Julius-Maximilians-
UNIVERSITÄT
WÜRZBURG

ep4

Elemental and elementary fun with topological insulators: α-Sn, stanene, bismuthene

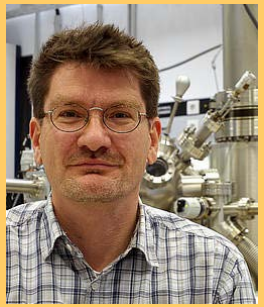
Ralph Claessen

Physikalisches Institut and
Röntgen Center for Complex Materials (RCCM),
Universität Würzburg, Germany

- Sn as 3D and 2D TI
- bismuthene/SiC: a quantum spin Hall paradigm
- electronic correlations in 1D edge states

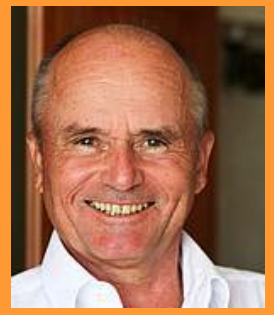
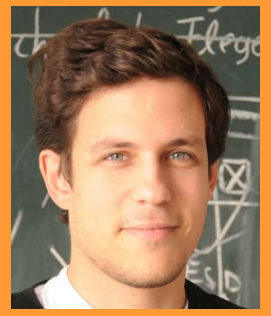
The team

Jörg Schäfer
Felix Reis
Raul Stühler
Florian Adler
Arne Barfuss
Max Bauernfeind
Lenart Dudy
Stefan Glass
Victor Rogalev
Markus Scholz



experiments

Gang Li *(now Shanghai Tech)*
Werner Hanke
Ronny Thomale
Domenico Di Sante
Andrzei Fleszar
Congjun Wu *(UCSD)*
Ewelina Hankiewicz
Fernando Dominguez
Dimitri Jungblut
Benedikt Scharf

theory

(almost) all @ U Würzburg

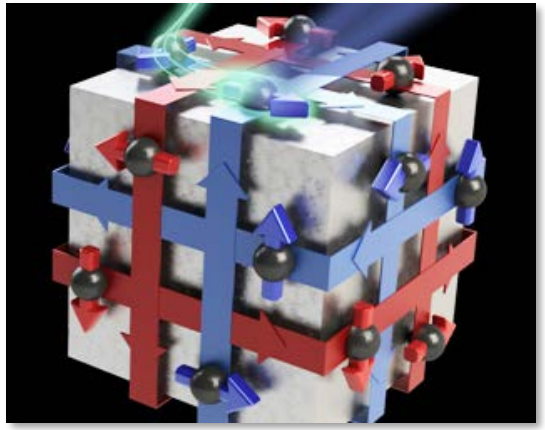
SFB1170
ToCoTronics*

*Topological and correlated electronics
at surfaces and interfaces

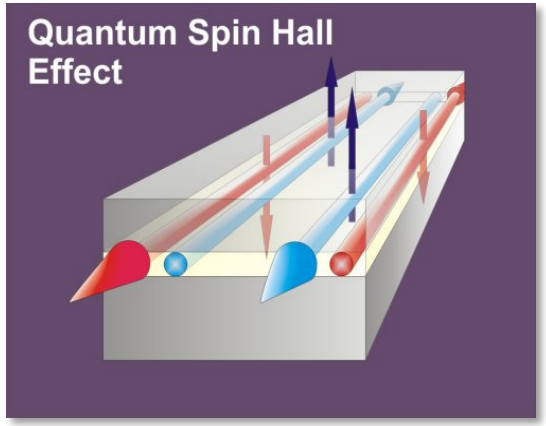
funded by DFG

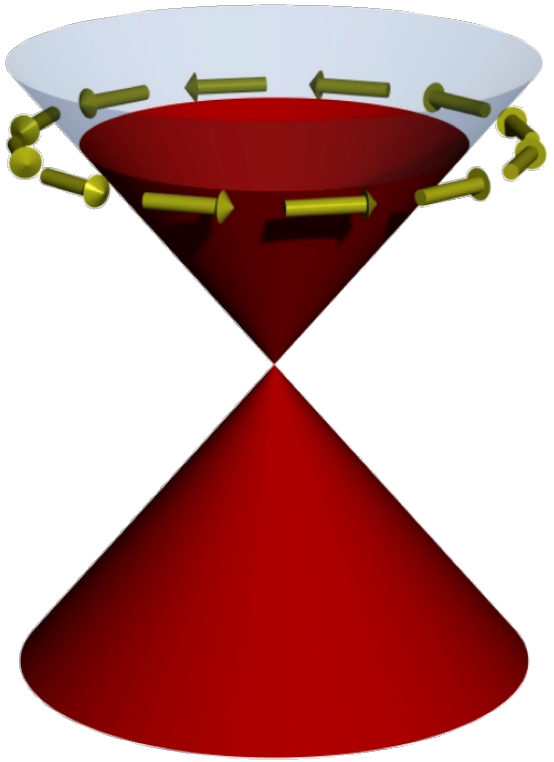
Helical surface/edge states in topological insulators

3D TIs
with 2D surface states



2D TIs
with 1D edge states





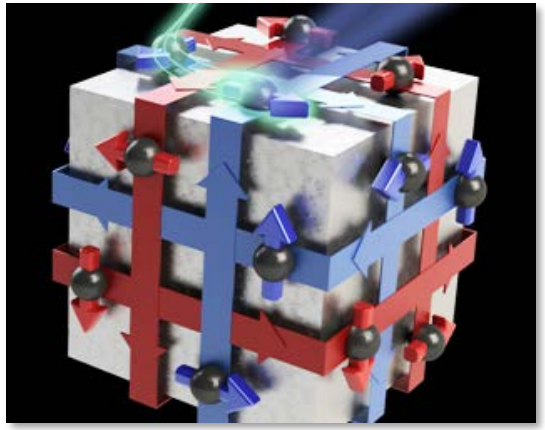
"topologically protected" surface/edge states in the bulk band gap:

- metallic
- spin-polarized
- helical

➡ search for Dirac materials & quantum spin Hall (QSH) insulators for **electronic/spintronic applications at room temperature**

Helical surface/edge states in topological insulators

3D TIs
with 2D surface states



2D TIs
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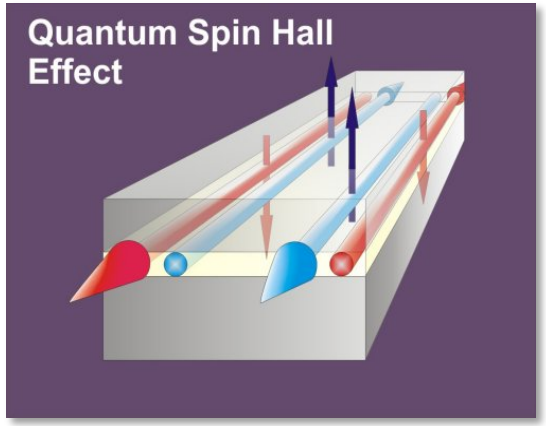

"topologically protected" surface/edge states in the bulk band gap:

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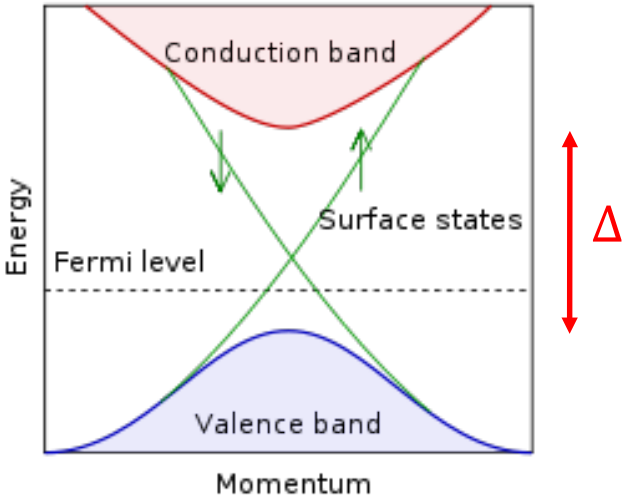
➡ search for Dirac materials & quantum spin Hall (QSH) insulators for **electronic/spintronic applications at room temperature**

Quantum Spin Hall Effect (QSHE) in 2D TIs

theoretical proposal:
semiconductor quantum wells with inverted band gap
Bernevig, Hughes & Zhang, Science (2006)



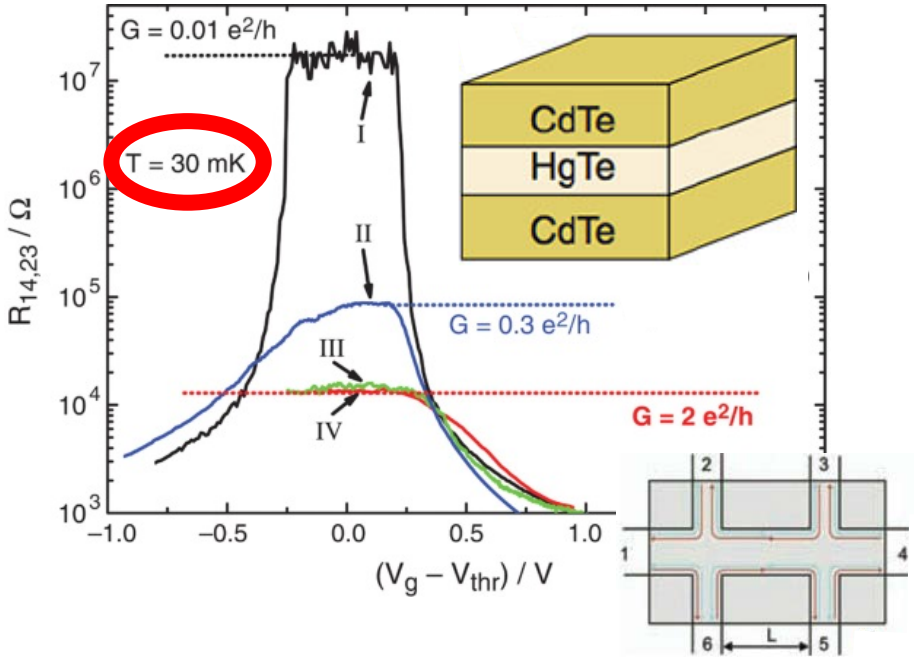
experimental realizations:

- HgTe/CdTe quantum well structures
  M. König et al., Science (2007)

  → effective band gap: $\Delta < 40$ meV

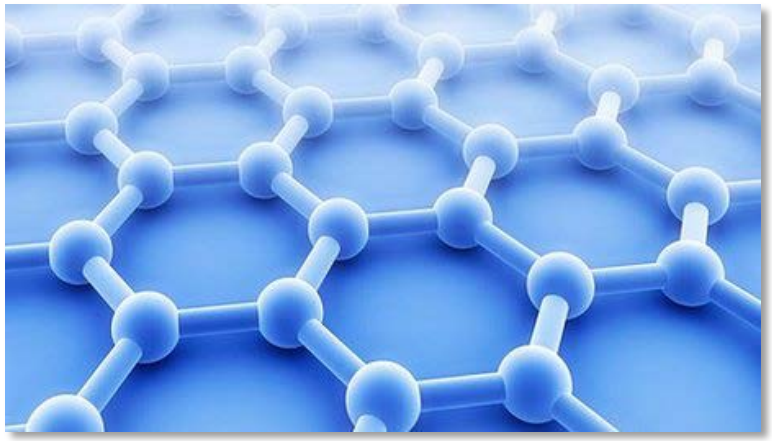
- InAs/GaSb QWs
  Knez, Du & Sullivan, PRL (2011)

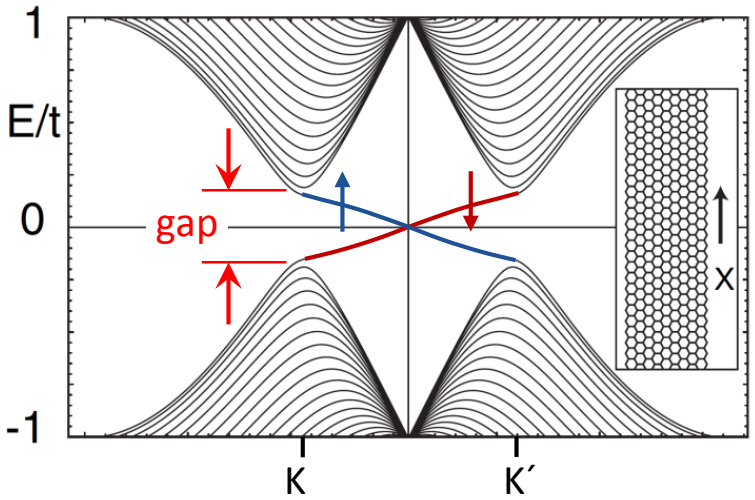
  → $\Delta \approx 4$ meV



Quantum spin Hall effect in honeycomb lattices

Kane & Mele, PRL (2005): **QSHE in graphene**





SOC-induced energy gap:

24 µeV
graphene

2 meV

24 meV

100 meV
stanene

Y. Xu et al., PRL 2013

spin-orbit coupling

Z^4

IV

6	12,011	C Carbon
14	28,086	Si Silicon
32	72,64	Ge Germanium
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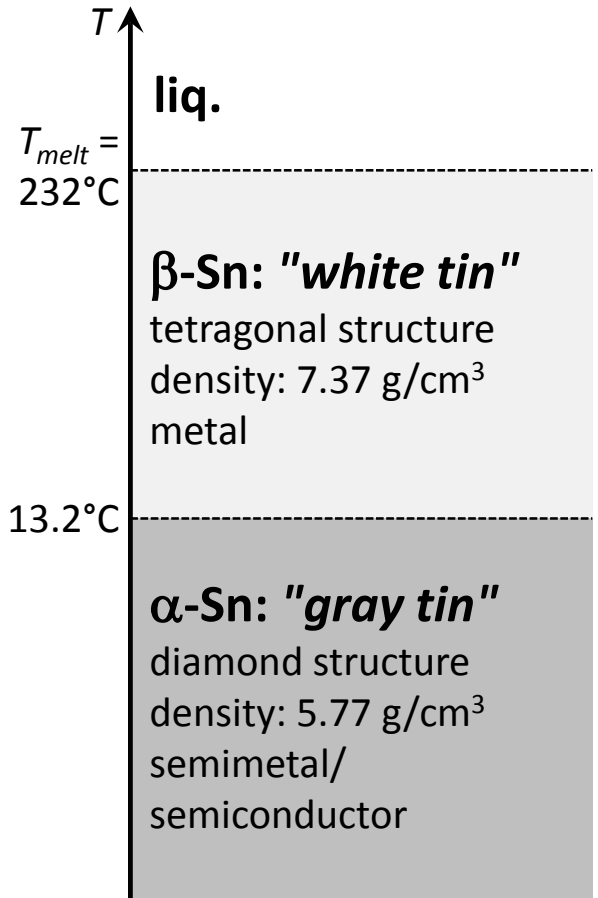
82	207,2	Pb Lead

→ **spin-polarized (helical) metallic edge states**

Elemental Sn as 3D and 2D topological insulator

Sn as elemental TI



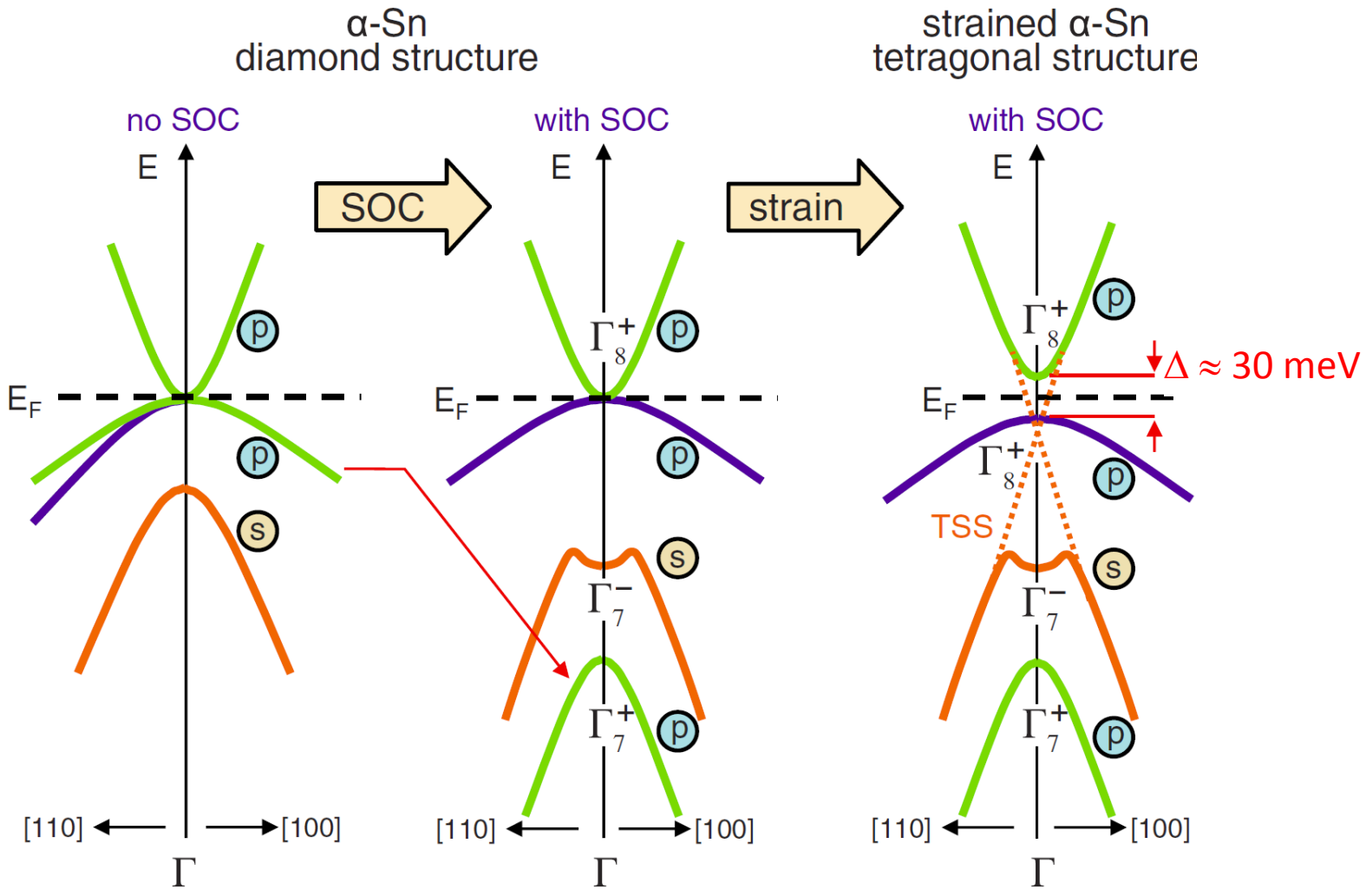
		13 IIIA 3A	14 IVA 4A	15 VA 5A	16 VIA 6A	17 VIIA 7A
		5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998
11 IB 1B	12 IIB 2B	13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453
29 Cu Copper 63.546	30 Zn Zinc 65.39	31 Ga Gallium 69.732	32 Ge Germanium 72.61	33 As Arsenic 74.922	34 Se Selenium 78.09	35 Br Bromine 79.904
47 Ag Silver 107.868	48 Cd Cadmium 112.411	49 In Indium 114.818	50 Sn Tin 118.71	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904
79 Au Gold 196.967	80 Hg Mercury 200.59	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium [208.982]	85 At Astatine 209.987

- **strained α-Sn – *diamond lattice***
  can be stabilized on suitable substrate

- **strained HgTe - *zincblende structure***
  → 3dim topological insulator

  (Brüne et al., PRL 2011)

Strained α-Sn/InSb(001): electronic band structure

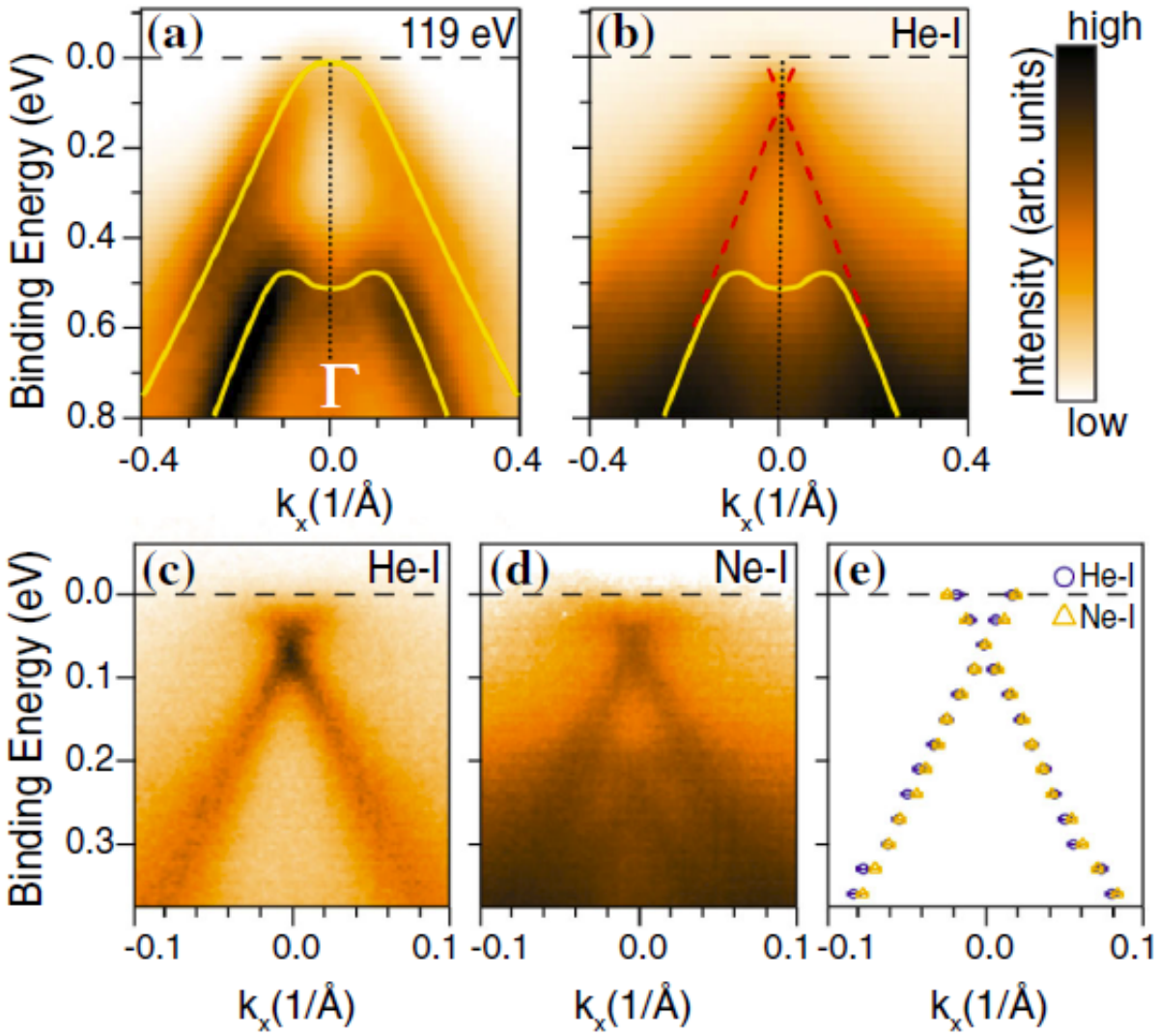


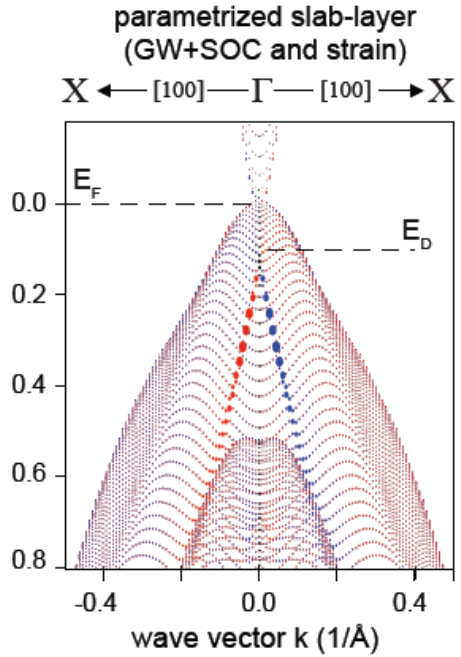
experimental realization:

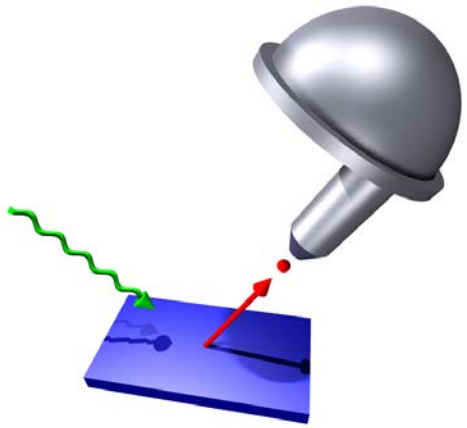
- epitaxial growth of α-Sn on InSb(001)
- compressive strain: -0.14%
- thickness: ~ 10 nm

*PRL **111**, 157205 (2013)*

Strained α-Sn/InSb(001): ARPES of topological surface states and Dirac cone

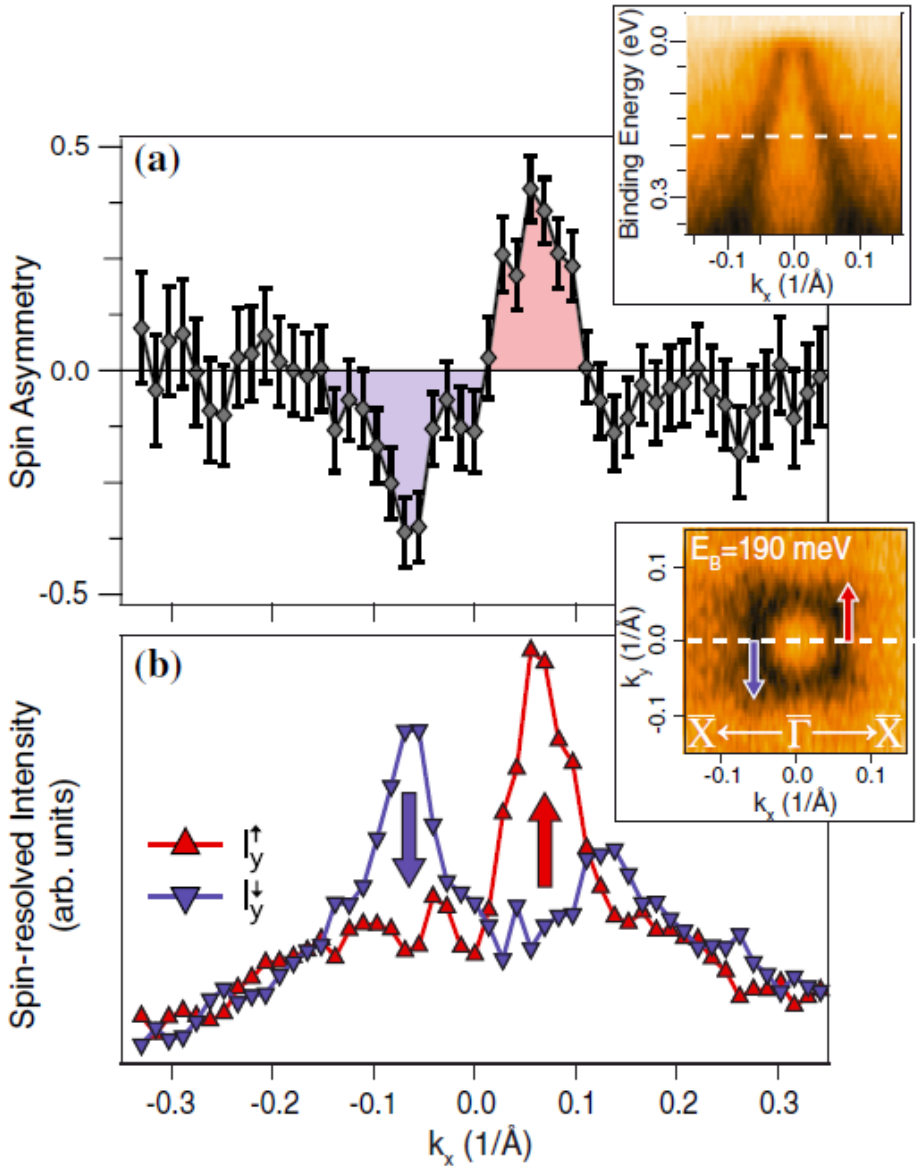


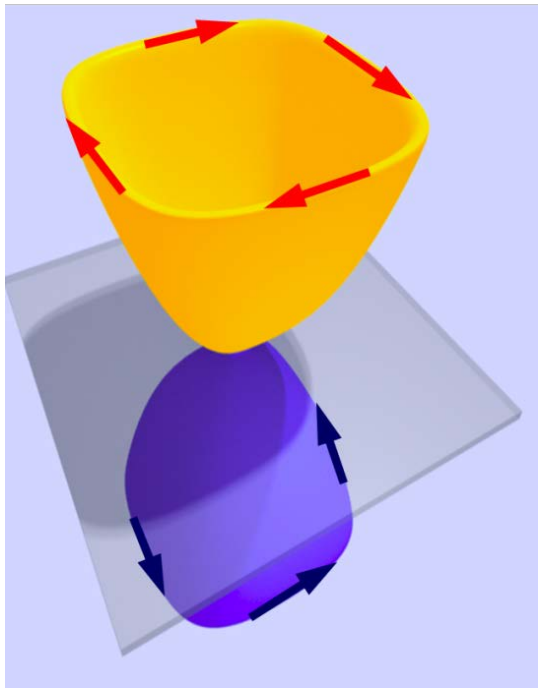




*PRL **111**, 157205 (2013)*

Strained α-Sn/InSb(001): spin-resolved ARPES





→ spin-momentum locking !

*PRL **111**, 157205 (2013)*

Quantum spin Hall effect in honeycomb lattices

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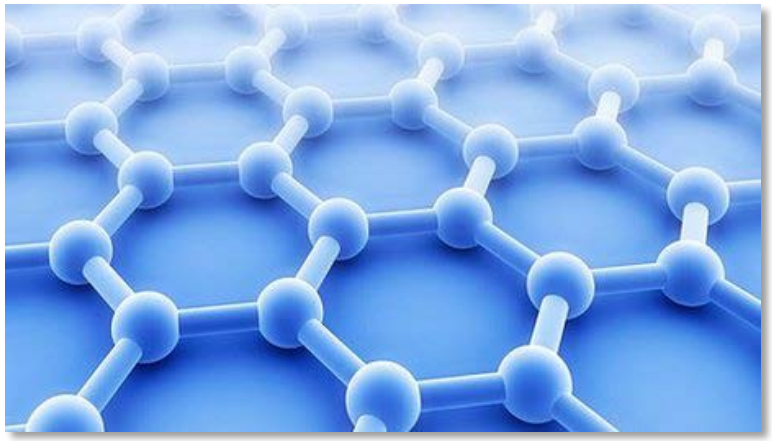

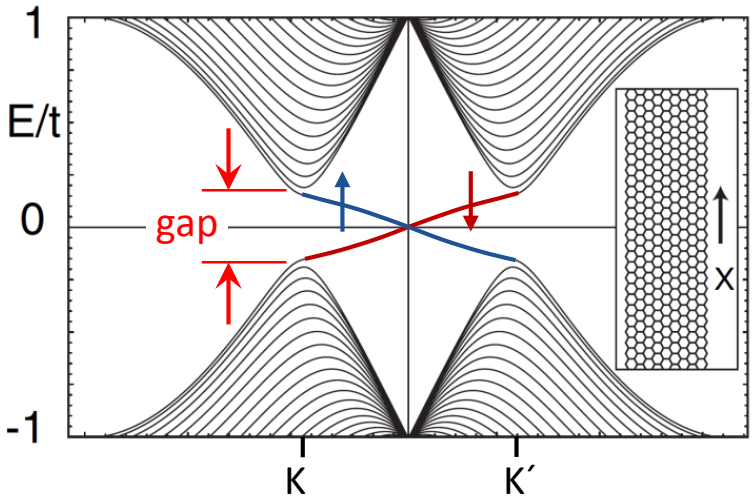

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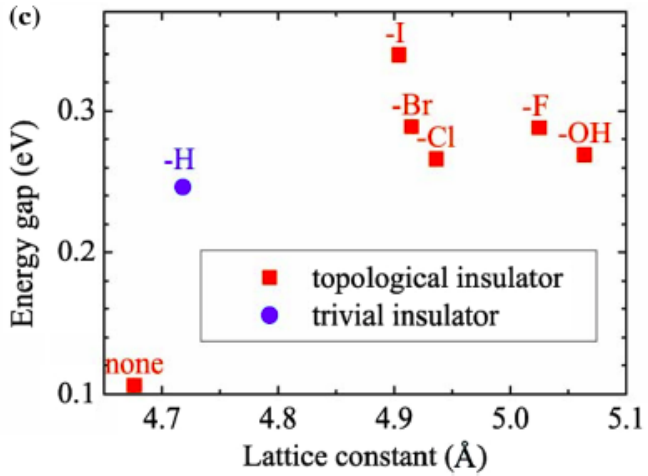
→ **spin-polarized (helical) metallic edge states**

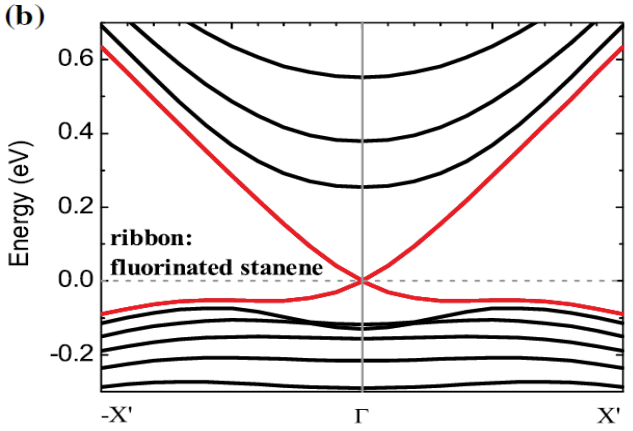
Sn as 2D topological insulator: stanene

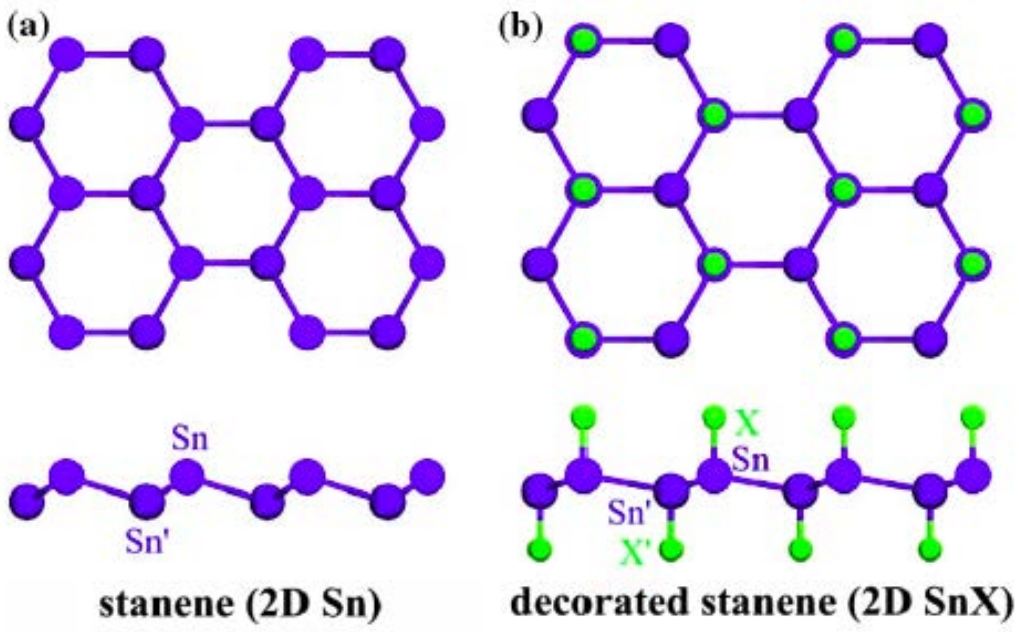
free-standing stanene

predicted to be a QSHE system/2D TI

Y. Xu et al., PRL 2013







control parameters

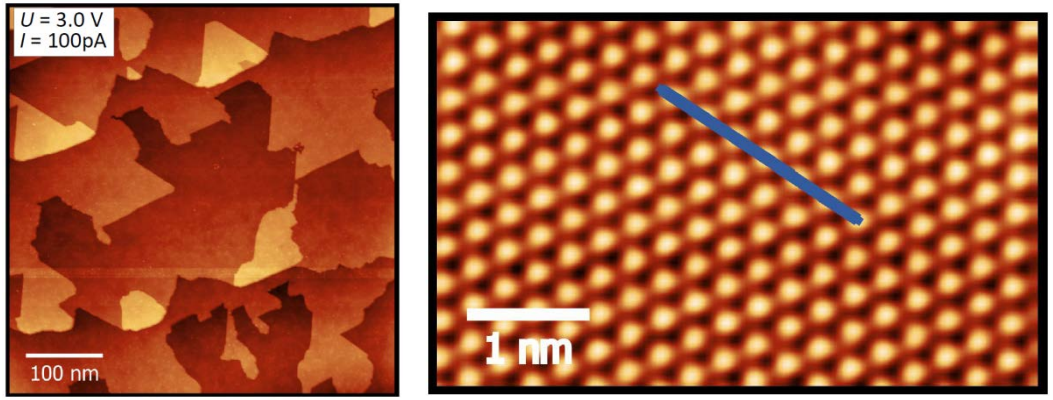
- strain
- functionalization

***real* stanene requires suitable substrate**

→ SiC(0001)

Epitaxial Sn sub-monolayers on SiC(0001)

substrate: 4H-SiC(0001)



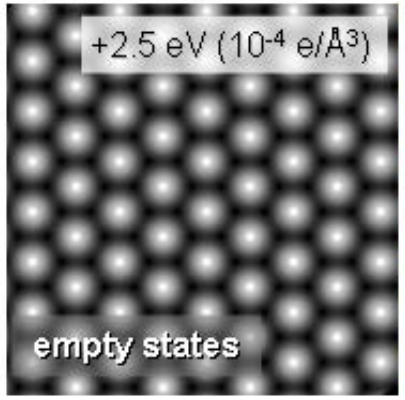
large, well-ordered terraces
prepared by hydrogen etching
(1 bar, 1200 °C)

J. Phys. Chem. C ***120****, 10361 (2016)*

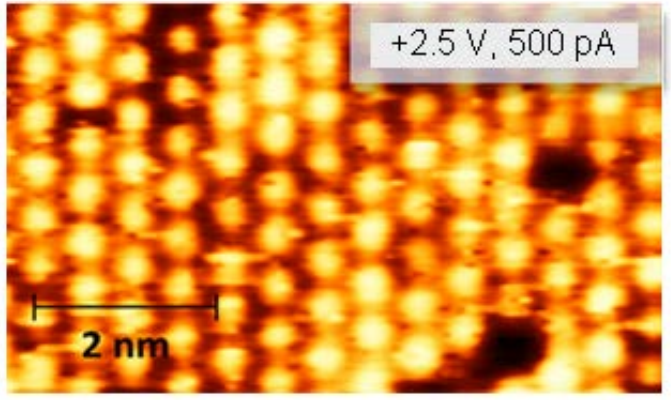
Sn epitaxy on SiC(0001)

√3x√3 reconstruction (dilute phase: 1/3 ML)

theory



experiment (STM)



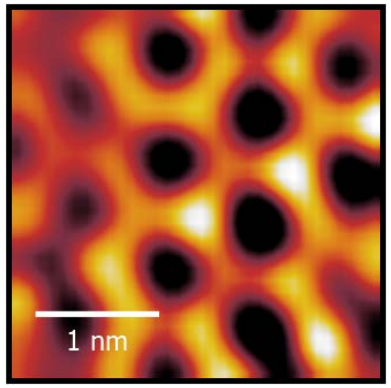
Mott insulator on a triangular lattice

PRL ***114****, 247602 (2015)*
Nat. Comm. ***4****, 1620 (2013)*

Epitaxial Sn sub-monolayers on SiC(0001)

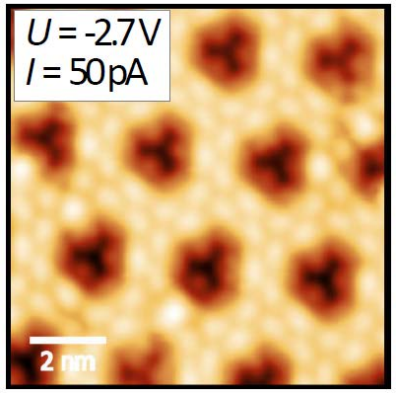
More Sn on SiC(0001): "honeycomb" reconstructions

3x3

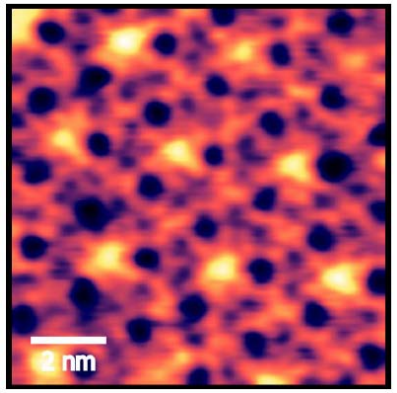


6√3 x 6√3

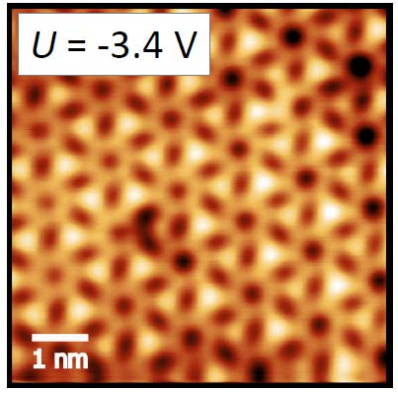
STM topography

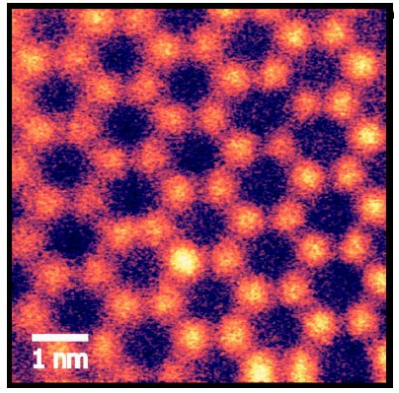


LDOS



√21x√21





multidude of phases for increasing Sn coverage/ decreasing substrate temp.:

"super-stanene" - lattice constants too large for real stanene

→ **real topological stanene yet to be realized !**

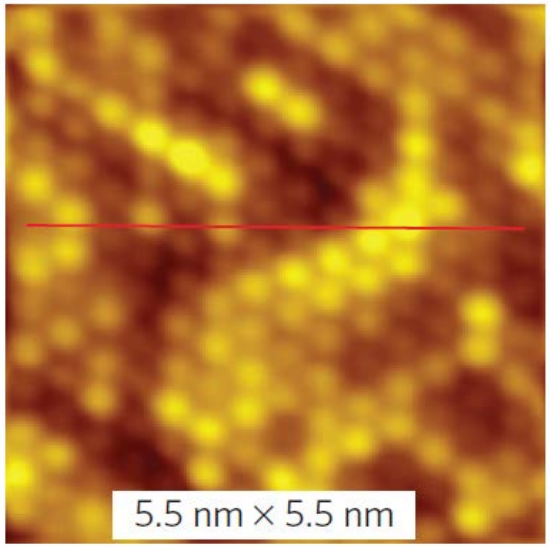
Stanene on Bi_2Te_3 ?

ARTICLES
PUBLISHED ONLINE: 3 AUGUST 2015 | DOI: 10.1038/NMAT4384
Nat.Mat. ***14****, 1020 (2015)*
nature materials

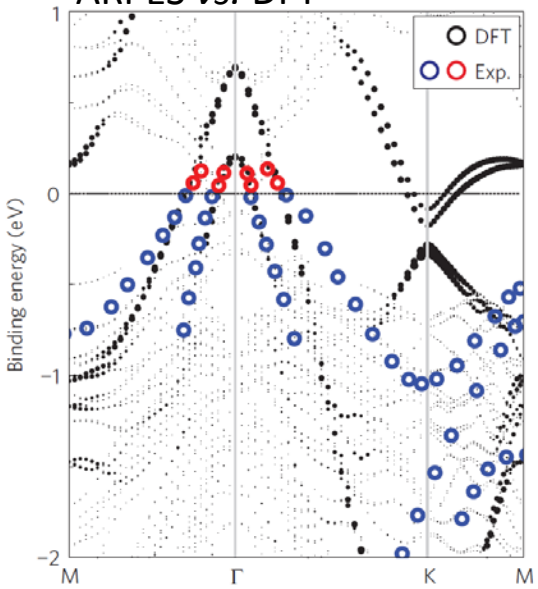
Epitaxial growth of two-dimensional stanene

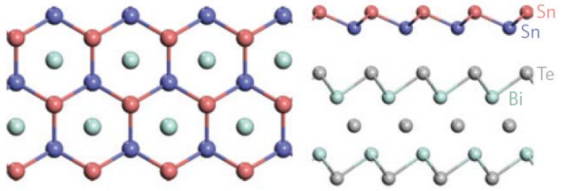
Feng-feng Zhu[1†], Wei-jiong Chen[1†], Yong Xu[2,3,4†], Chun-lei Gao[1,5], Dan-dan Guan[1,5], Can-hua Liu[1,5], Dong Qian[1,5*], Shou-Cheng Zhang[2,3,4] and Jin-feng Jia[1,5*]

STM



ARPES *vs.* DFT





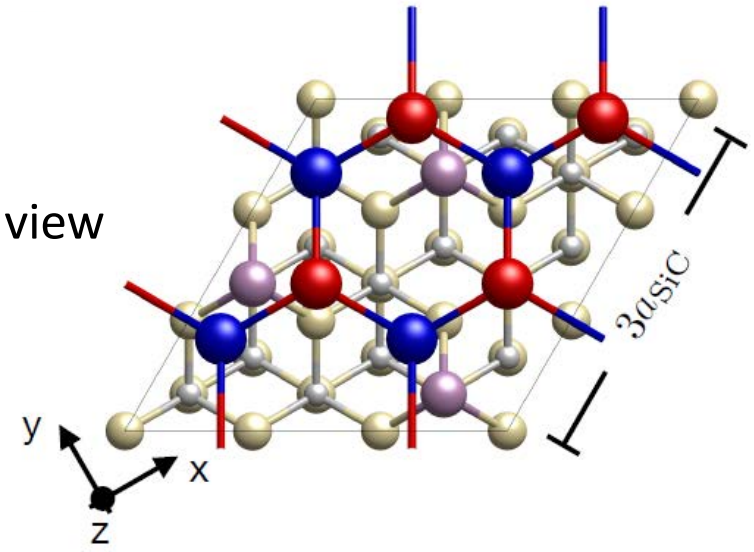
?

- STM shows hexagonal (triangular) lattice, **not honeycomb**
- ARPES finds **metal, not 2D TI**

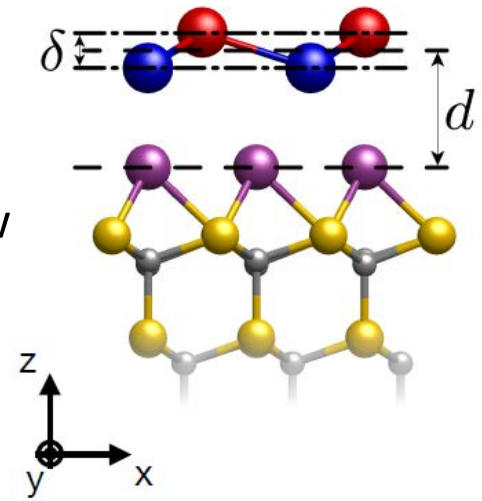
→ **real topological stanene yet to be realized !**

Quasi-freestanding stanene via substrate engineering: a proposal

top view



side view



stanene

buffer layer

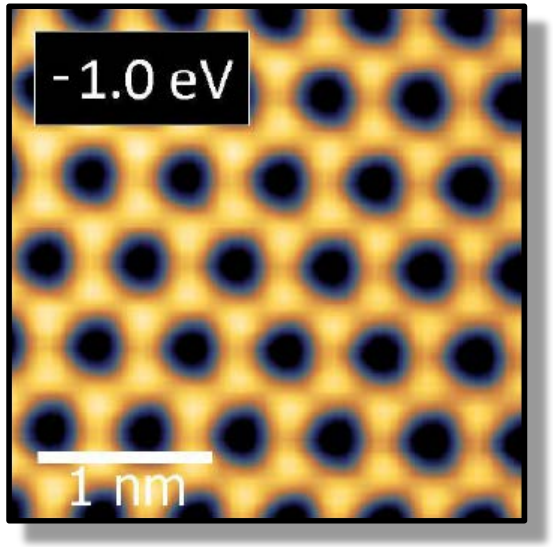
SiC substrate

		P	As	Sb	Bi
Si					
	ΔE_K(meV)	68	43	40	61
	d_{Buf}(Å)	1.8	1.9	2.2	2.3
	d(Å)	3.2	3.5	3.6	3.6
	δ(Å)	0.46	0.45	0.46	0.46
	$\mathbb{Z}_2$	0	0	0	0
C					
	ΔE_K(meV)	69	55	42	11
	d_{Buf}(Å)	1.3	1.4	1.6	1.8
	d(Å)	3.9	3.8	3.9	3.7
	δ(Å)	0.44	0.44	0.44	0.45
	$\mathbb{Z}_2$	1	1	1	0

DFT calculations by D. Di Sante, P. Eck, R. Thomale, and G. Sangiovanni

arXiv:1807.09006

A new quantum spin Hall paradigm: bismuthene/SiC(0001)



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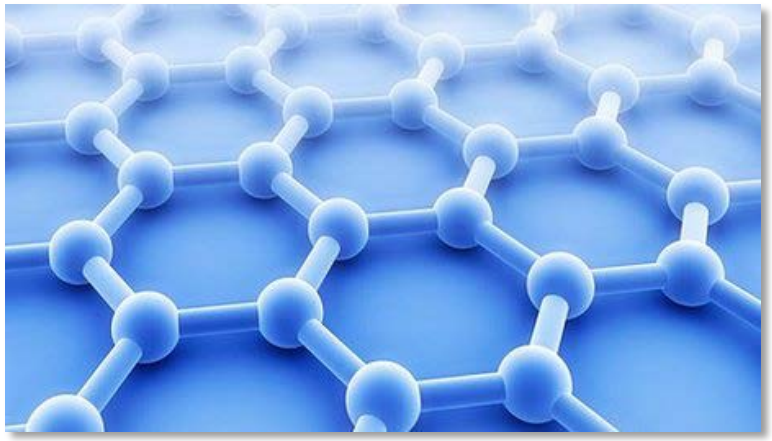

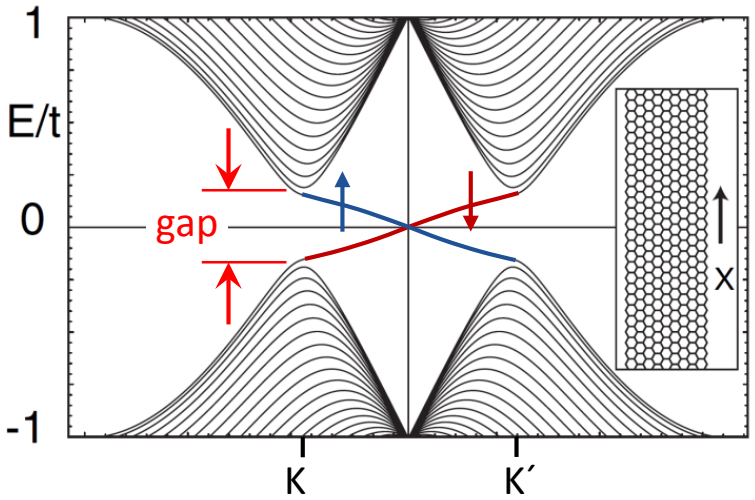

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Y. Xu et al., PRL 2013

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Z^4

IV	V
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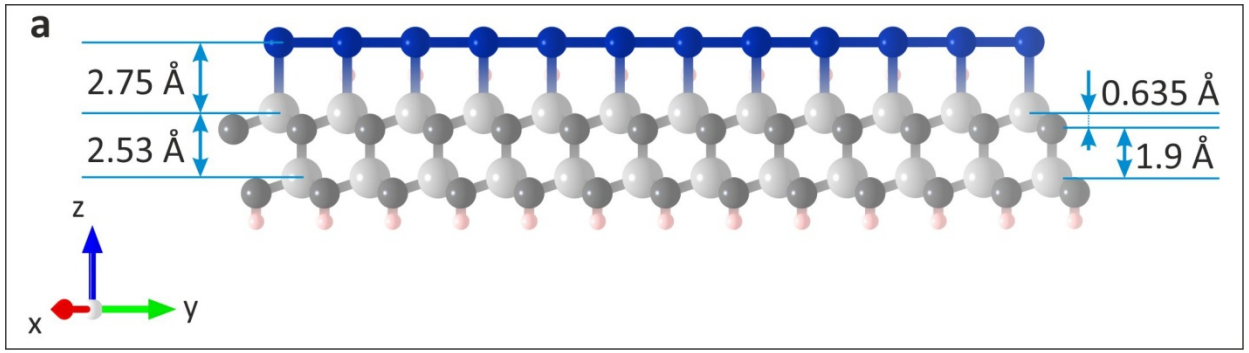
32 72,64 Ge Germanium	33 74,922 As Arsenic
50 118,71 Sn Tin	51 121,76 Sb Antimony
82 207,2 Pb Lead	83 208,98 Bi Bismuth

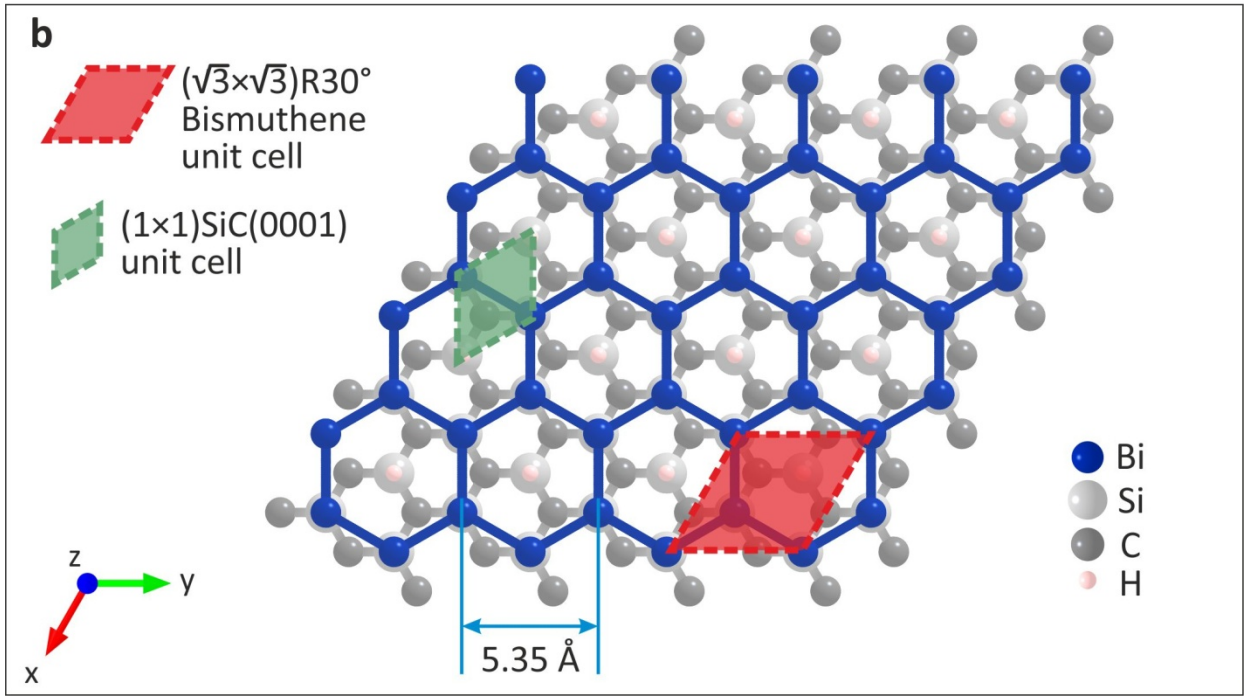
bismuthene:
Bi/SiC(0001)
Hsu et al., NJP 2015

→ **spin-polarized (helical) metallic edge states**

Bismuthene/SiC(0001): structure



18% tensile strain
→ planar honeycombs

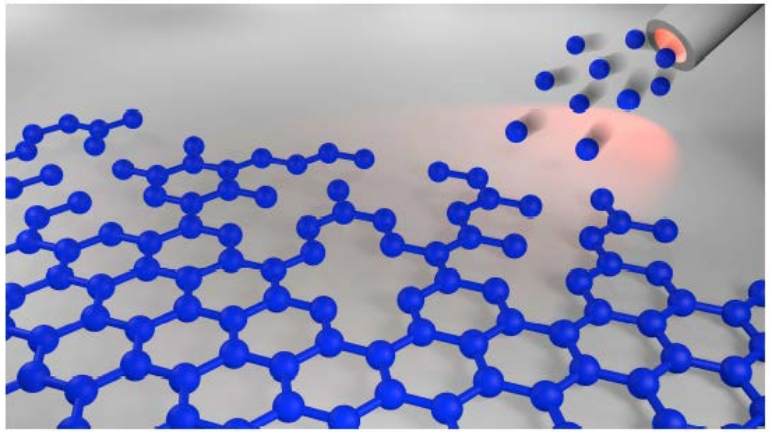


(√3x√3)R30°
reconstruction

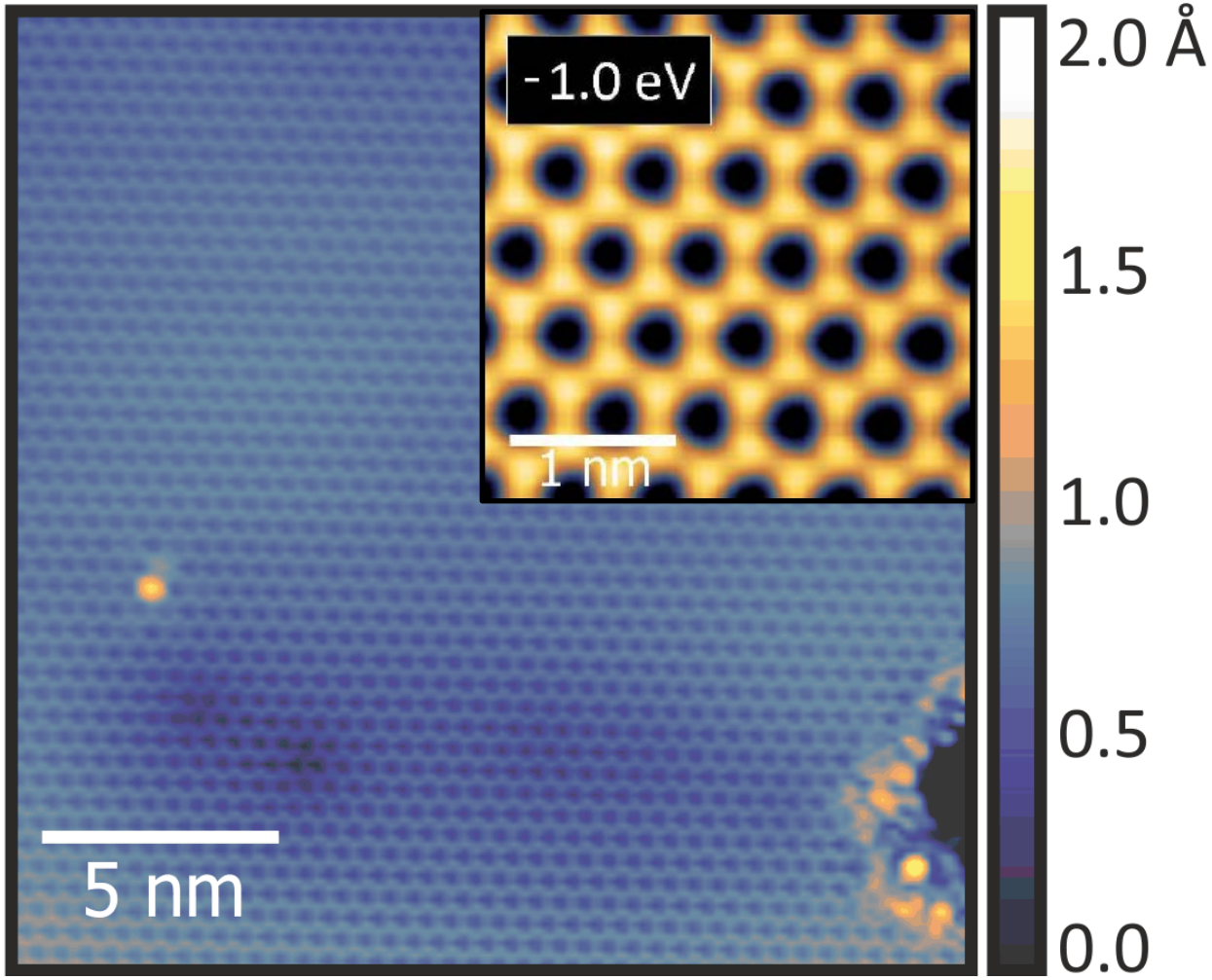
*Science **357**, 287 (2017)*

Bismuthene/SiC(0001): experimental realization by monolayer epitaxy

Bi-epitaxy on H-etched *4H*-SiC(0001)
@ T_{SiC} ~ 500°C



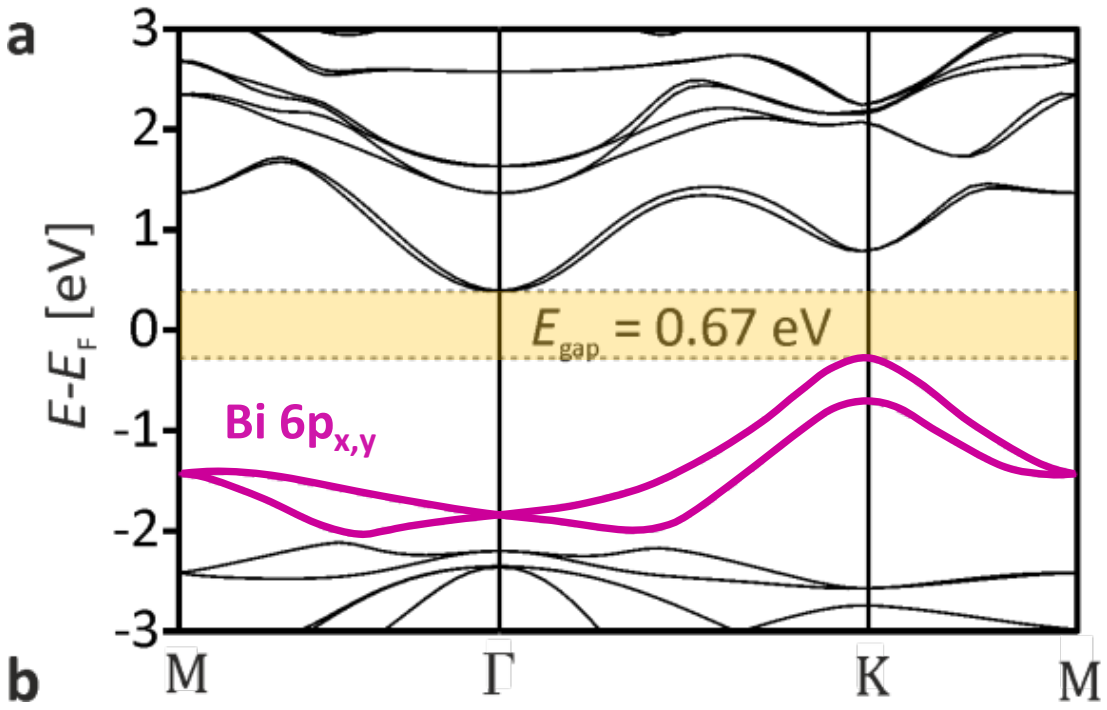
STM topography



Science ***357****, 287 (2017)*

Bismuthene/SiC(0001): band structure and energy gap

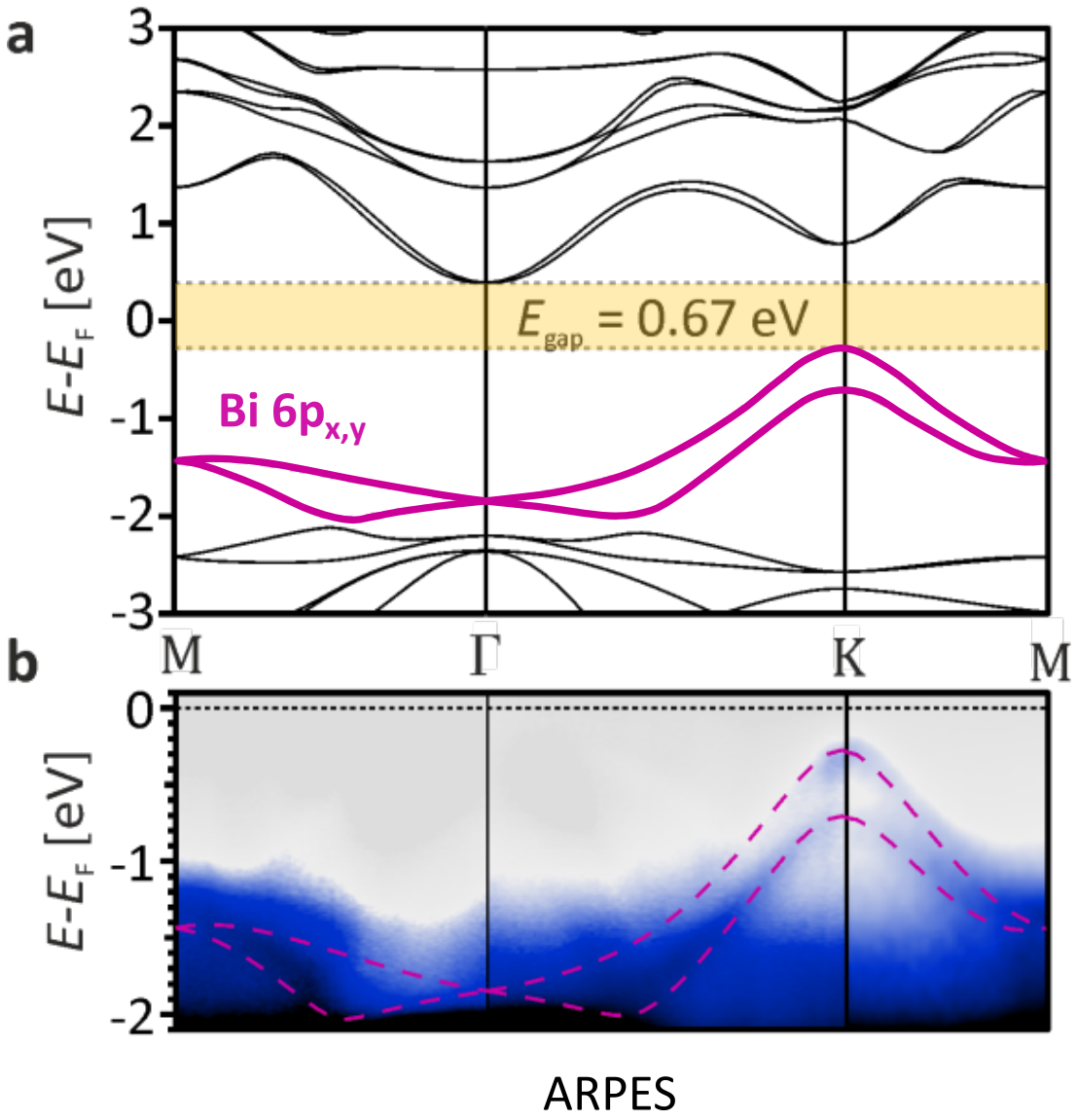
density functional theory



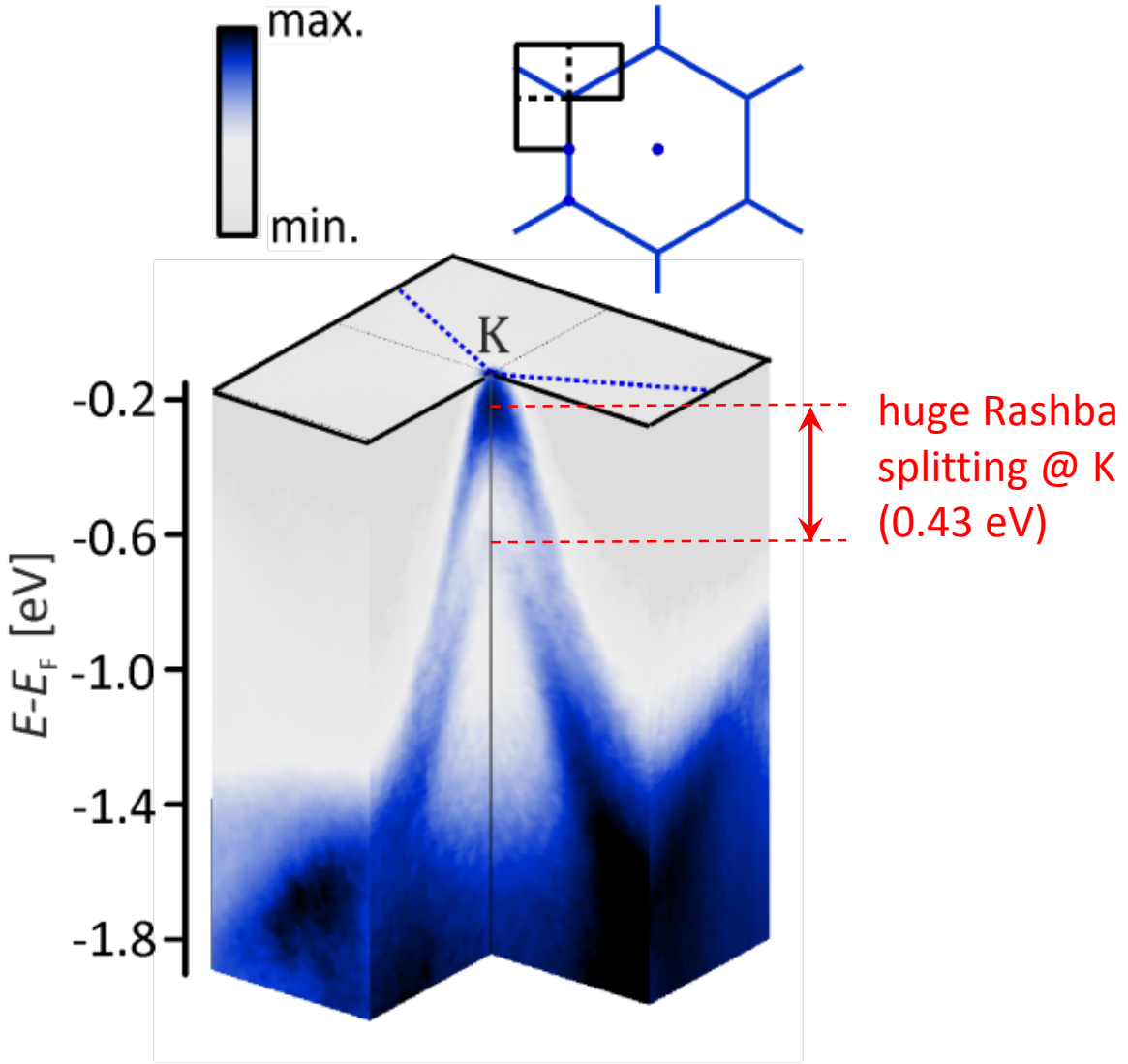
Science ***357***, *287 (2017)*

Bismuthene/SiC(0001): band structure and energy gap

density functional theory



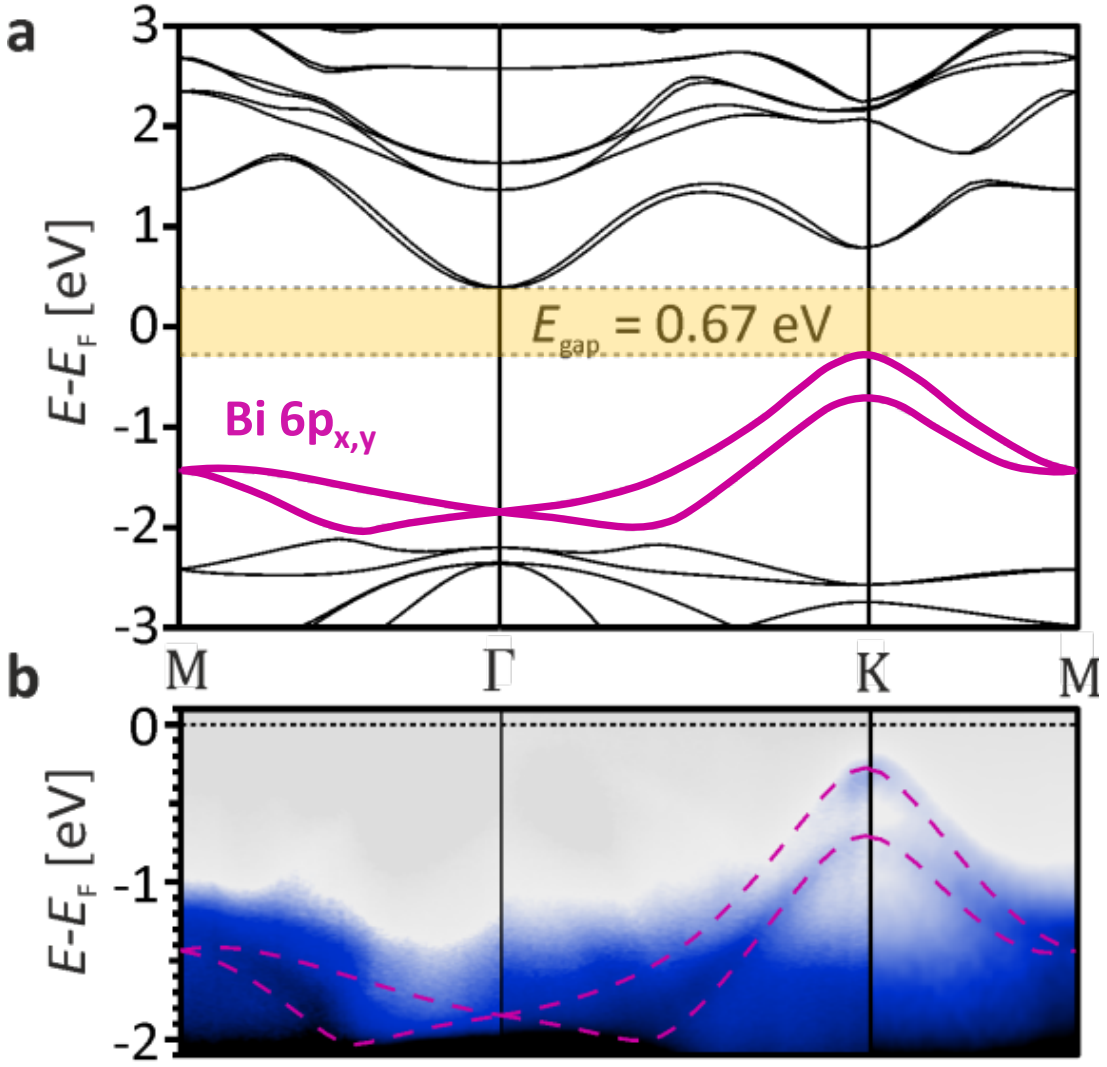
ARPES



Science ***357****, 287 (2017)*

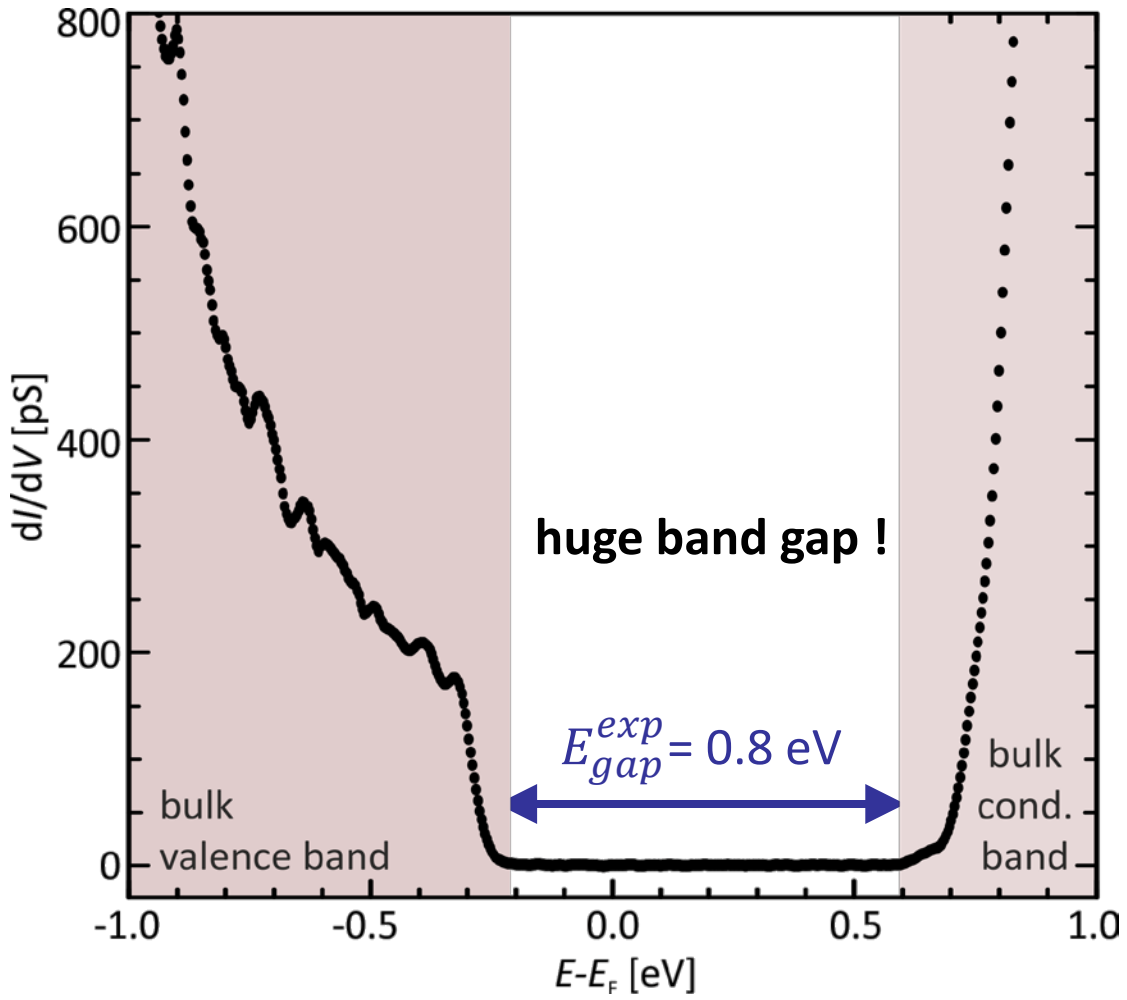
Bismuthene/SiC(0001): band structure and energy gap

density functional theory



ARPES

tunneling spectroscopy



*Science **357**, 287 (2017)*

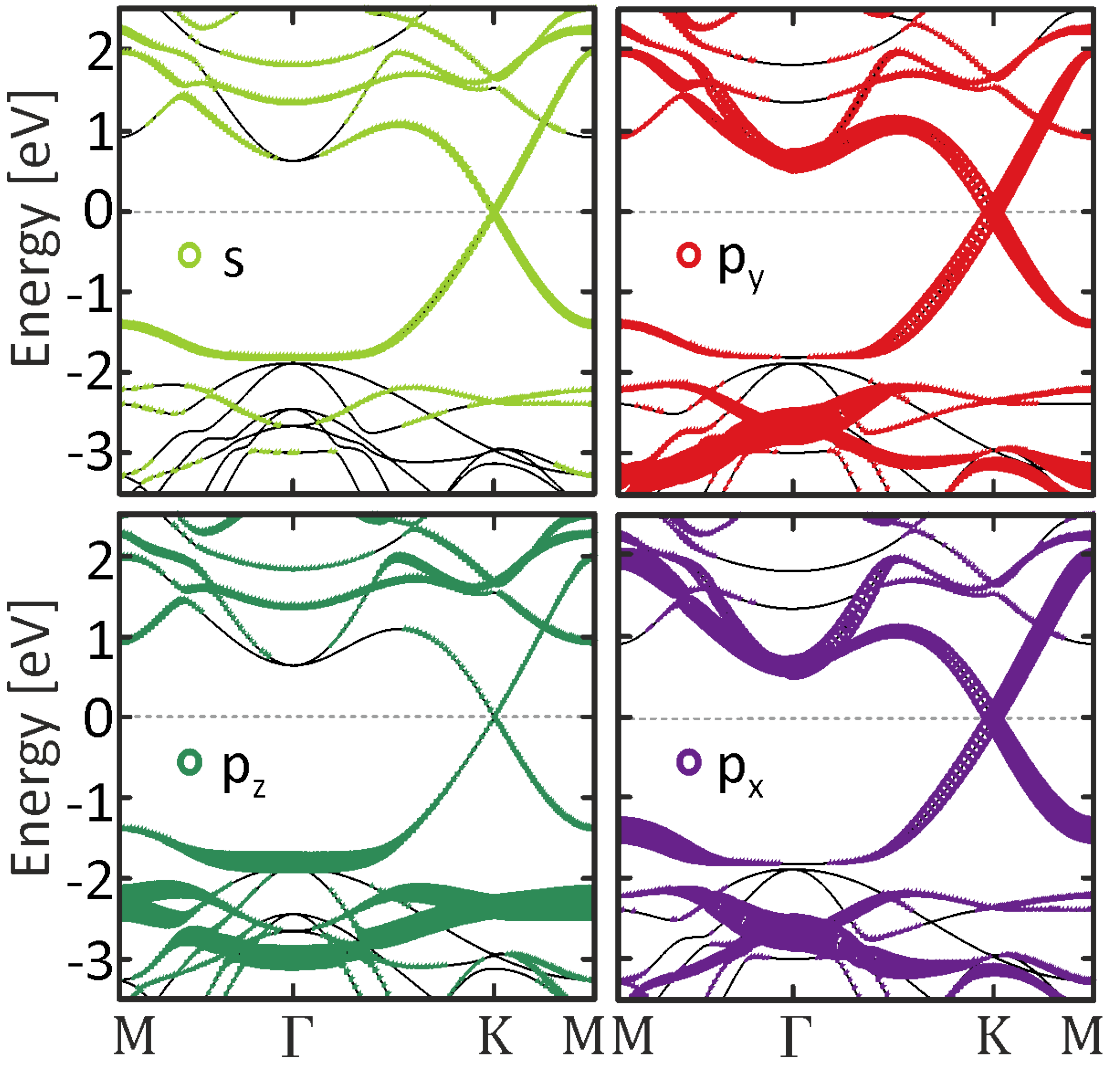
Bismuthene/SiC(0001): effective model

band structure analysis w/o spin-orbit coupling:

- sp^2-type σ-bonding
- p_x and p_y orbitals dominate at low energies
- **important role of substrate:**
  removes p_z from Fermi level
  → *"orbital filtering"*

→ exploitation of ***local*** $(L_z S_z)$ SOC

→ distinctly different from graphene & Kane-Mele model !



*Science **357**, 287 (2017)*

Bismuthene/SiC(0001): effective model *including SOC*

basis states: $\left|p^A_{x\uparrow}\right\rangle, \left|p^A_{y\uparrow}\right\rangle, \left|p^B_{x\uparrow}\right\rangle, \left|p^B_{y\uparrow}\right\rangle;$ $\left|p^A_{x\downarrow}\right\rangle, \left|p^A_{y\downarrow}\right\rangle, \left|p^B_{x\downarrow}\right\rangle, \left|p^B_{y\downarrow}\right\rangle$

tight-binding Hamiltonian: $H^{\sigma\sigma}_{eff} = \begin{pmatrix} H^{\sigma\sigma}_{\uparrow\uparrow} & H^{\sigma\sigma}_{\uparrow\downarrow} \\ H^{\sigma\sigma}_{\downarrow\uparrow} & H^{\sigma\sigma}_{\downarrow\downarrow} \end{pmatrix}$ with

$$H^{\sigma\sigma}_{\uparrow\uparrow/\downarrow\downarrow} = H^{\sigma\sigma}_{0,\uparrow\uparrow/\downarrow\downarrow} \pm \boldsymbol{\lambda_{SOC}} \begin{pmatrix} 0 & \boldsymbol{-i} & 0 & 0 \\ \boldsymbol{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & \boldsymbol{-i} \\ 0 & 0 & \boldsymbol{i} & 0 \end{pmatrix}$$

off-diagonal orbital term
mixes in local (atomic) SOC

$$H^{\sigma\sigma}_{\uparrow\downarrow} = (H^{\sigma\sigma}_{\downarrow\uparrow})^{+} = \lambda_R \begin{pmatrix} 0 & 0 & m_1 & m_2 \\ 0 & 0 & m_2 & m_3 \\ m_4 & m_5 & 0 & 0 \\ m_5 & m_6 & 0 & 0 \end{pmatrix}$$

Rashba

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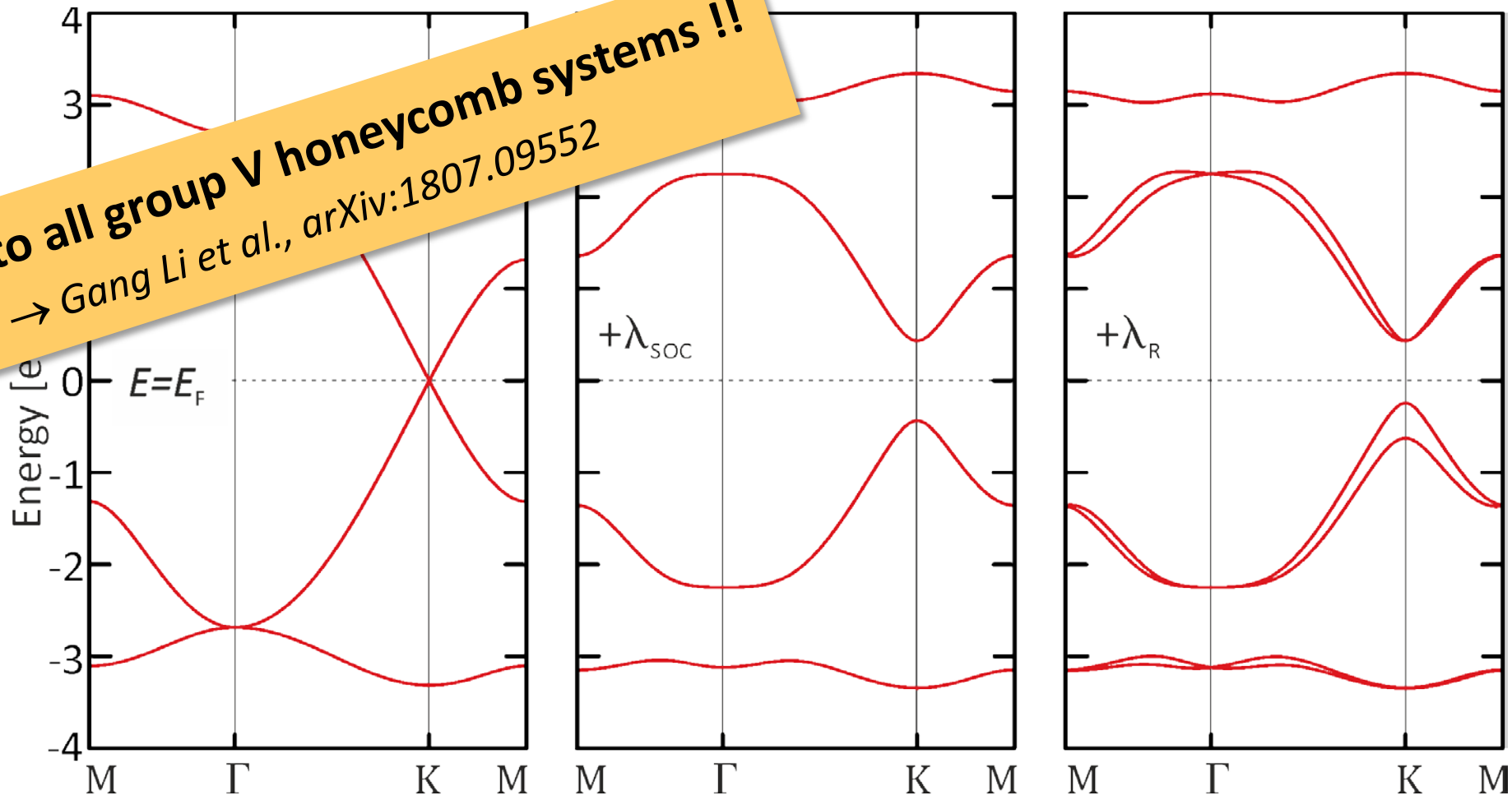
Bismuthene/SiC(0001): effective model *including SOC*

generic to all group V honeycomb systems !!

→ *Gang Li et al., arXiv:1807.09552*

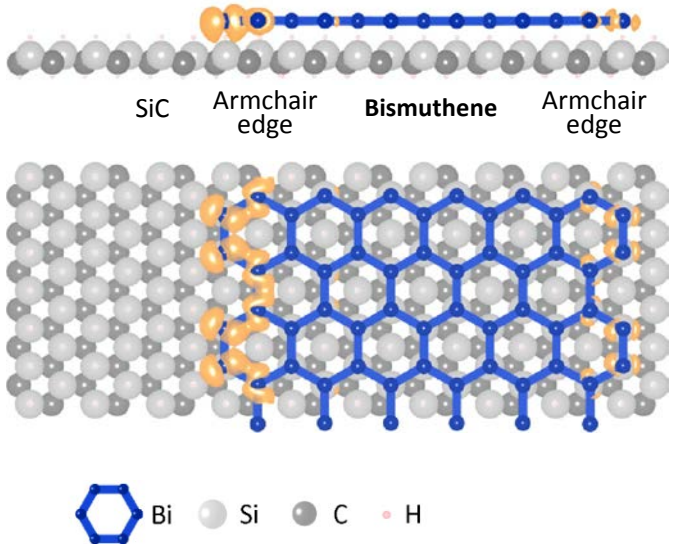


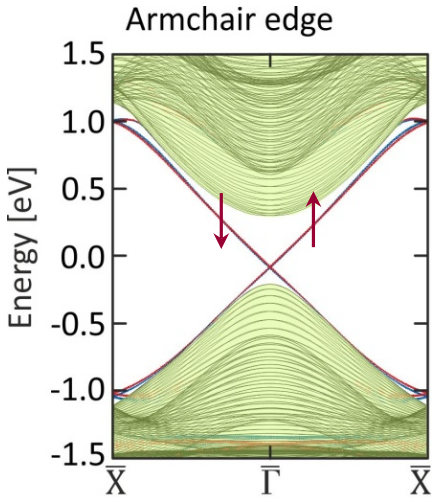
$$H_{eff}^{\sigma\sigma} = H_0^{\sigma\sigma} + \lambda_{SOC} H_{SOC}^{\sigma\sigma} + \lambda_R H_R^{\sigma\sigma}$$

*Science **357**, 287 (2017)*

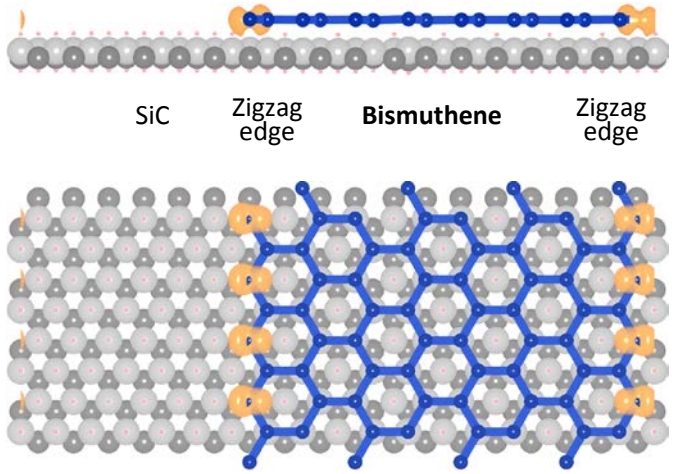
Bismuthene/SiC(0001): topological edge states

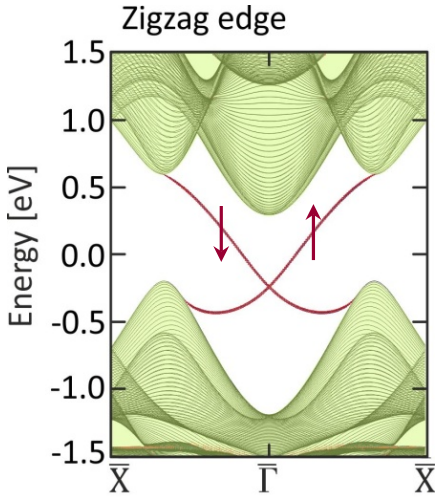
Armchair edge ribbon





Zigzag edge ribbon





TB calculations for nanoribbon geometries:

→ helical metallic edge states

→ topological invariant $Z_2 = 1$

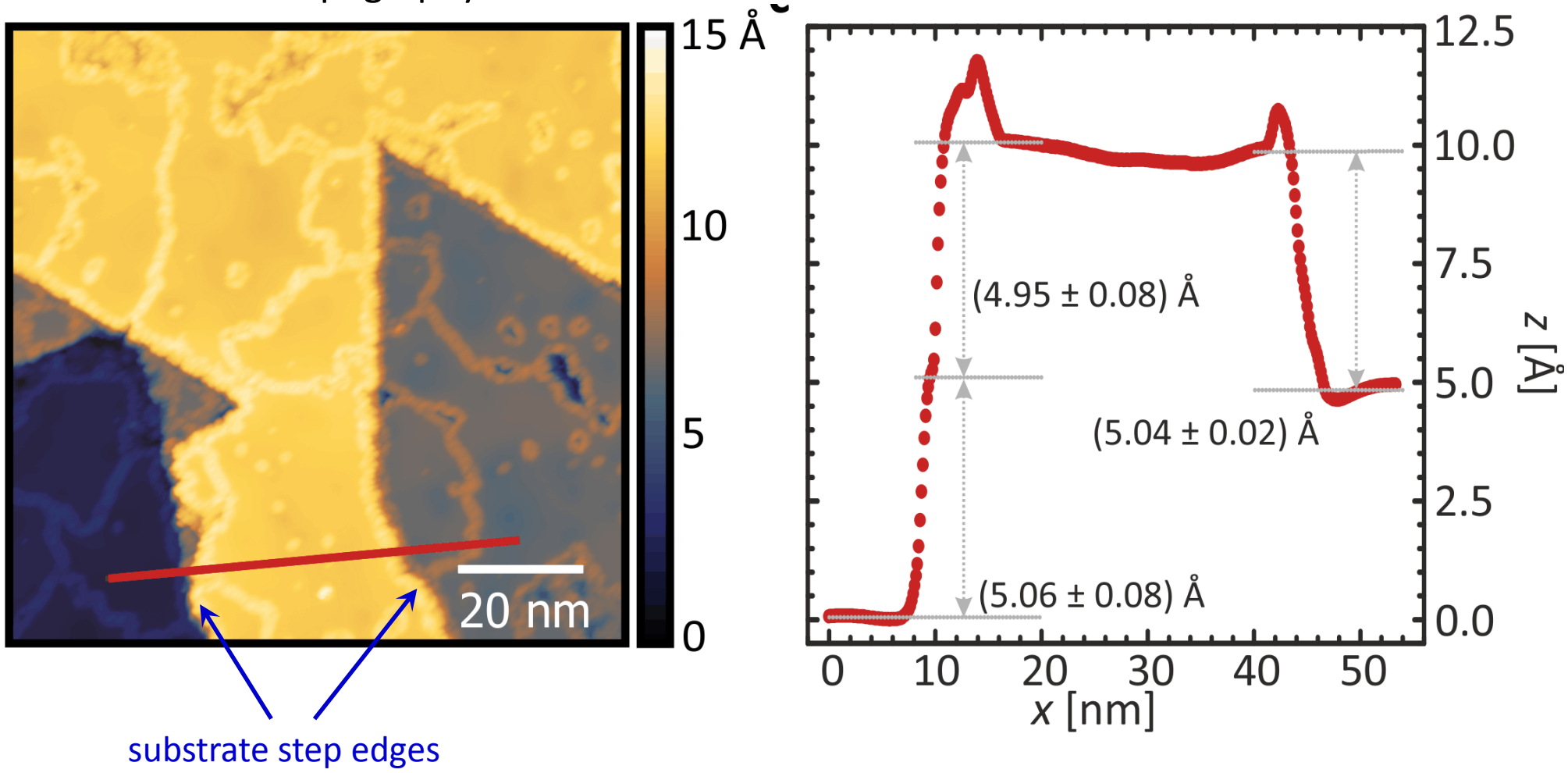
→ **bismuthene/SiC is a QSH system !**

(cf. Hsu et al., NJP 2015)

*Science **357**, 287 (2017)*

Bismuthene/SiC(0001): edge states at substrate terrace steps

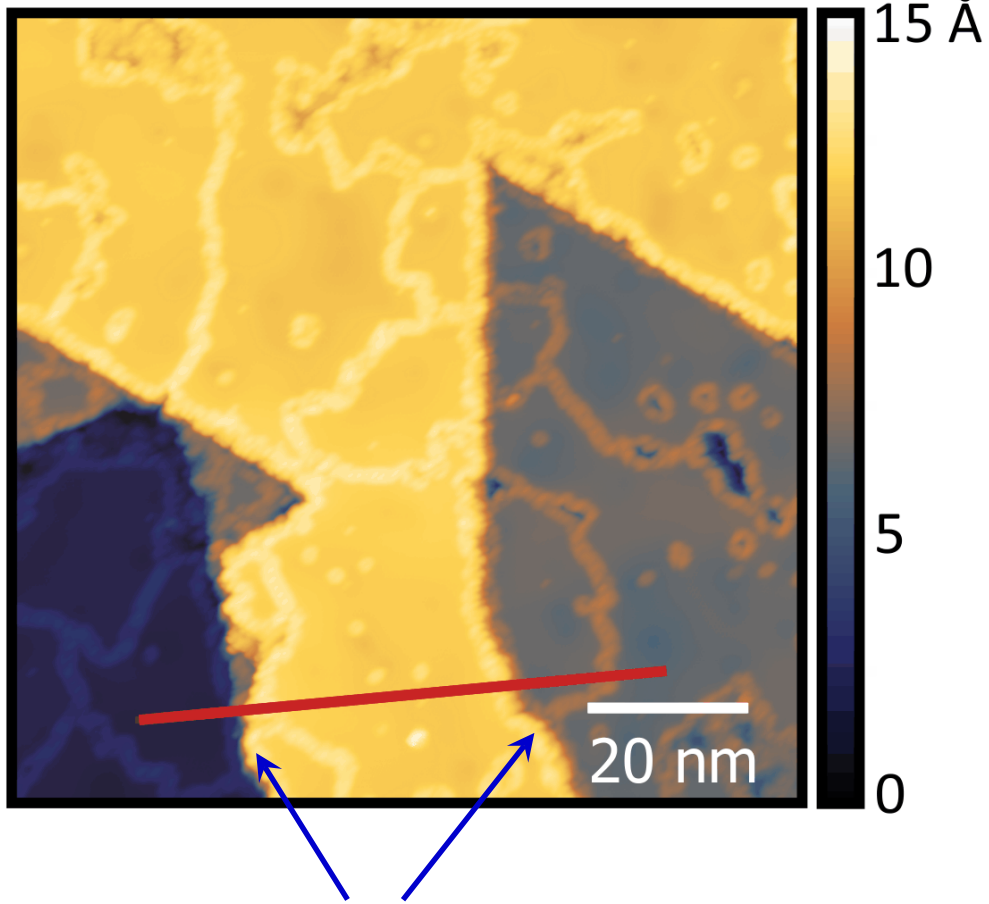
STM topography

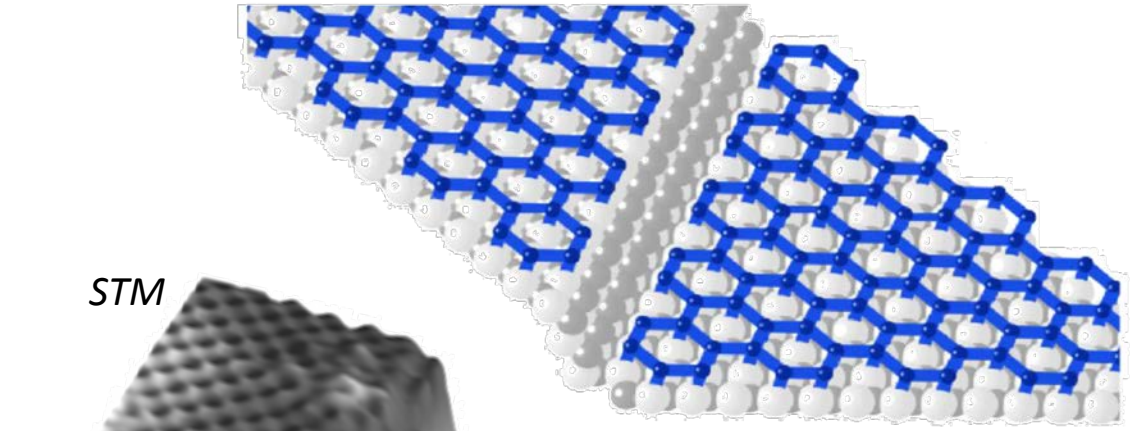


*Science **357**, 287 (2017)*

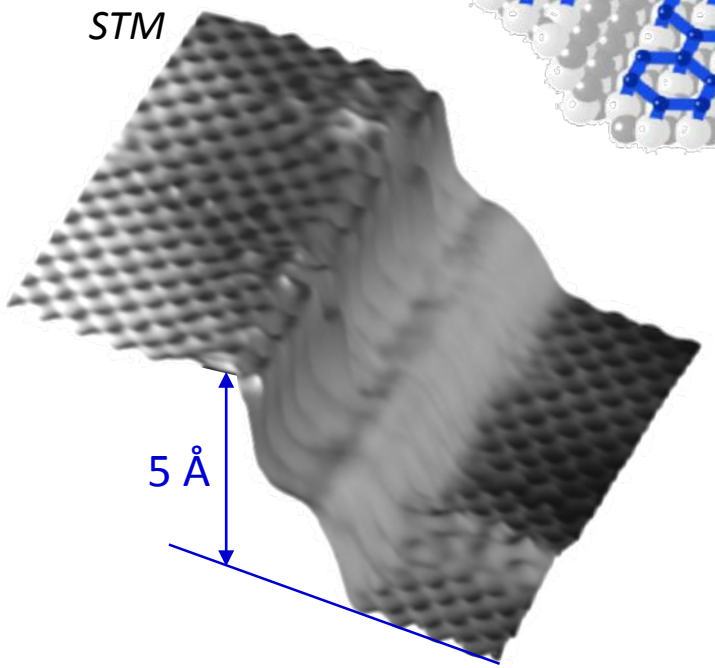
Bismuthene/SiC(0001): edge states at substrate terrace steps

STM topography





schematically

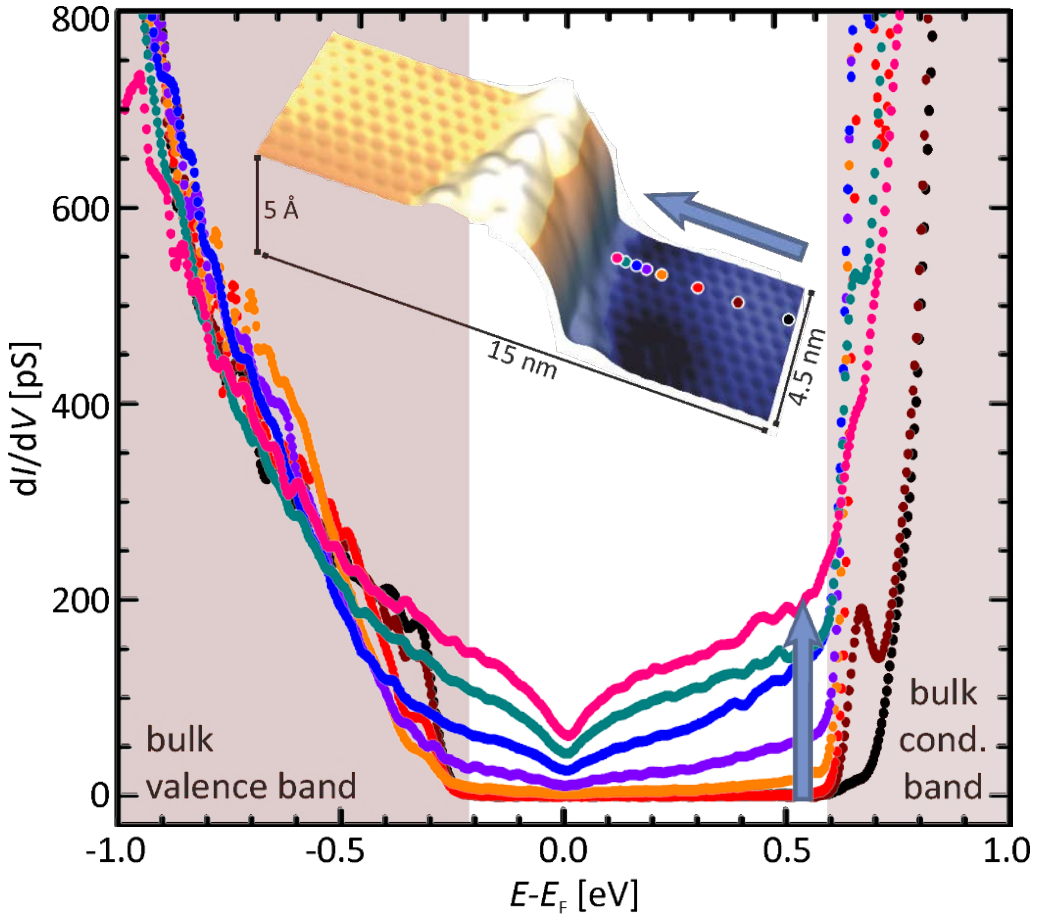


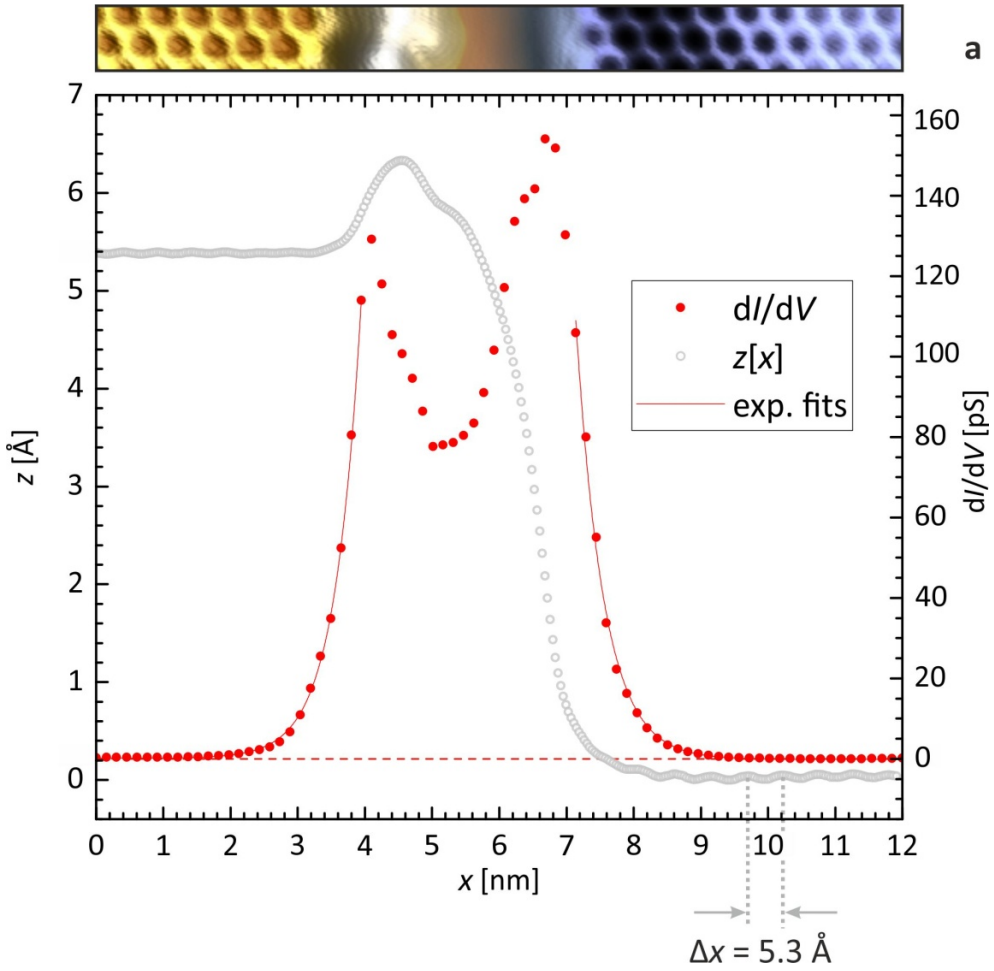
bismuthene
armchair egdes

*Science **357**, 287 (2017)*

Bismuthene/SiC(0001): edge state spectroscopy

tunneling spectra





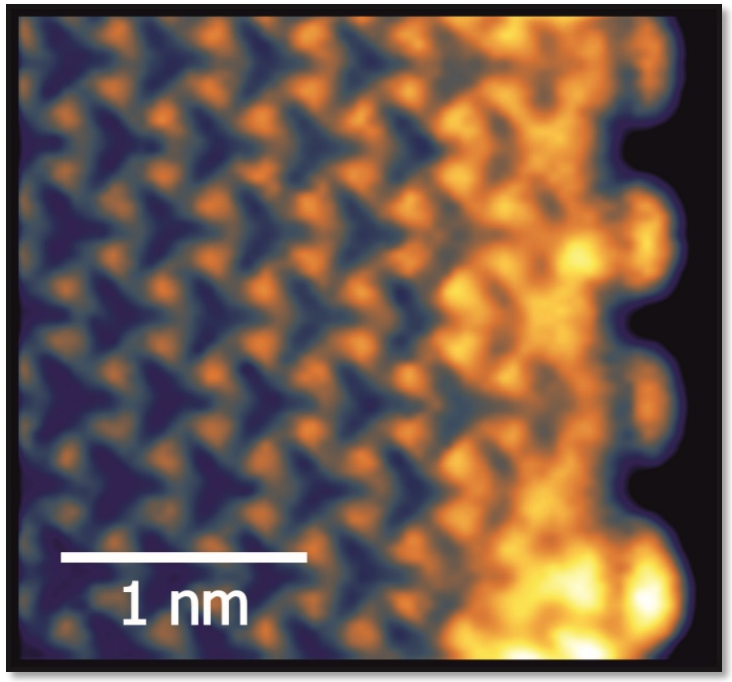
- **metallic edge states in bulk gap**
- **exponential decay into bulk**
  quantitatively consistent with theory

Science ***357****, 287 (2017)*

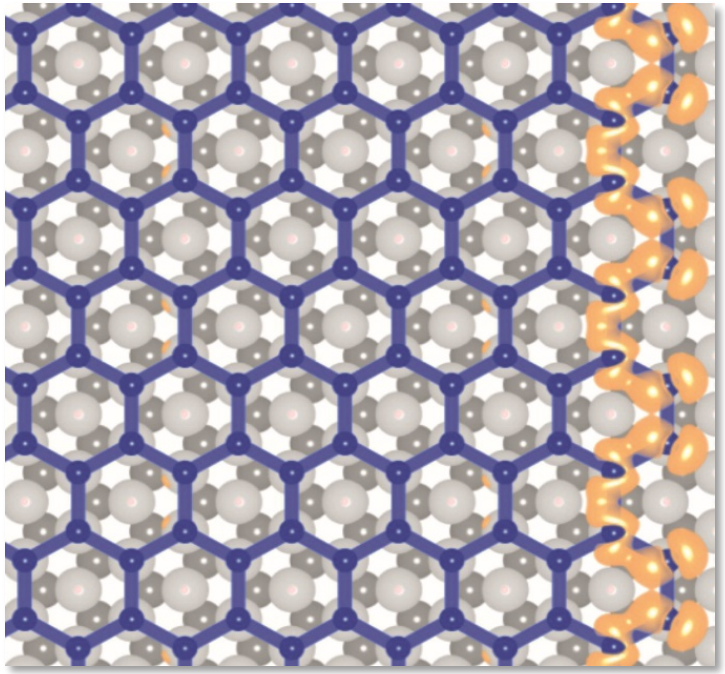
Bismuthene/SiC(0001): edge state STM vs. theory

charge density @ arm chair edge

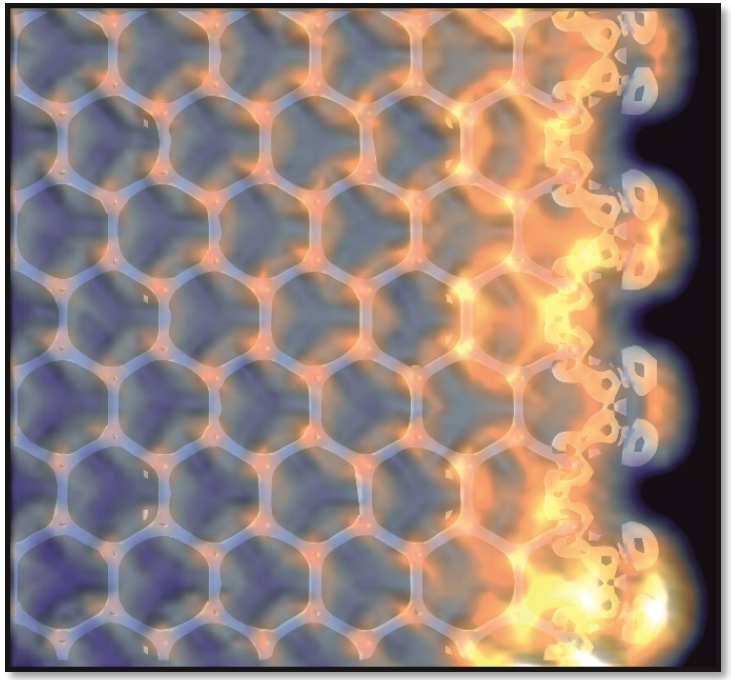
STM



nano-ribbon calculation

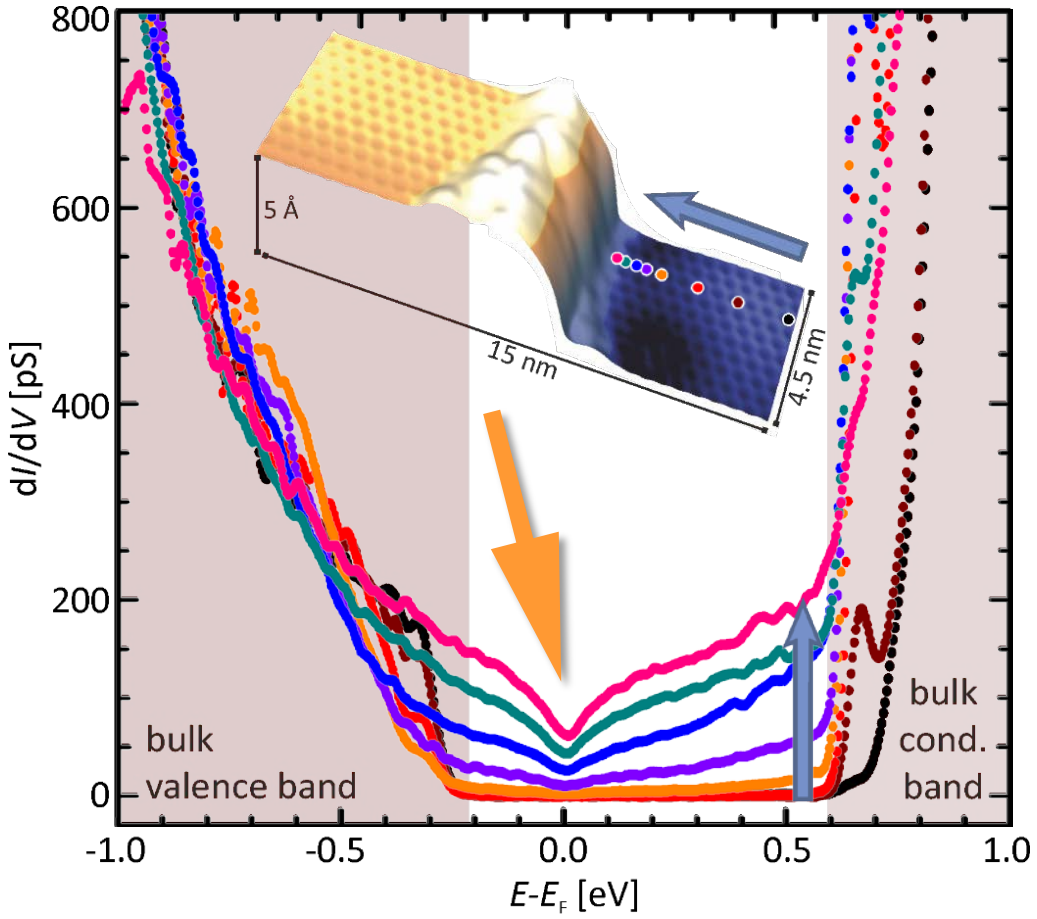


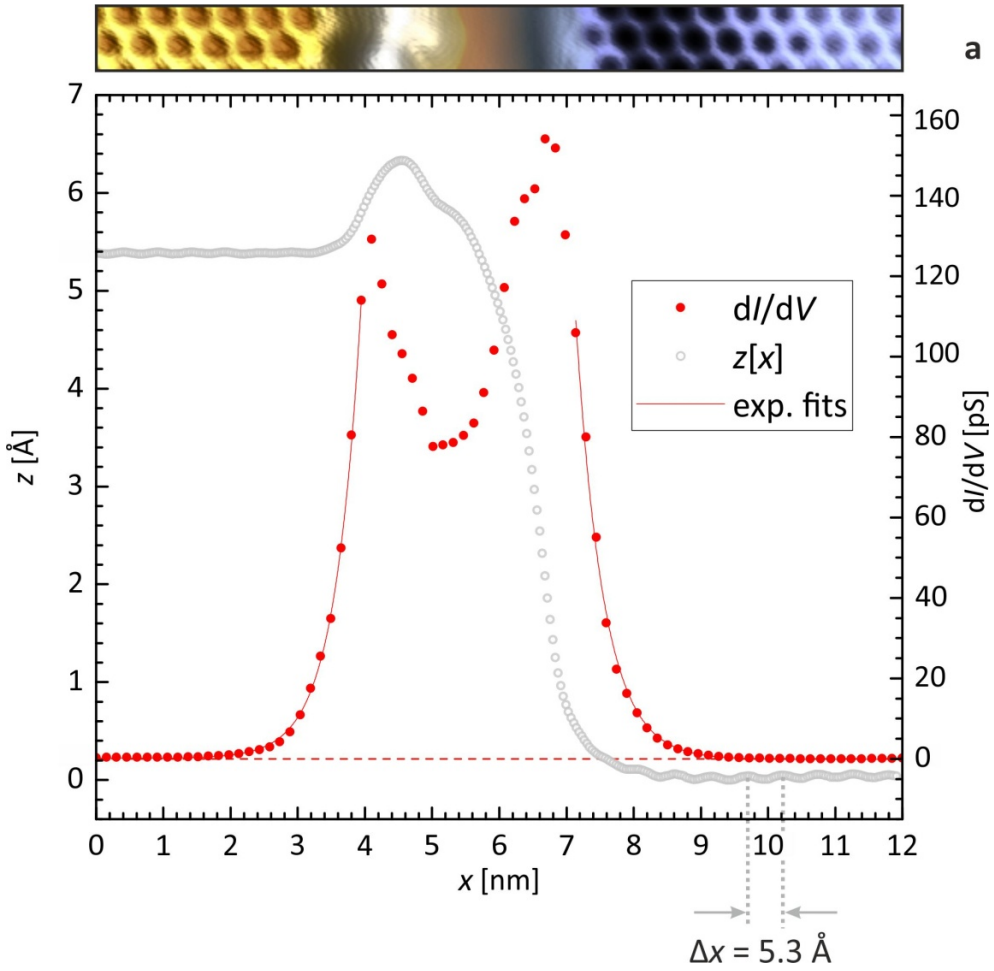
overlay theory/STM



Bismuthene/SiC(0001): edge state spectroscopy

tunneling spectra

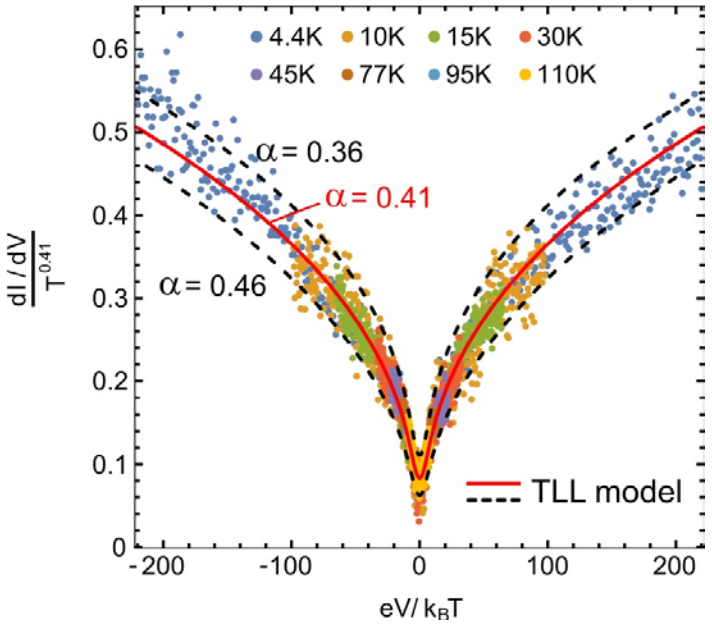




- **metallic edge states in bulk gap**
- **zero bias anomaly (ZBA)**
- **exponential decay into bulk**
  quantitatively consistent with theory

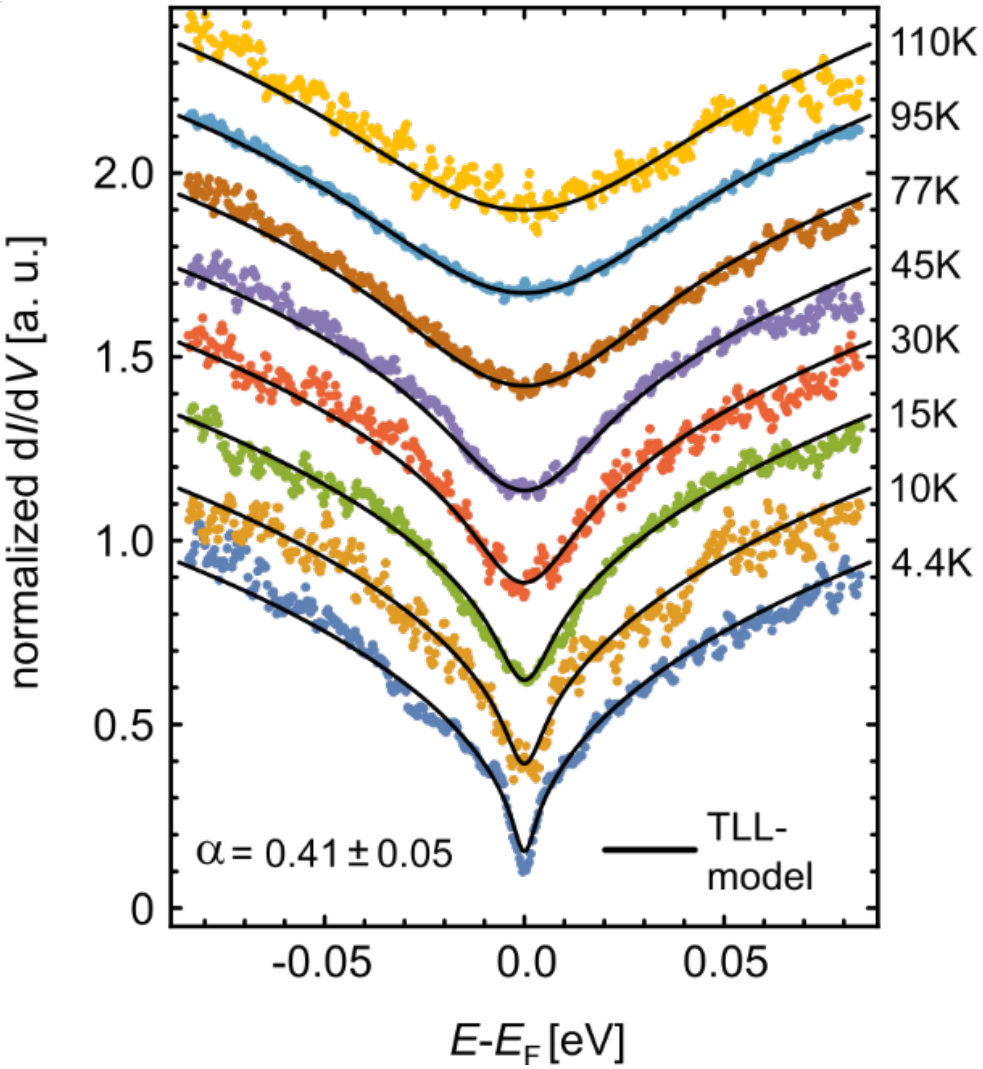
Science ***357****, 287 (2017)*

Bismuthene/SiC(0001):
edge states as helical Tomonaga-Luttinger liquid



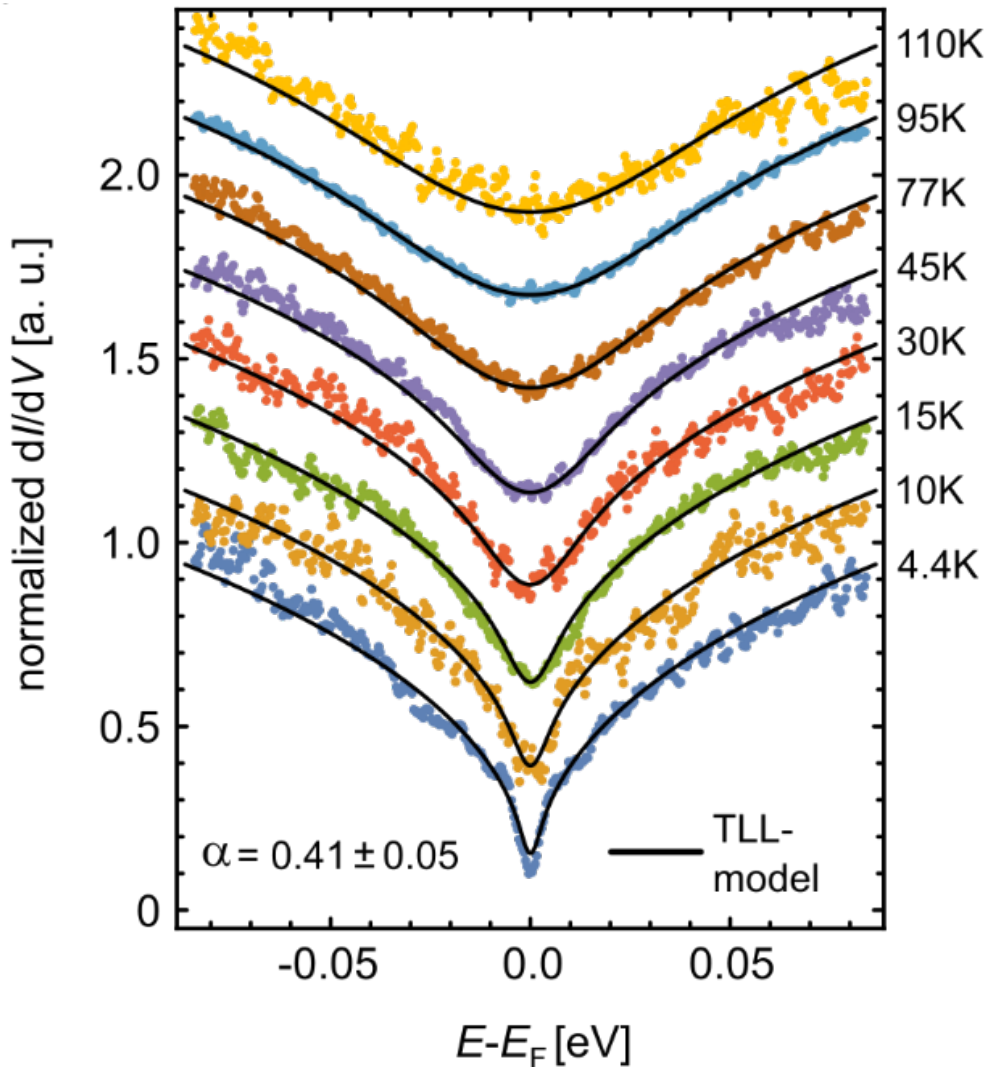
Bismuthene/SiC(0001): zero bias anomaly

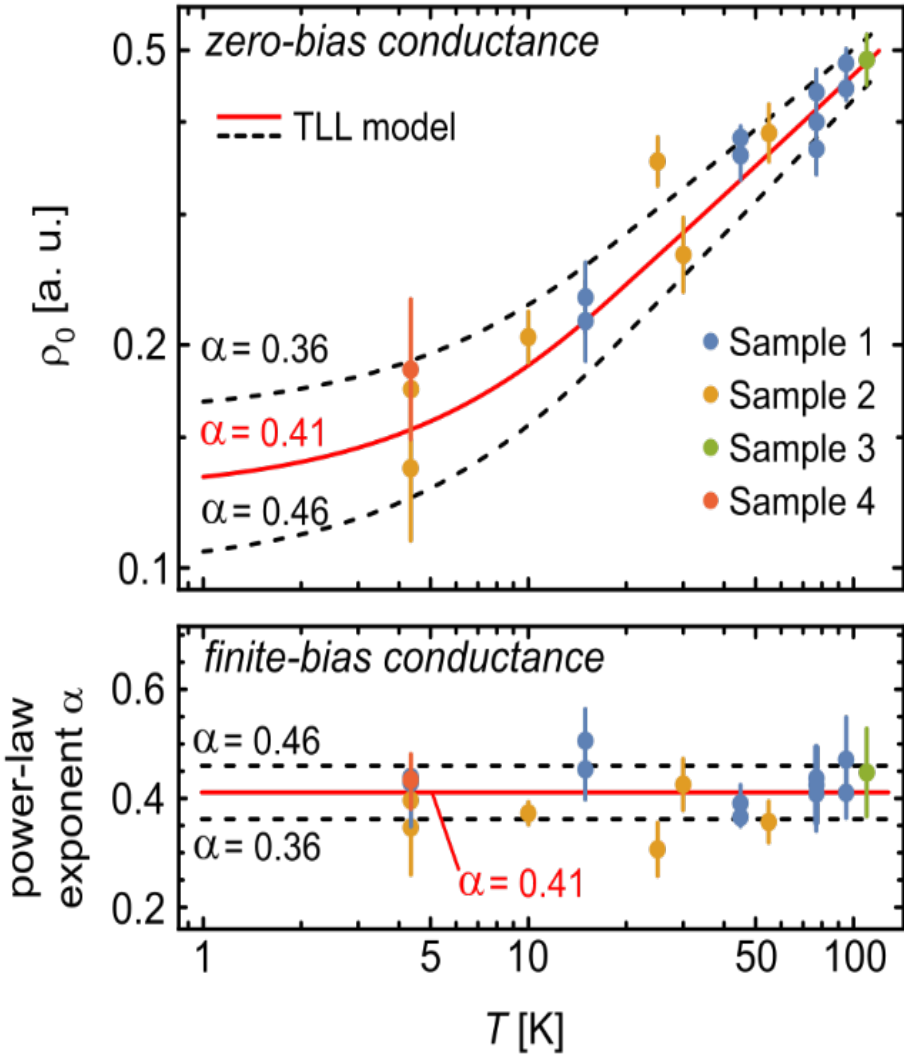
ZBA: bias and T dependence



Bismuthene/SiC(0001): zero bias anomaly

ZBA: bias and T dependence





→ **power laws**

$\propto T^{\alpha}$

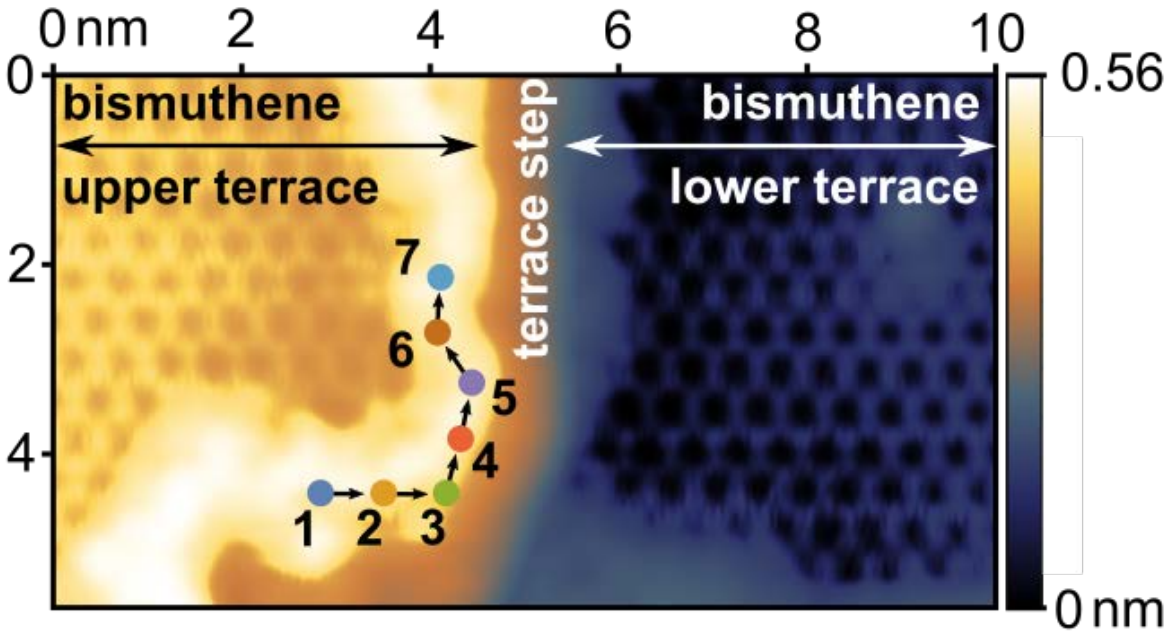
$\propto V^{\alpha}$

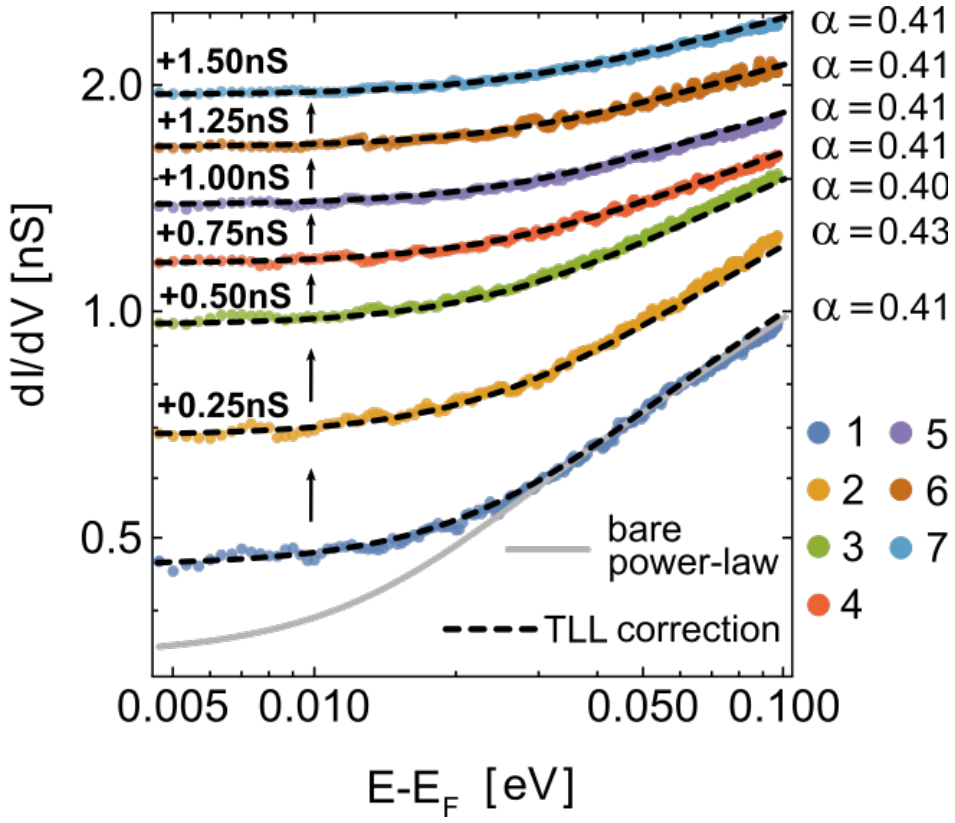
same exponent

$\alpha = 0.41$

Bismuthene/SiC(0001): zero bias anomaly

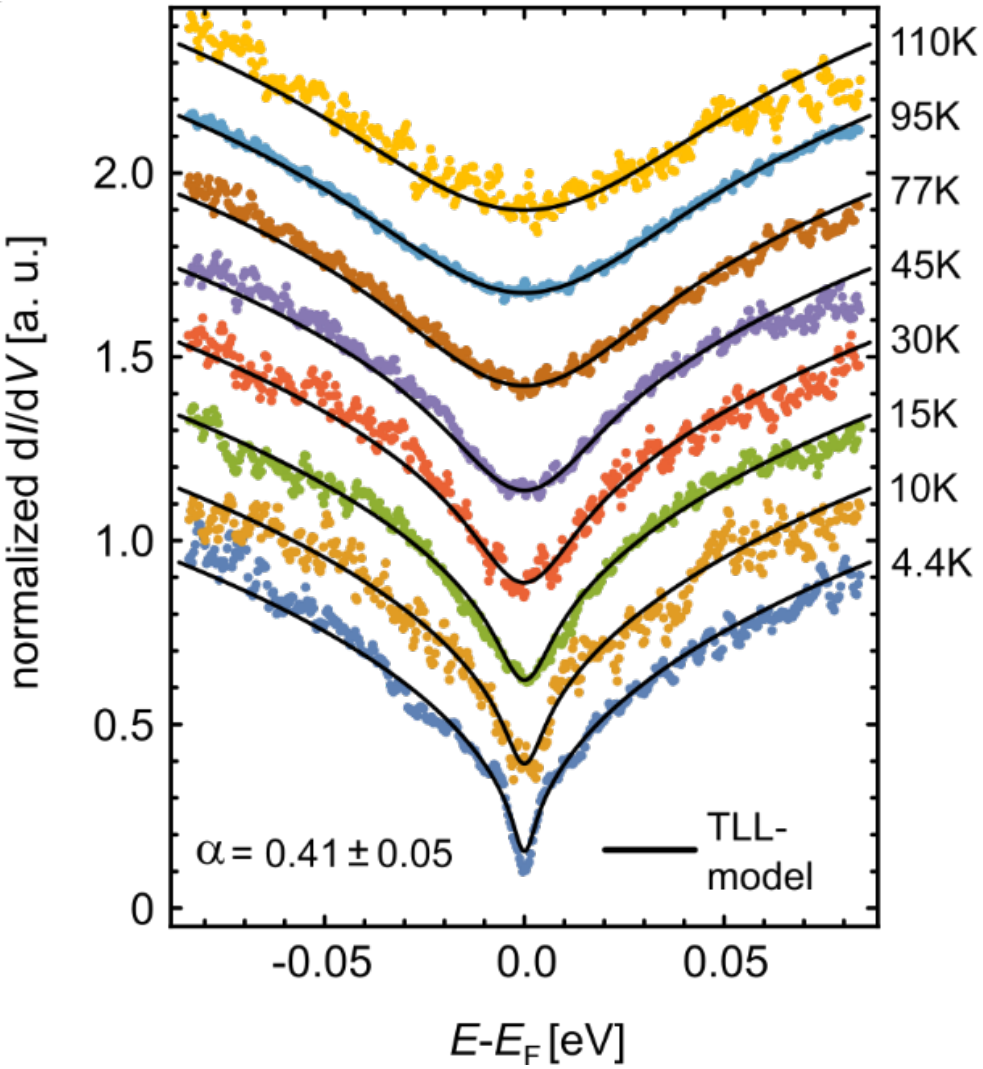
persistent power-law dependence of ZBA even in "kinky" edge



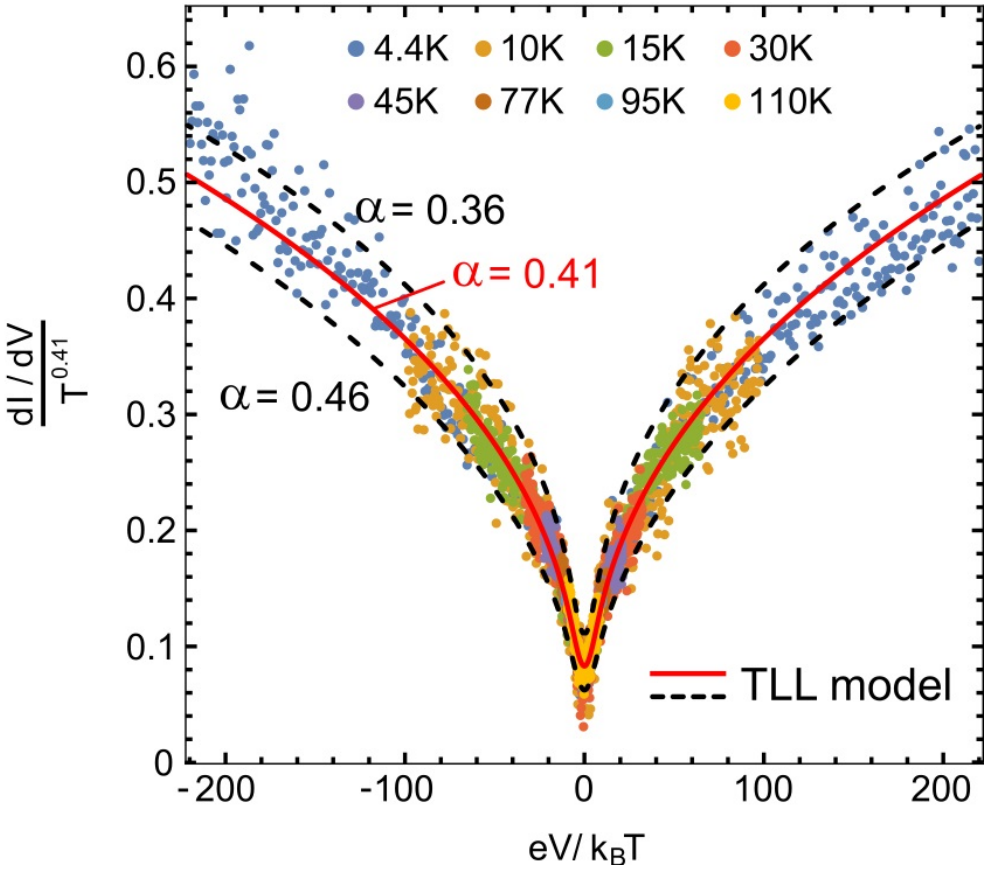


Bismuthene/SiC(0001): zero bias anomaly

ZBA: bias and T dependence



scaled spectra

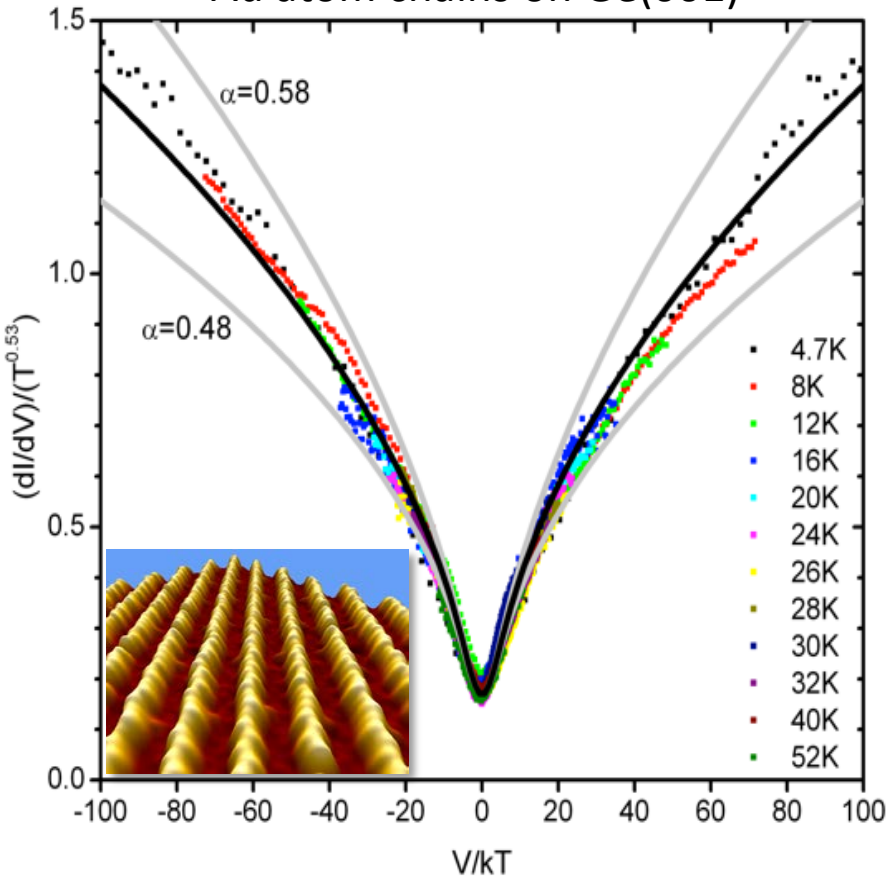


same power law in V and T: **universal scaling**

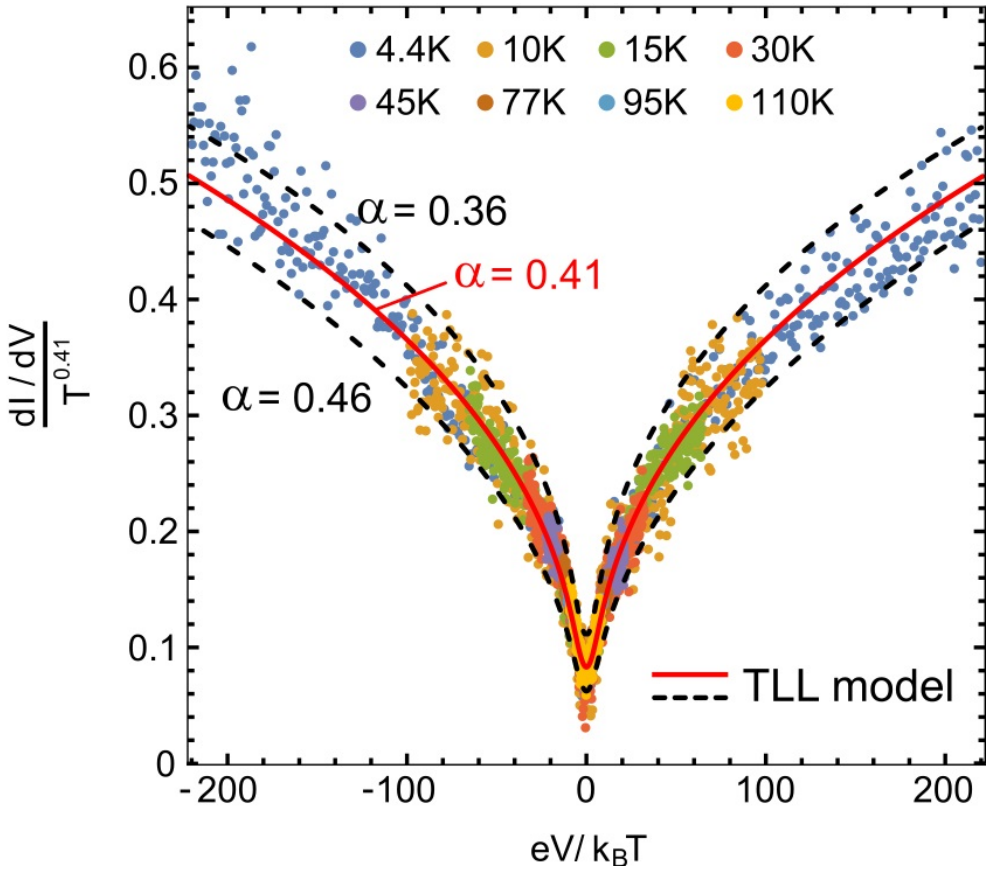
→ el. correlations in 1D: Tomonaga-Luttinger liquid

Bismuthene/SiC(0001): 1D edge states as helical TLL

Au atom chains on Ge(001)



scaled spectra



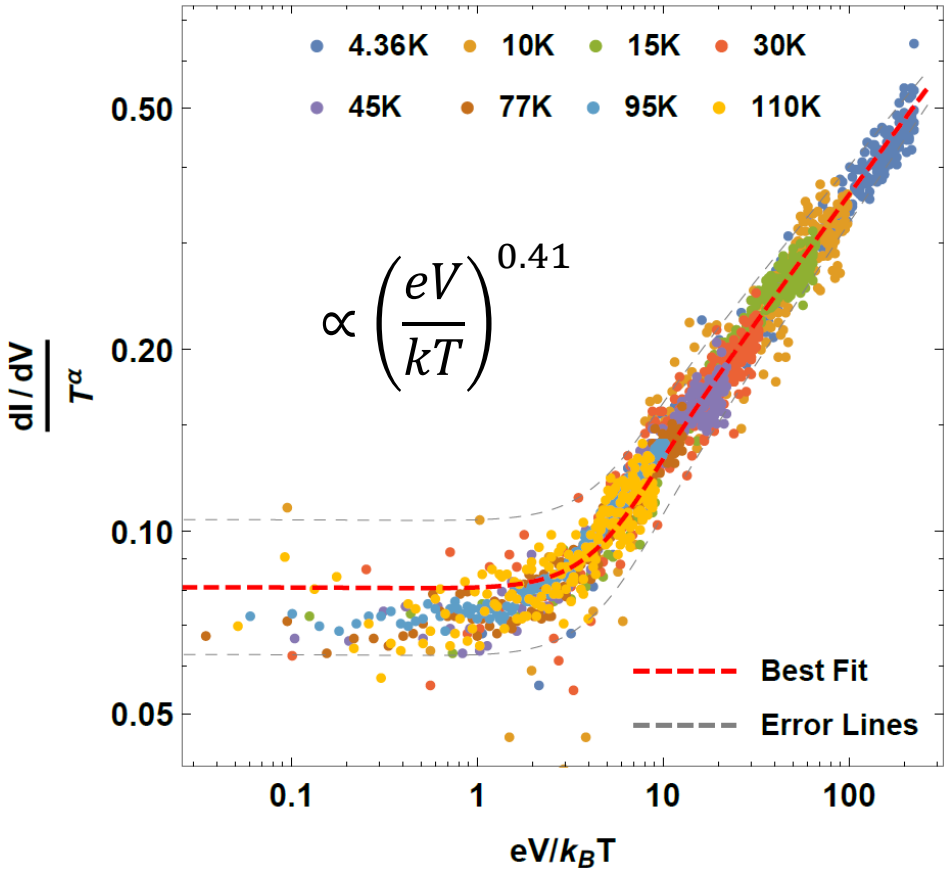
$$\frac{dI}{dV} \propto T^{\alpha} cosh\left(\frac{eV}{kT}\right)\left|\Gamma\left(\frac{1+\alpha}{2}+i\frac{eV}{2\pi kT}\right)\right|^2 \otimes \frac{df}{dE}$$

→ **el. correlations in 1D: Tomonaga-Luttinger liquid**

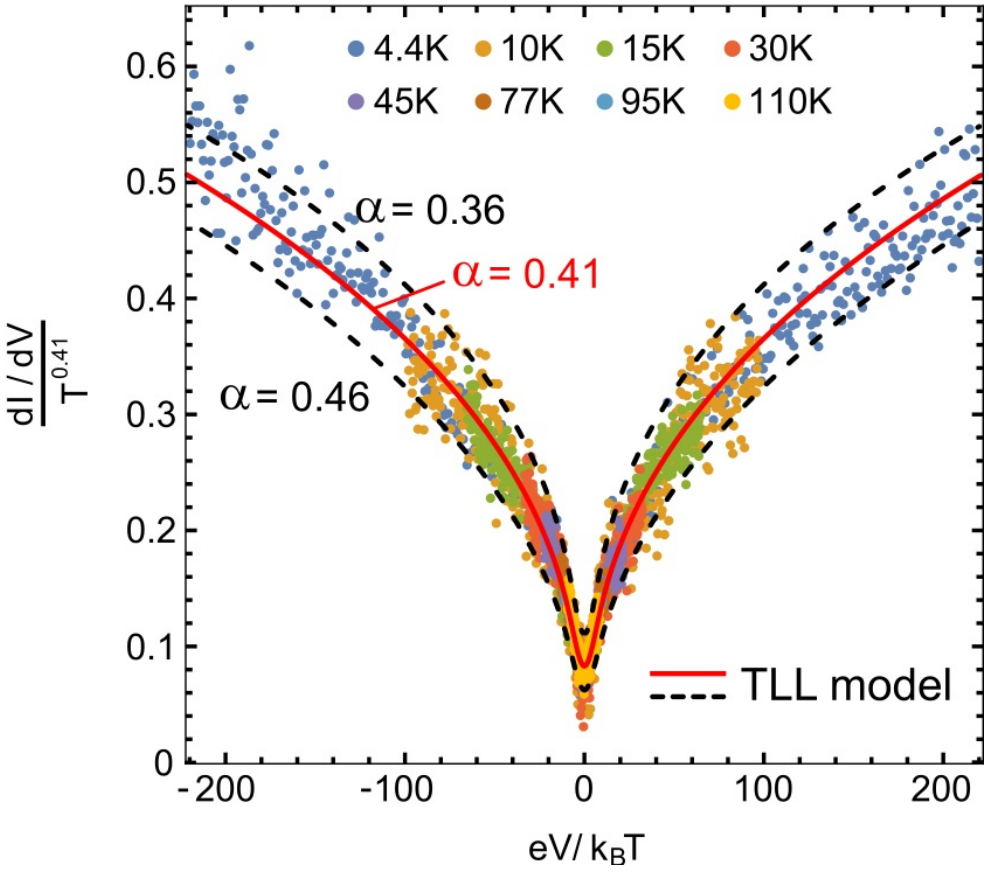
Nat. Phys. ***7****, 776 (2011)*

Bismuthene/SiC(0001): 1D edge states as helical TLL

scaled log-log plot

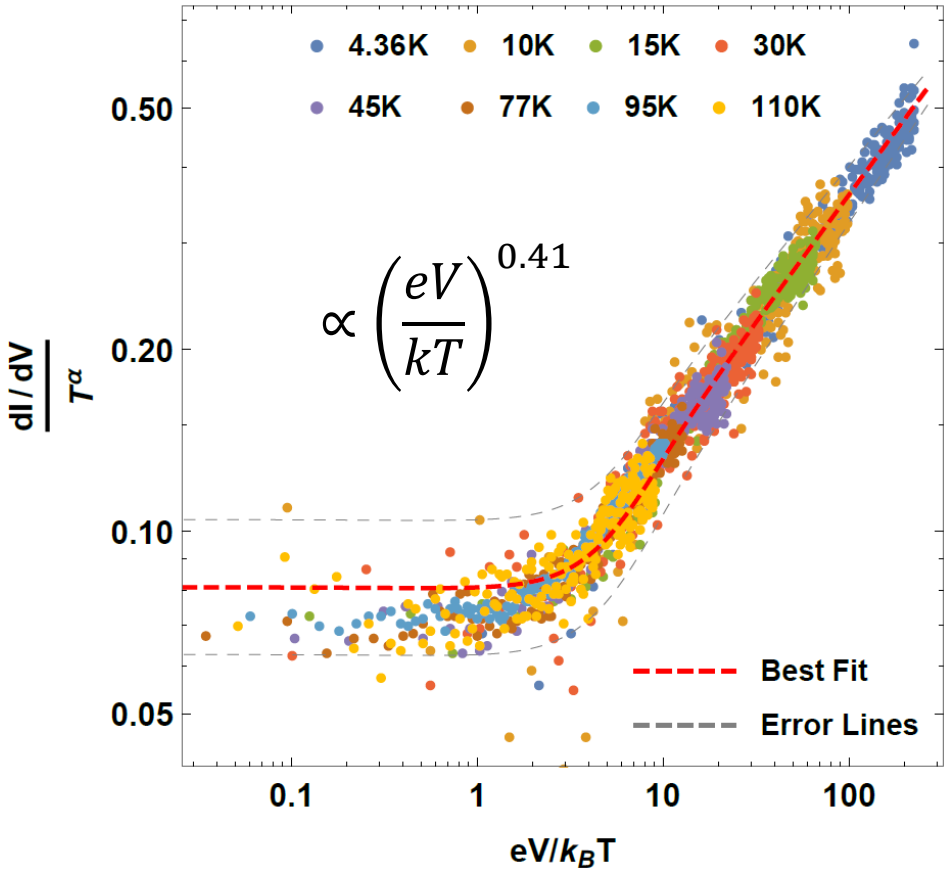


scaled spectra

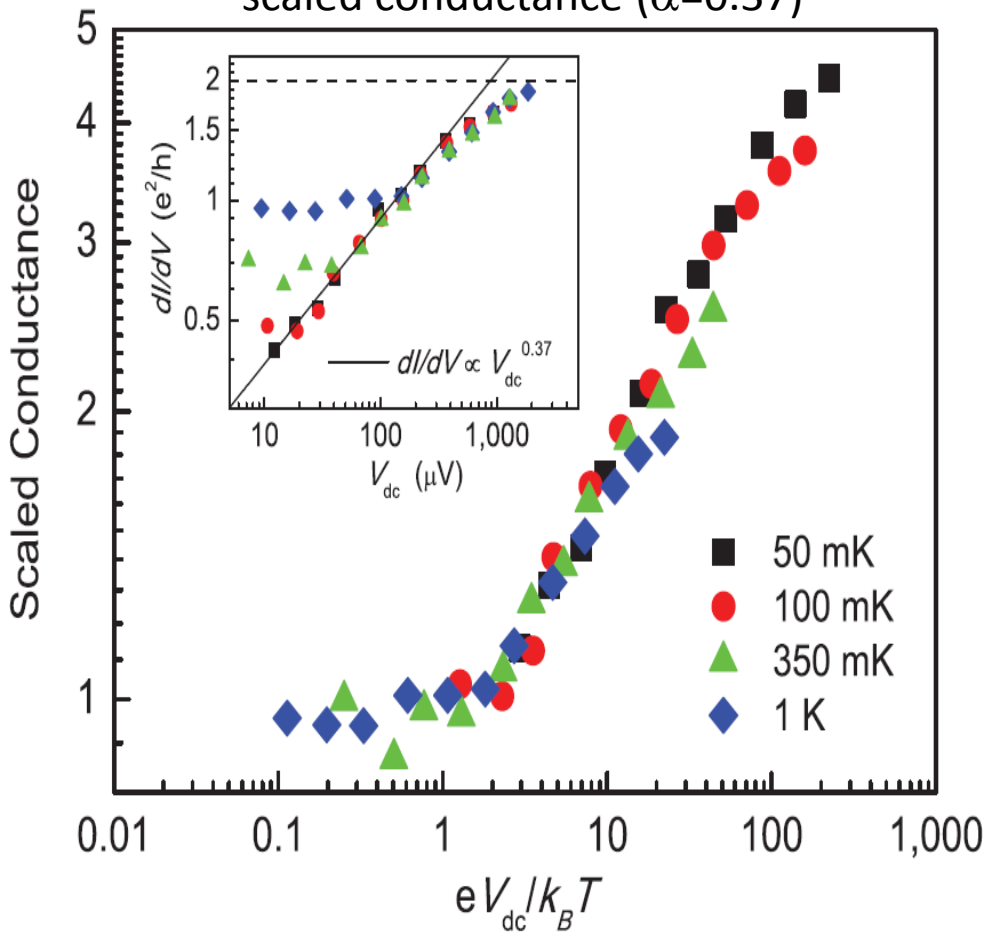


Bismuthene/SiC(0001): 1D edge states as helical TLL

scaled log-log plot



scaled conductance (α=0.37)



TLL scaling behavior in

Bi^{ene}/SiC

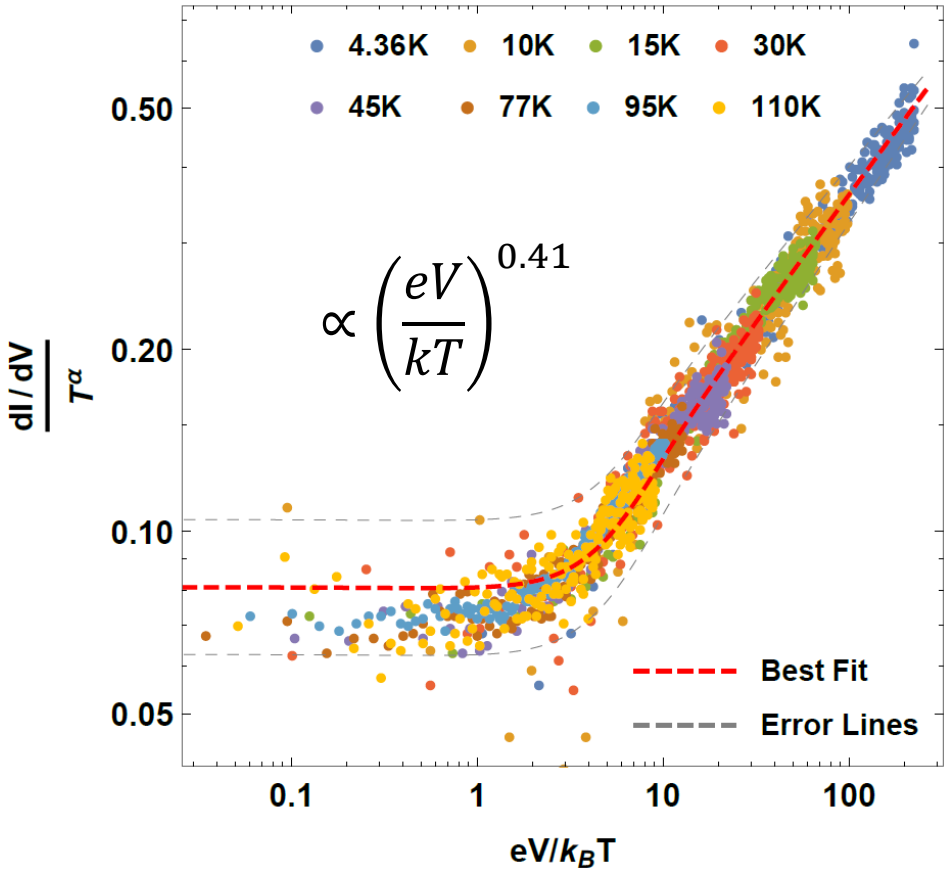
for comparison:

InAs/GaSb QWs

*Li et al., PRL **115**, 136804 (2015)*

Bismuthene/SiC(0001): Tomonaga-Luttinger parameter

scaled log-log plot



TLL scaling behavior in

Bi^{ene}/SiC

TLL parameter K = $\sqrt{\frac{1+\tilde{g}_4-\tilde{g}_2}{1+\tilde{g}_4+\tilde{g}_2}}$ with $\tilde{g}_i = \frac{g_i}{2\pi\hbar v_F}$

= 0.42 ± 0.05 from $\alpha = \frac{1}{2}\left(K + \frac{1}{K} - 2\right)$

for helical TLL, see Braunecker et al., PRB (2012)

	K	source
non-interacting limit	1	
HgTe/CdTe QW	~0.5…0.9	theor. estimate *Teo & Kane (PRB 2009)*
bismuthene/SiC	**0.42**	**tunneling DOS** *this work*
InAs/GaSb QW	0.21 *vs.* 0.8	exp. conductance *Li et al. (PRL 2015)* vs. *Väryrynen et al. (PRB 2016)*

Open questions and outlook

α-Sn: gap too small for practicable purposes, but nice (Hg-free!) 3D model TI for spectroscopic studies

stanene: potentially interesting QSH insulator, but still needs to be synthesized

bismuthene/SiC:

- **novel QSH paradigm**, extend to other group V elements
- **verify helical nature** of edge states:
  - → in $\vec{B}$-field (characteristic gap openings: *arXiv:1803.02648*)
  - → magnetic impurities (local breaking of TRS)
  - → ultimately:

    QSHE, conductance quantization ($\frac{2e^2}{h}$) **at room temperature !**

role of 1D correlations?