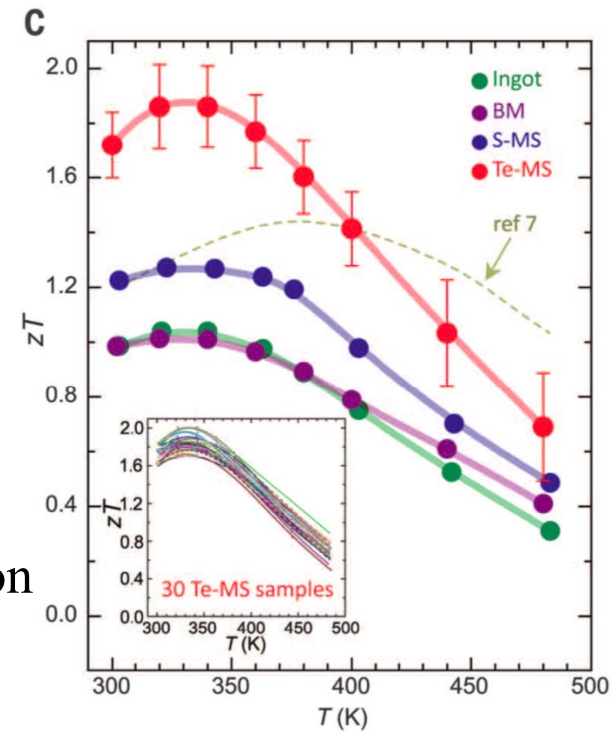
Outlook

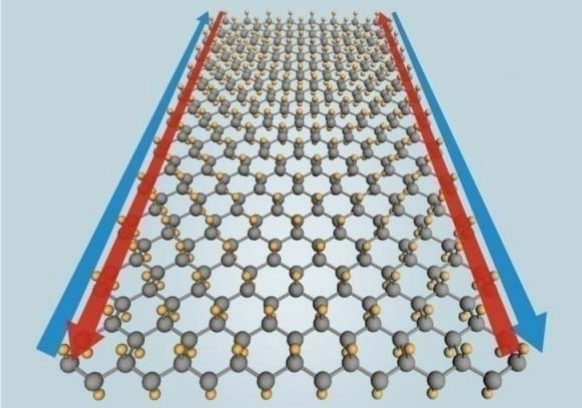
3D TI $Bi_{0.5}Sb_{1.5}Te_3$: p-type ***zT* ~ 1.86 at *T* = 320 K**
(by Samsung Electronics) Science **348**, 109 (2015).



Low energy grain boundary by liquid phase compaction

The underlying mechanism is unclear!





Future: more research on 2D TI
search large-gap materials, like stanene.

F. Zhu, W.-J. Chen, **YX** *et al*. Nature Mater. 14, 1020 (2015).
YX *et al*., Phys. Rev. B 92, 081112(R) (2015).

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Thanks for your attention!