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ep4

Bismuthene on SiC: A candidate material for a new high-temperature quantum spin Hall paradigm

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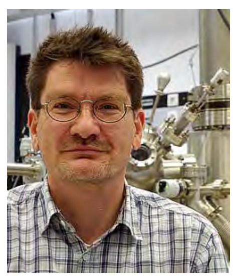
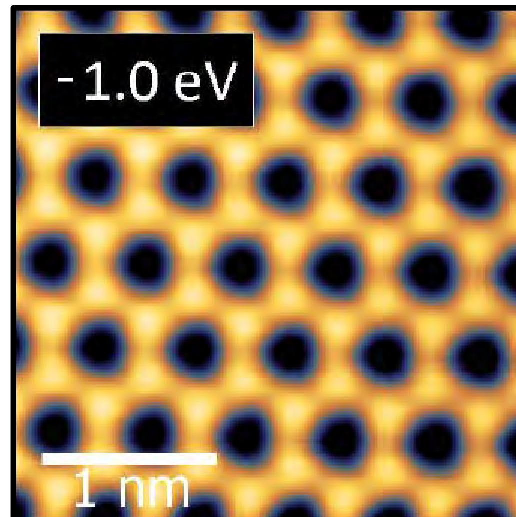


Jörg Schäfer



L. Dudy, M. Bauernfeind, S. Glass, W. Hanke & R. Thomale
all @ U Würzburg

SFB1170
ToCoTronics
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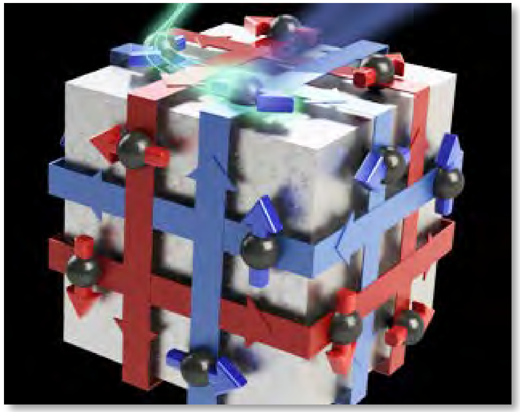
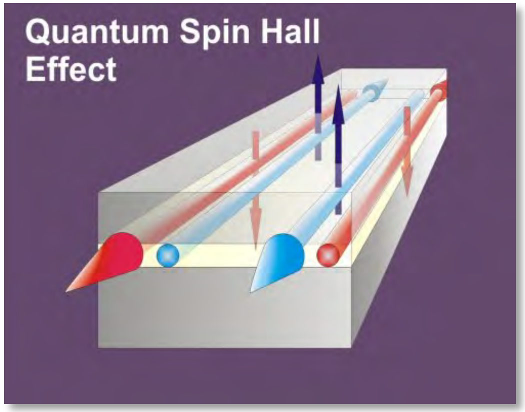
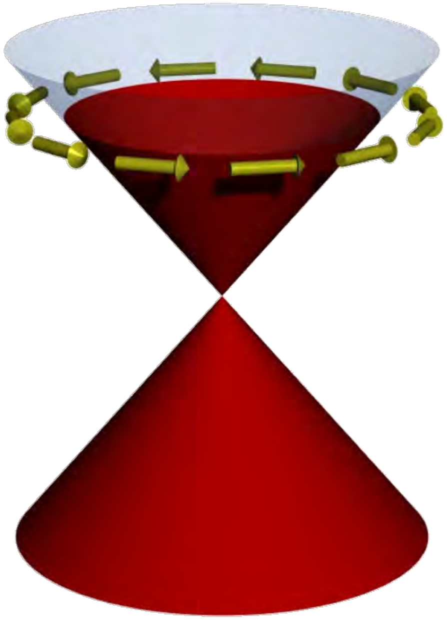
Helical edge states in topological insulators

3D TIs
with 2D surface states



2D TIs
with 1D edge states





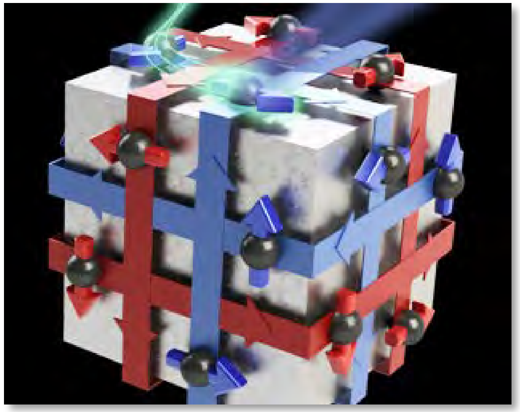
"topologically protected" surface/edge states in the bulk band gap:

- metallic
- spin-polarized
- helical

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

Helical edge states in topological insulators

3D TIs
with 2D surface states



2D TIs
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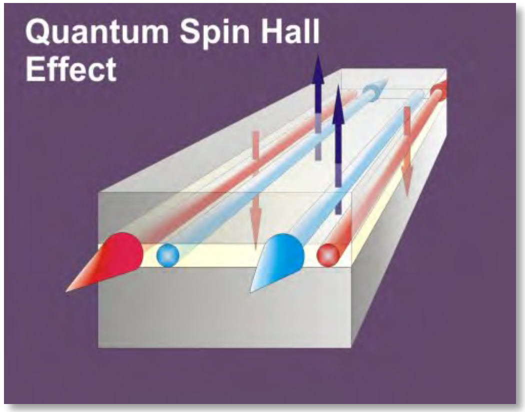

"topologically protected" surface/edge states in the bulk band gap:

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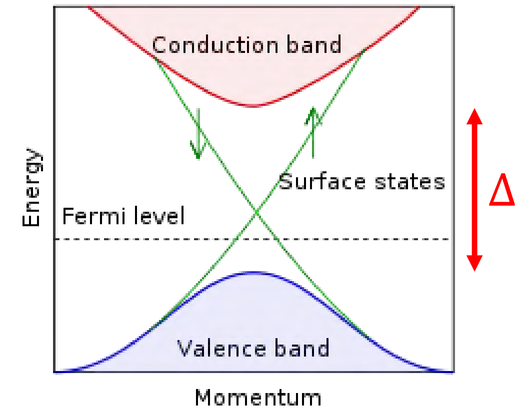
→ search for Dirac materials & quantum spin Hall (QSH) insulators for **electronic/spintronic applications at room temperature**

Quantum Spin Hall Effect (QSHE) in 2D TIs

theoretical proposal:

semiconductor quantum wells with inverted band gap

Bernevig, Hughes & Zhang, Science (2006)

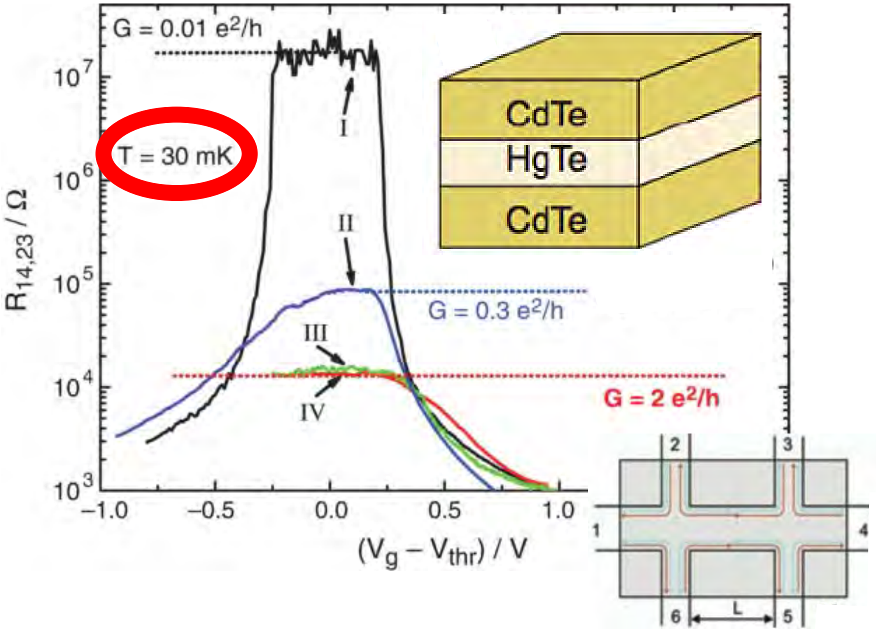


experimental realizations:

- HgTe/CdTe quantum well structures

  M. König et al., Science (2007)

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



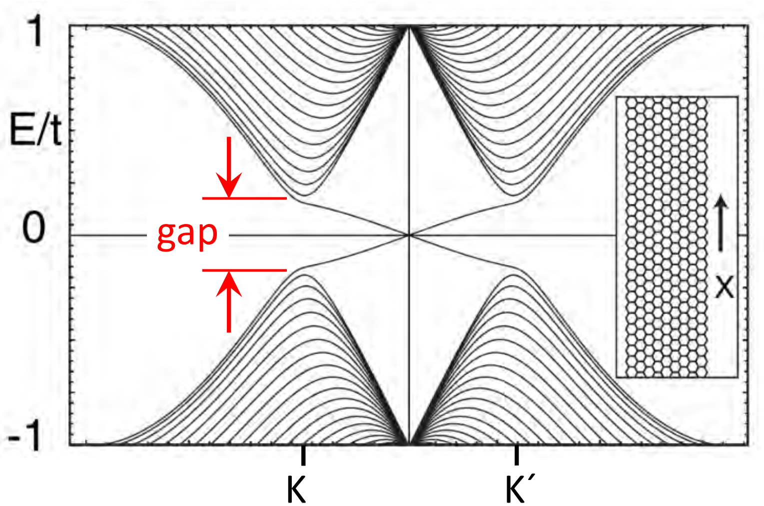
- InAs/GaSb QWs

  Knez, Du & Sullivan, PRL (2011)

  → $\Delta \approx 4$ meV

QSHE in 2D honeycomb lattices

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



→ metallic spin-polarized edge states

energy gap

24 µeV
graphene

2 meV

24 meV

100 meV
stanene

Y. Xu et al., PRL 2013

spin-orbit coupling

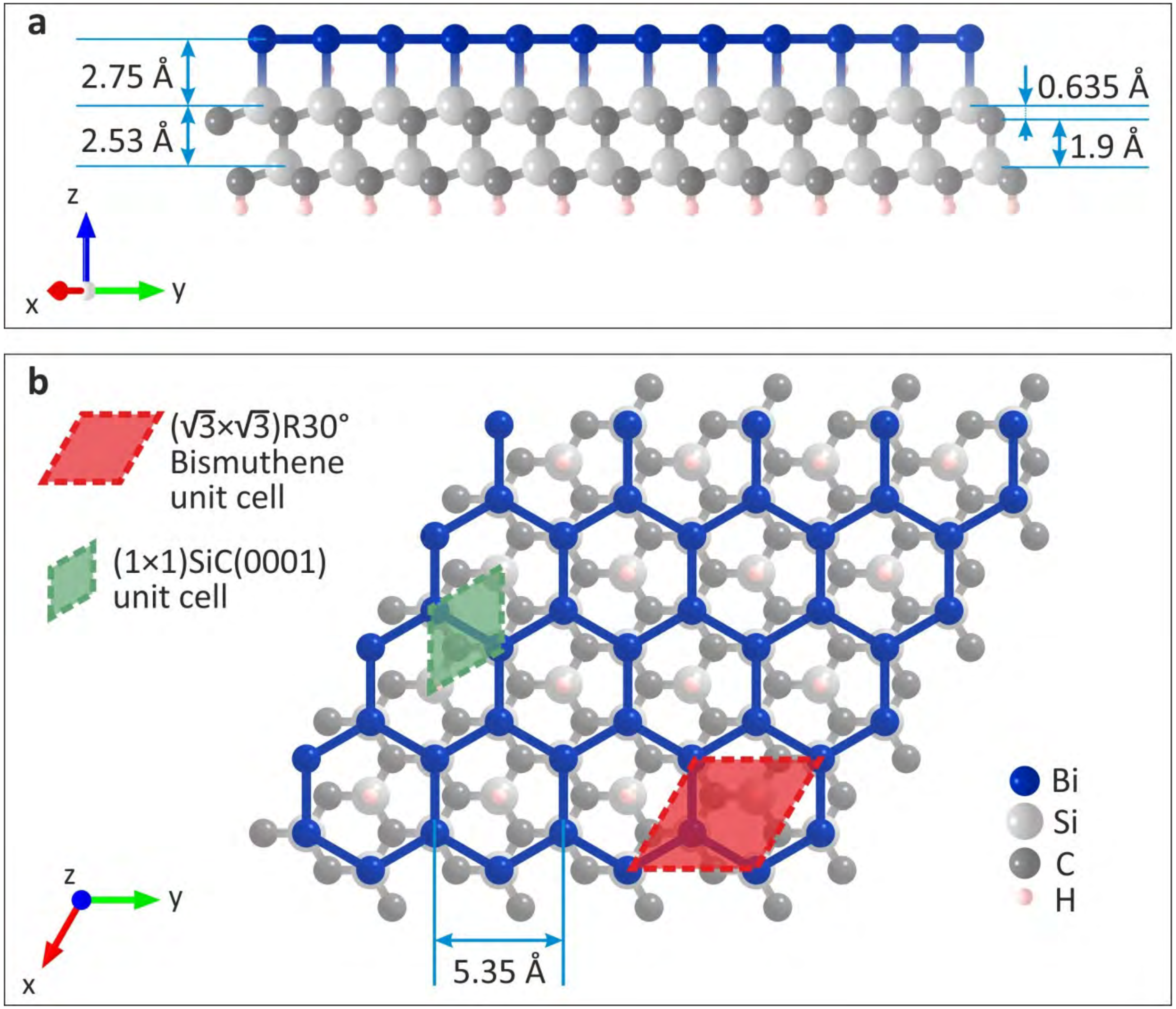
Z^4

group IV	V
6 12,011 C Carbon	7 14,007 N Nitrogen
14 28,086 Si Silicon	15 30,974 P Phosphorous
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

Bi/SiC(0001)

Hsu et al., NJP 2015

Bismuthene on SiC(0001): structure



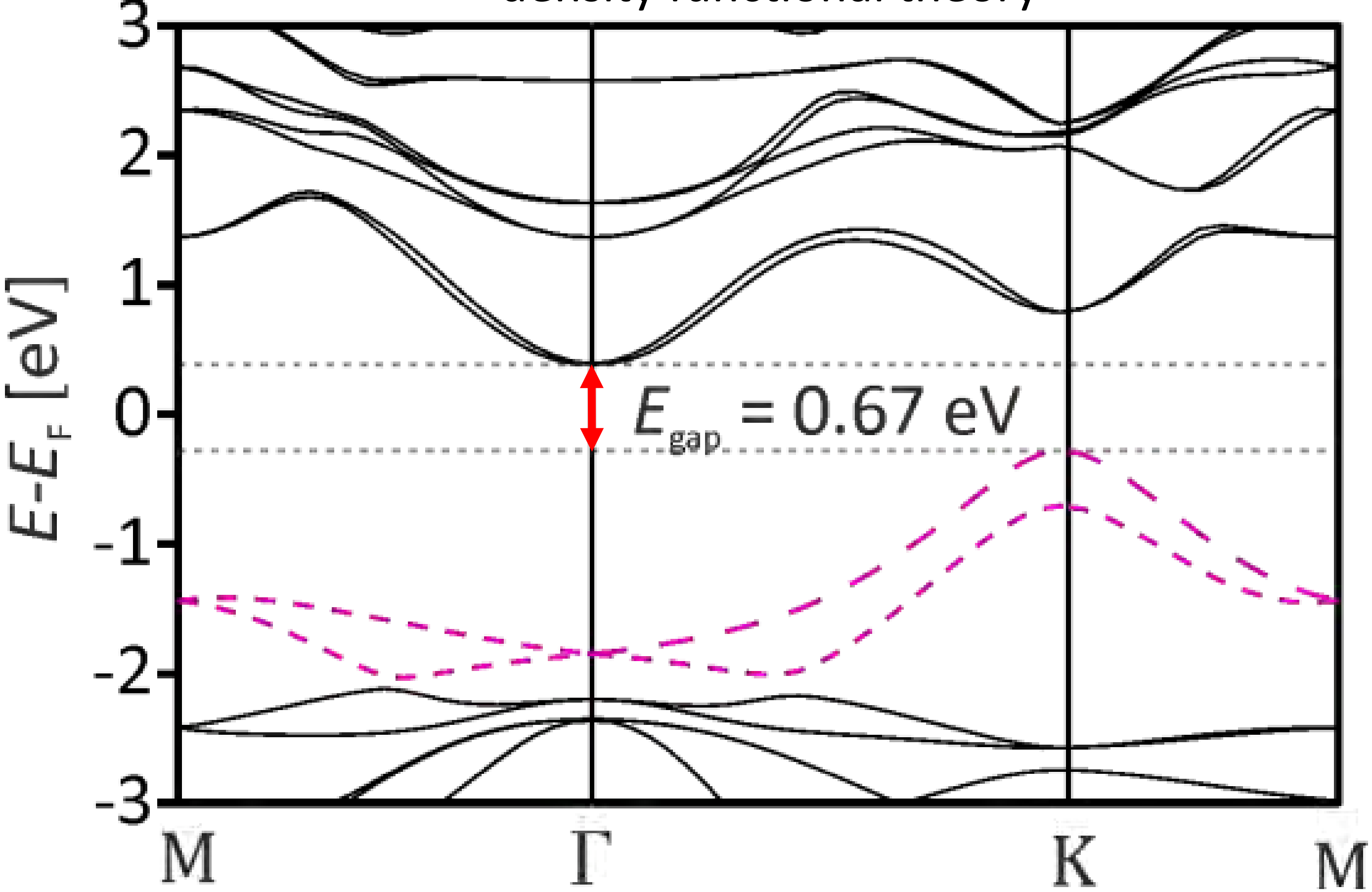
18% tensile strain
→ planar honeycombs

(√3x√3)R30°
reconstruction

arXiv:1608.00812

Bismuthene on SiC(0001): band structure and gap

density functional theory



arXiv:1608.00812

Bismuthene on SiC(0001): effective model

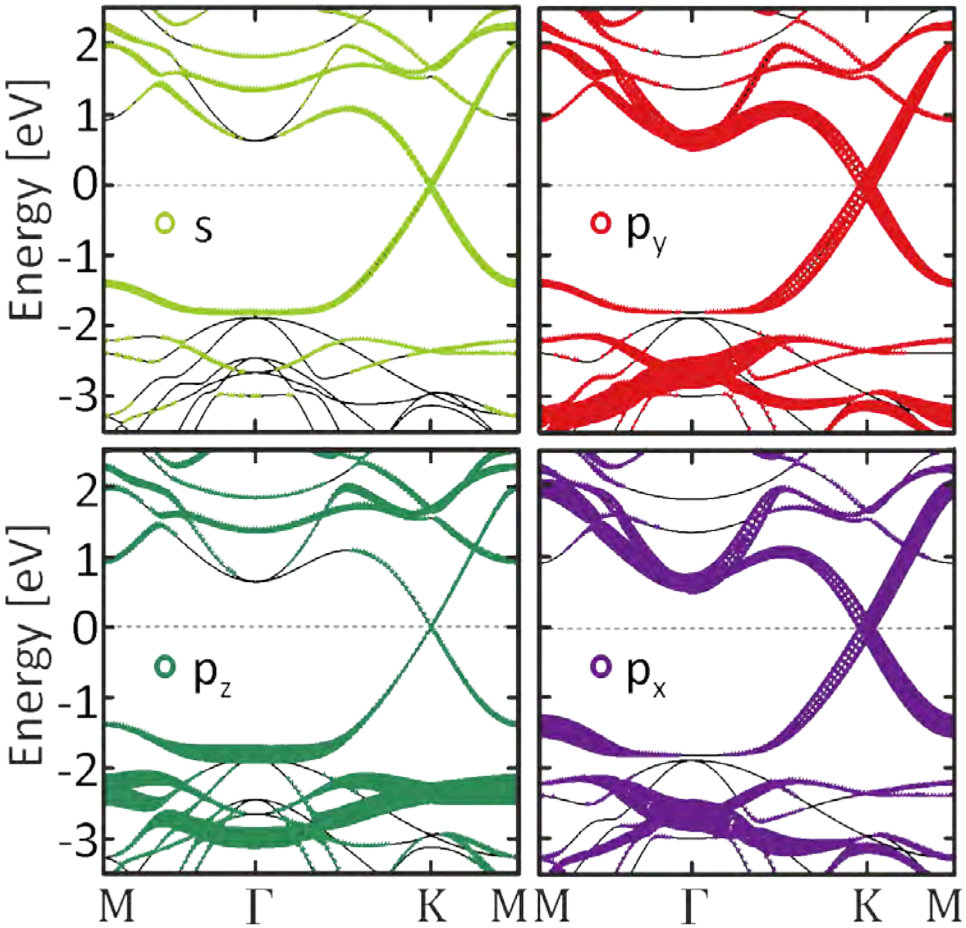
band structure analysis w/o spin-orbit coupling:

- *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 !

(and from Bernevig-Hughes-Zhang model for HgTe/CdTe)



arXiv:1608.00812

Bismuthene on SiC(0001): effective model

basis states: $|p_{x\uparrow}^A\rangle, |p_{y\uparrow}^A\rangle, |p_{x\uparrow}^B\rangle, |p_{y\uparrow}^B\rangle;$ $|p_{x\downarrow}^A\rangle, |p_{y\downarrow}^A\rangle, |p_{x\downarrow}^B\rangle, |p_{y\downarrow}^B\rangle$

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

$$H_{\uparrow\uparrow/\downarrow\downarrow}^{\sigma\sigma} = H_{0,\uparrow\uparrow/\downarrow\downarrow}^{\sigma\sigma} \pm \lambda_{soc} \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

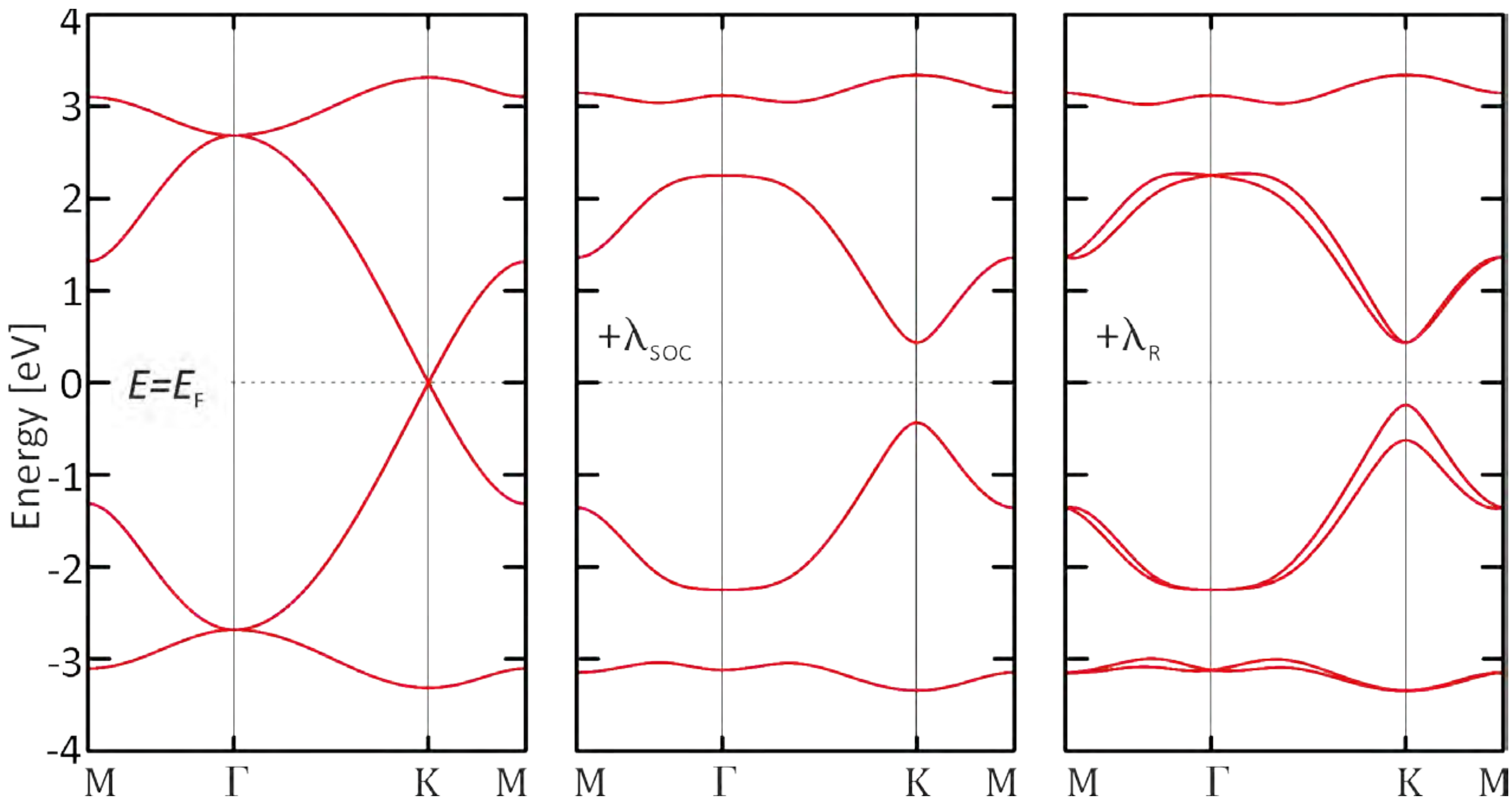
off-diagonal orbital term mixes in local (atomic) SOC

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

Rashba

arXiv:1608.00812

Bismuthene on SiC(0001): effective model



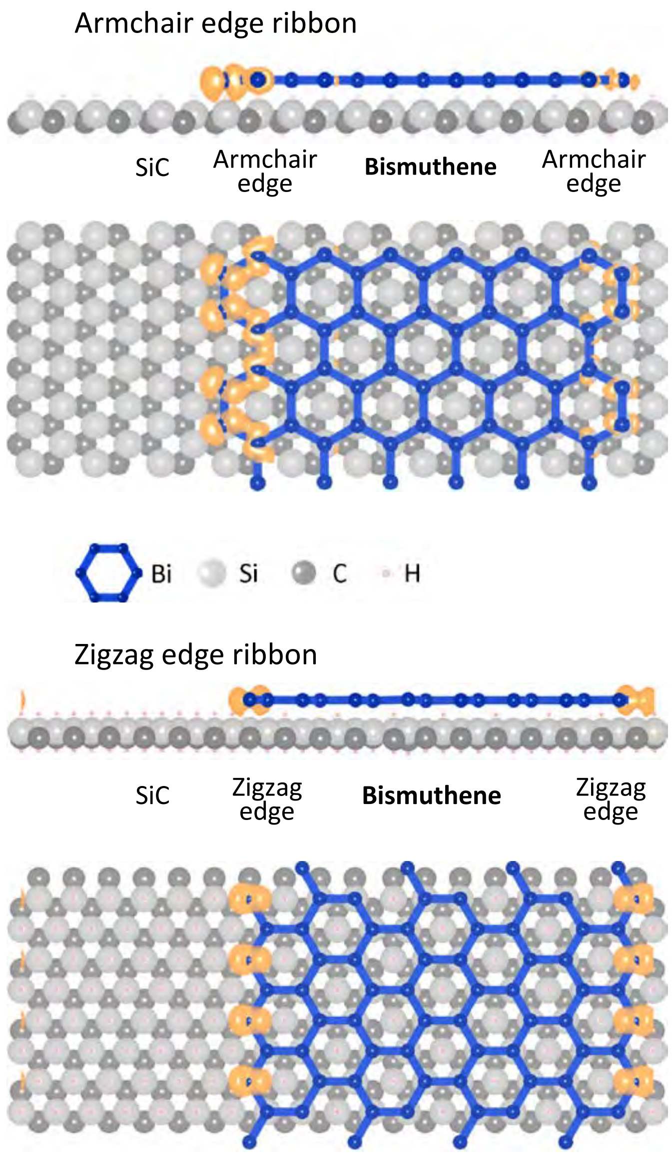
effective tight-binding model *with* SOC:

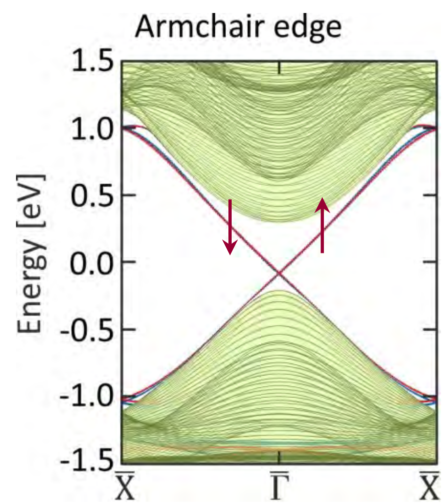
$$H_{eff}^{\sigma\sigma} = H_0^{\sigma\sigma} + \lambda_{SOC} H_{SOC}^{\sigma\sigma} + \lambda_R H_R^{\sigma\sigma}$$

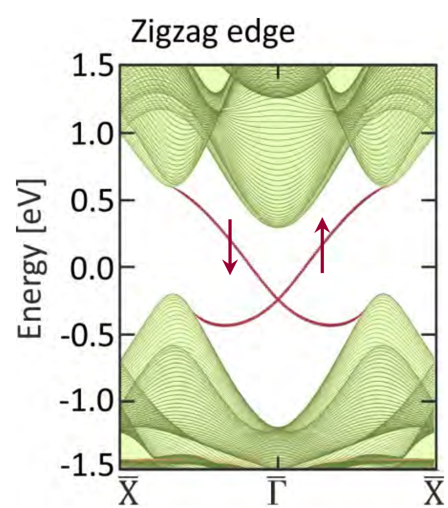
arXiv:1608.00812

Bismuthene on SiC(0001): topological edge states

TB calculations for edge situations:







helical metallic edge states,

topological invariant
$$Z_2 = 1$$

↓

bismuthene/SiC is a QSH system !

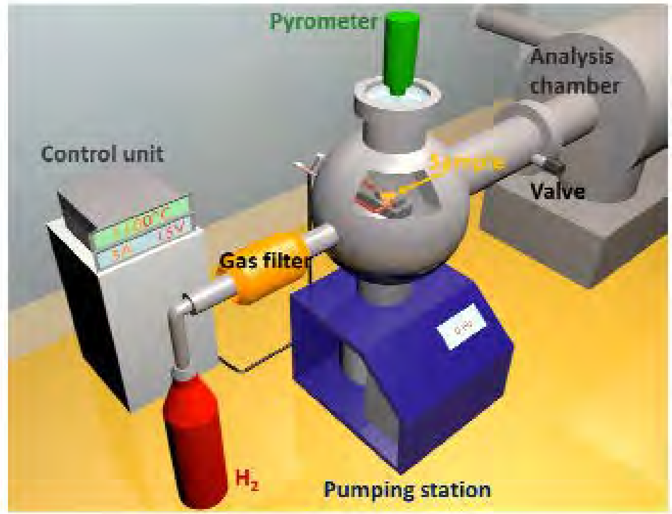
arXiv:1608.00812

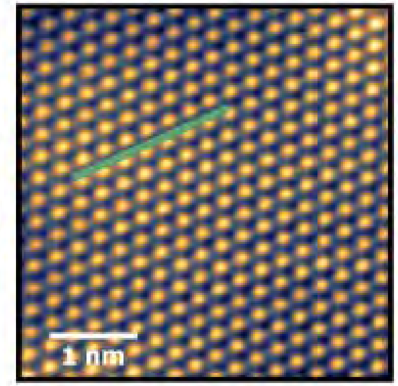
Bismuthene on SiC(0001): experimental realization

substrate prep:

4H-SiC(0001) wafers (n-doped, 0.02 Ωcm),

H-etching for smooth (1x1) surfaces

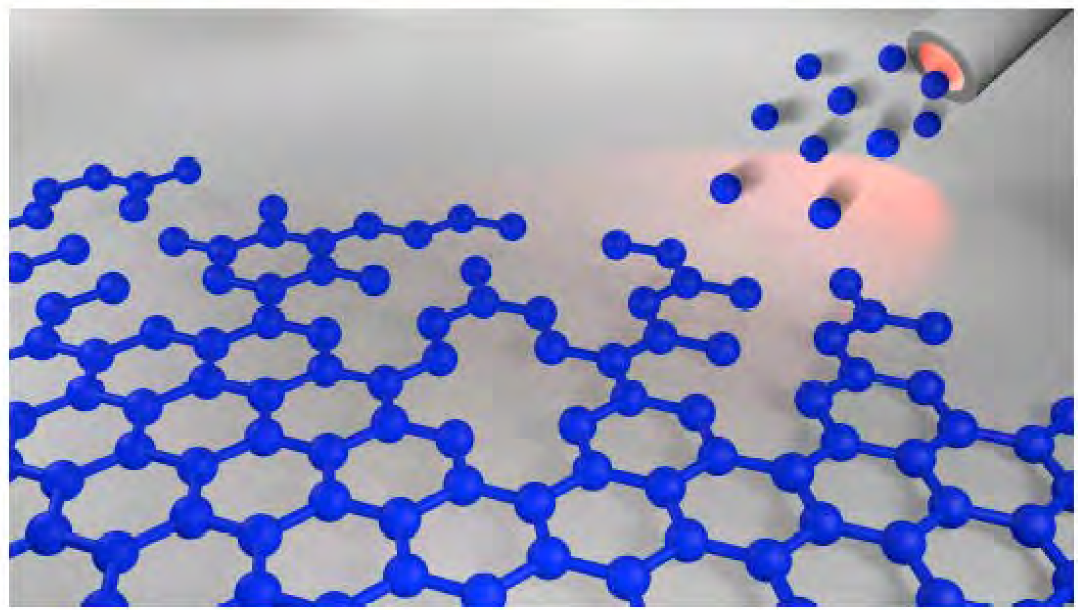




STM after etching

epitaxial film growth:

Bi-deposition at $T_{SiC} \sim 500$°C, monitored by LEED ($\sqrt{3}\times\sqrt{3}$)



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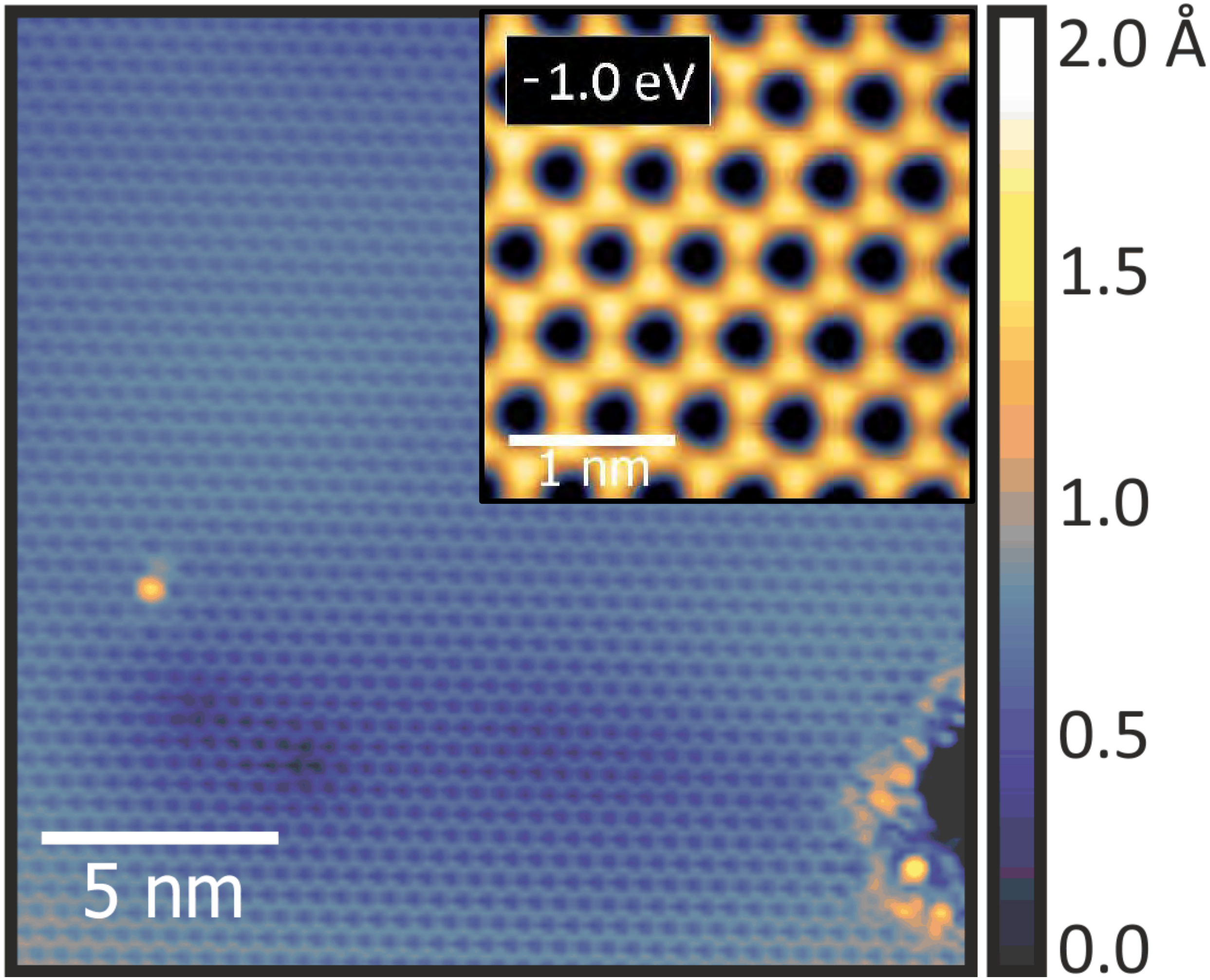
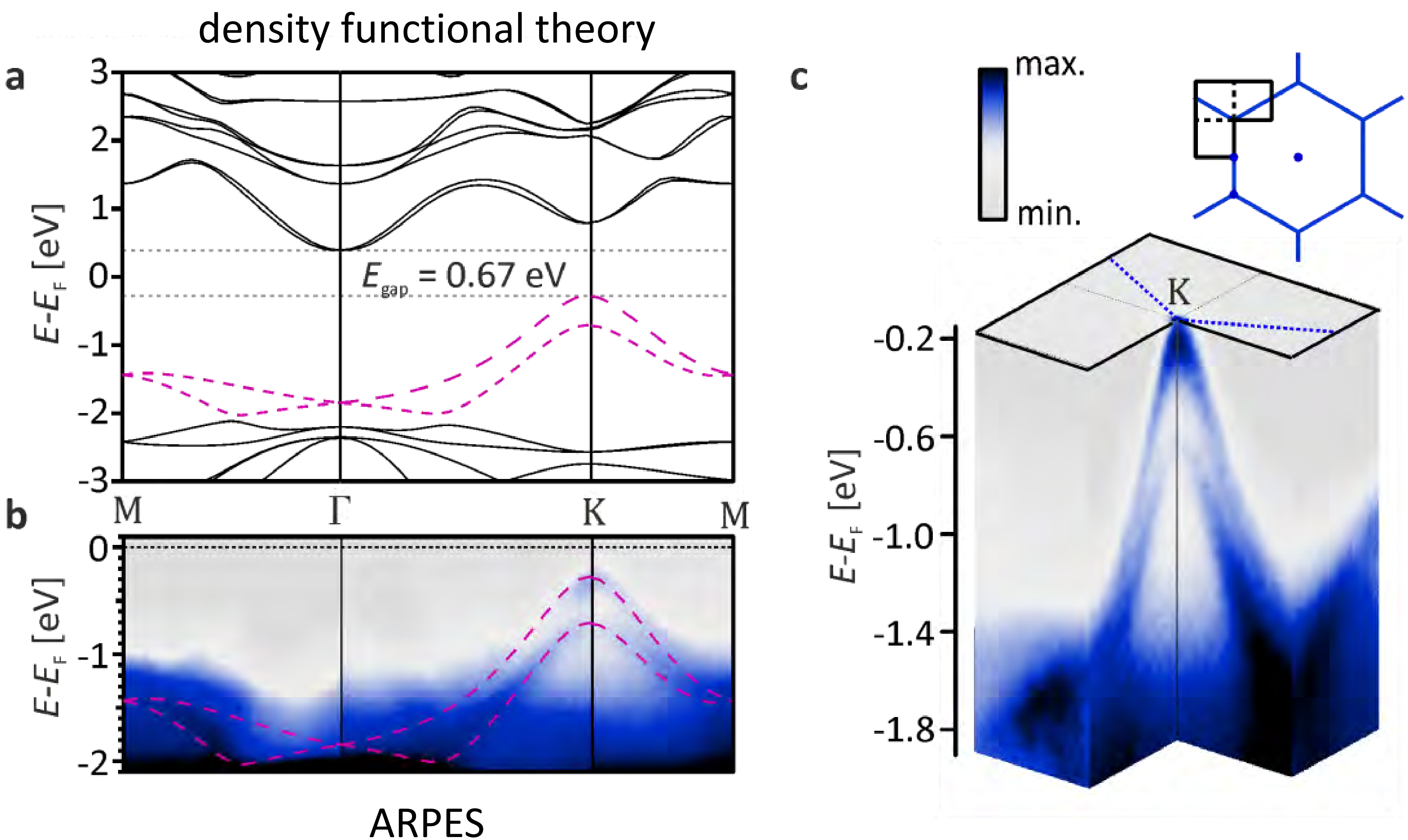
Bismuthene on SiC(0001): experimental realization

STM topography



arXiv:1608.00812

Bismuthene on SiC(0001): exp'tal band structure and gap



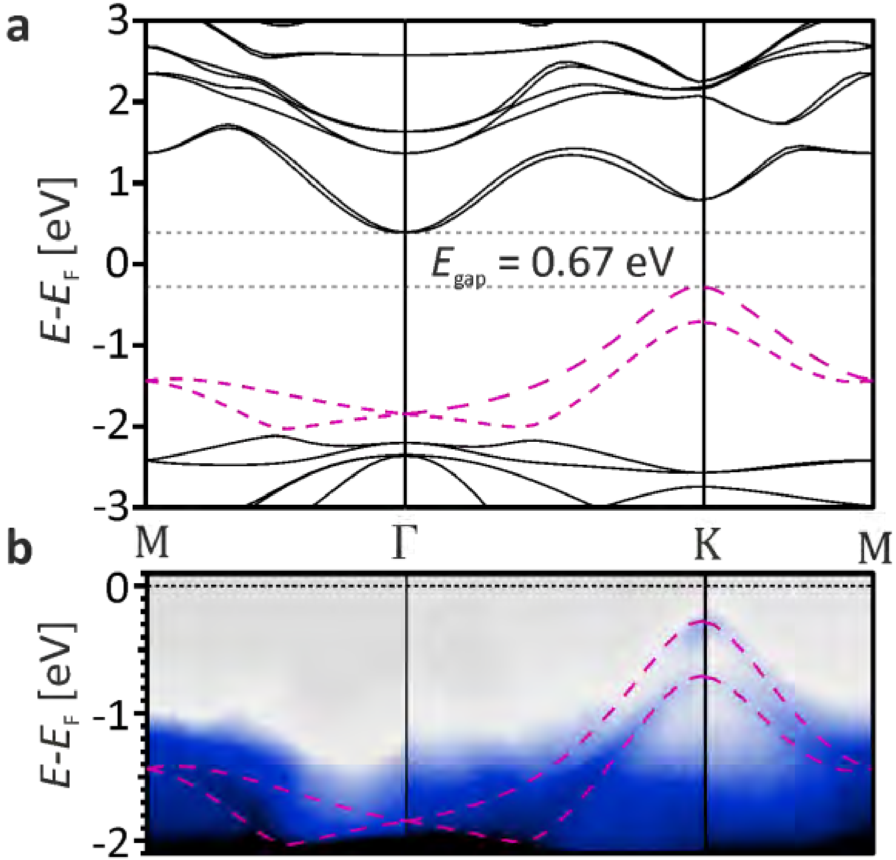
→ **valence band dispersion in excellent agreement**

→ **VB maximum @ K-point, huge Rashba splitting (0.43 eV)**

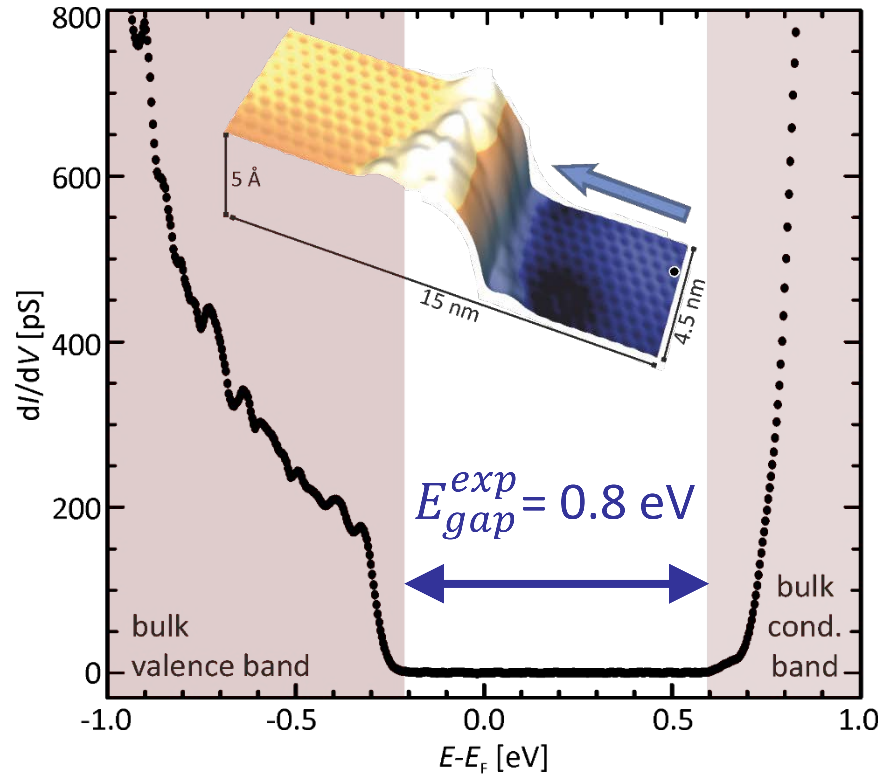
arXiv:1608.00812

Bismuthene on SiC(0001): exp'tal band structure and gap

density functional theory



ARPES



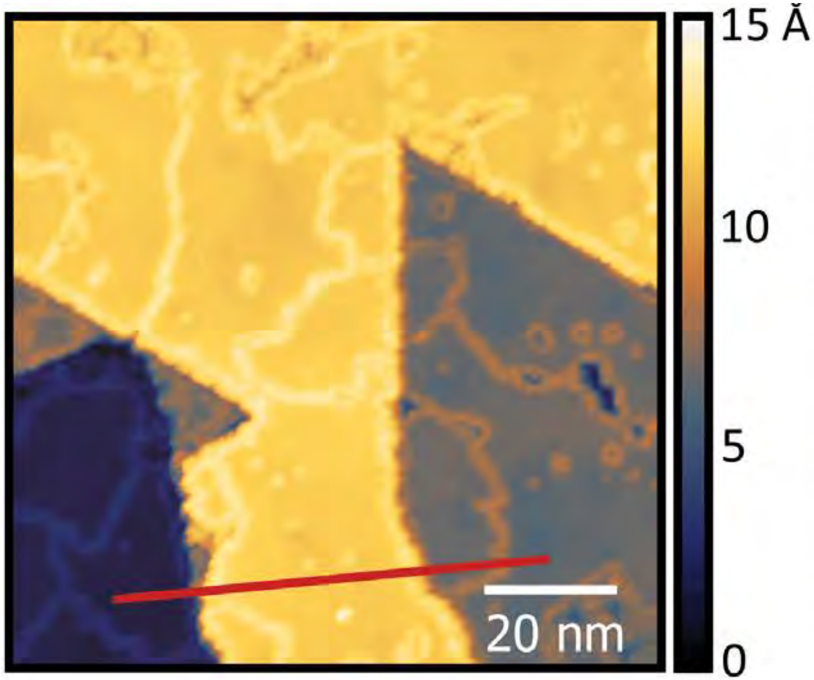
tunneling spectroscopy

→ **huge band gap !**

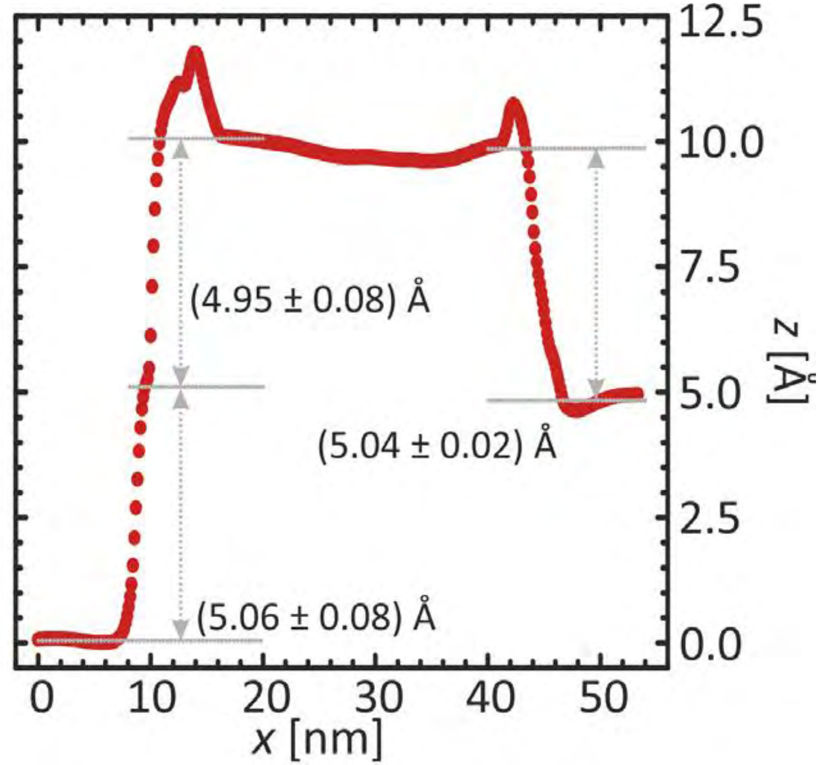
arXiv:1608.00812

Bismuthene on SiC(0001): edge states in experiment

STM topography



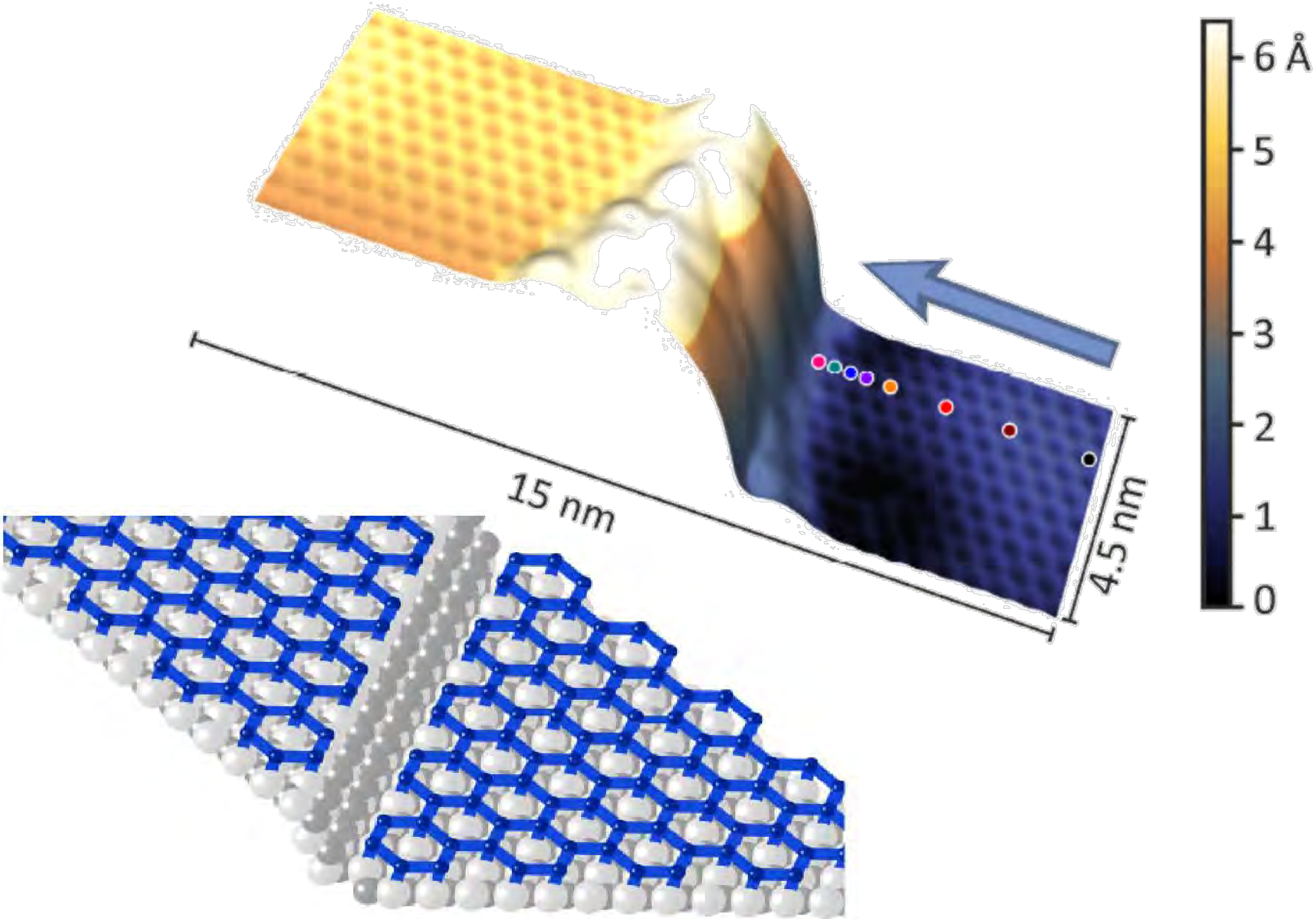
z-profile (along red line)



→ **bismuthene edges at terrace steps of SiC substrate**

arXiv:1608.00812

Bismuthene on SiC(0001): edge states in experiment



→ **bismuthene edges at terrace steps of SiC substrate**

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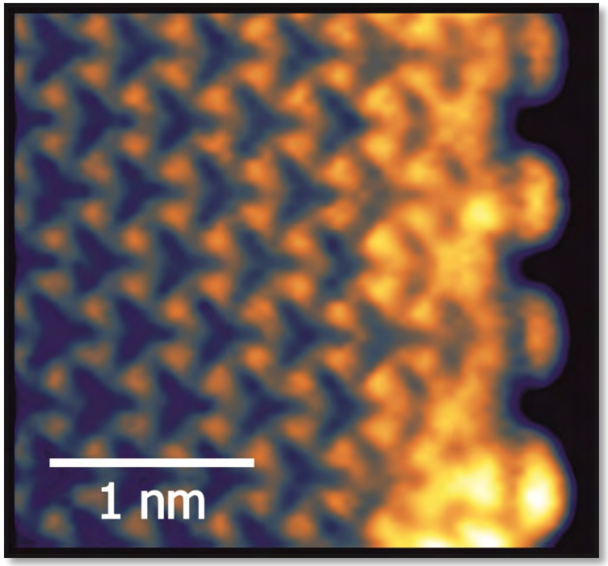
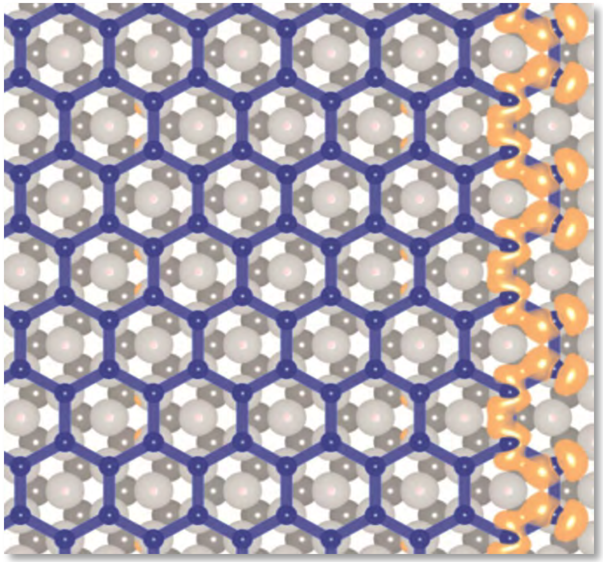
Bismuthene on SiC(0001): edge states in experiment

charge density @ arm chair edge

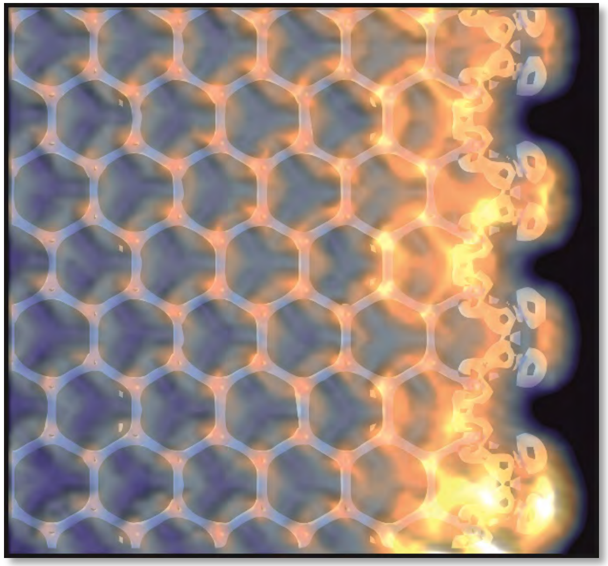
STM



DFT ribbon calculation

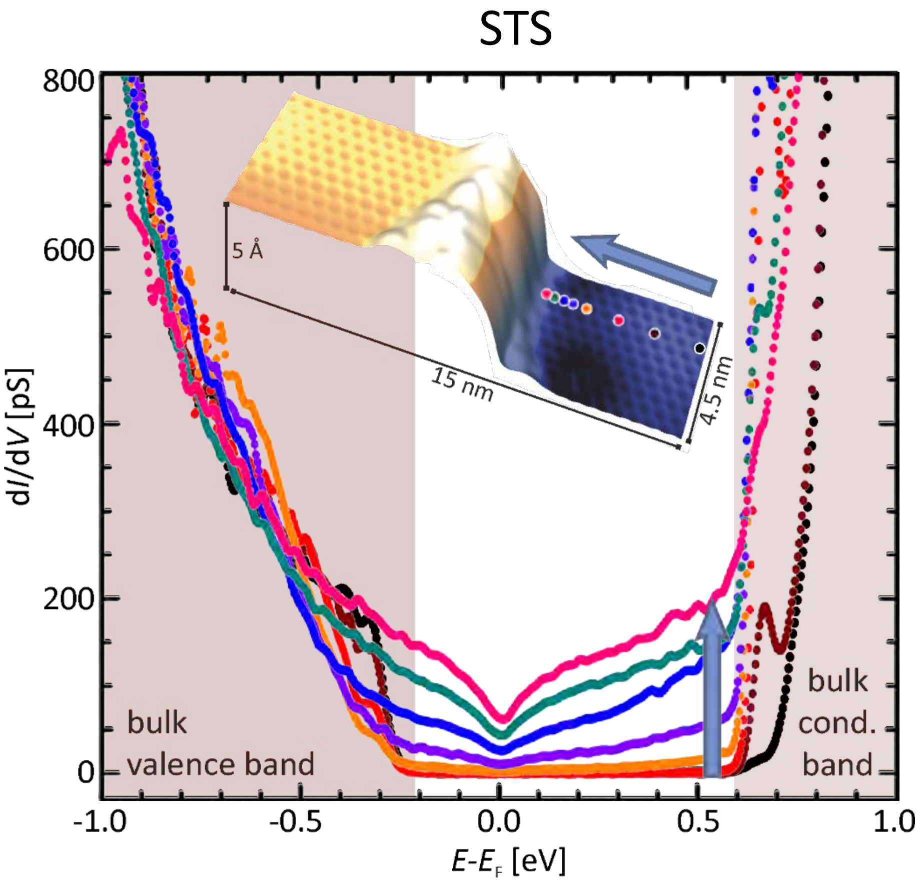


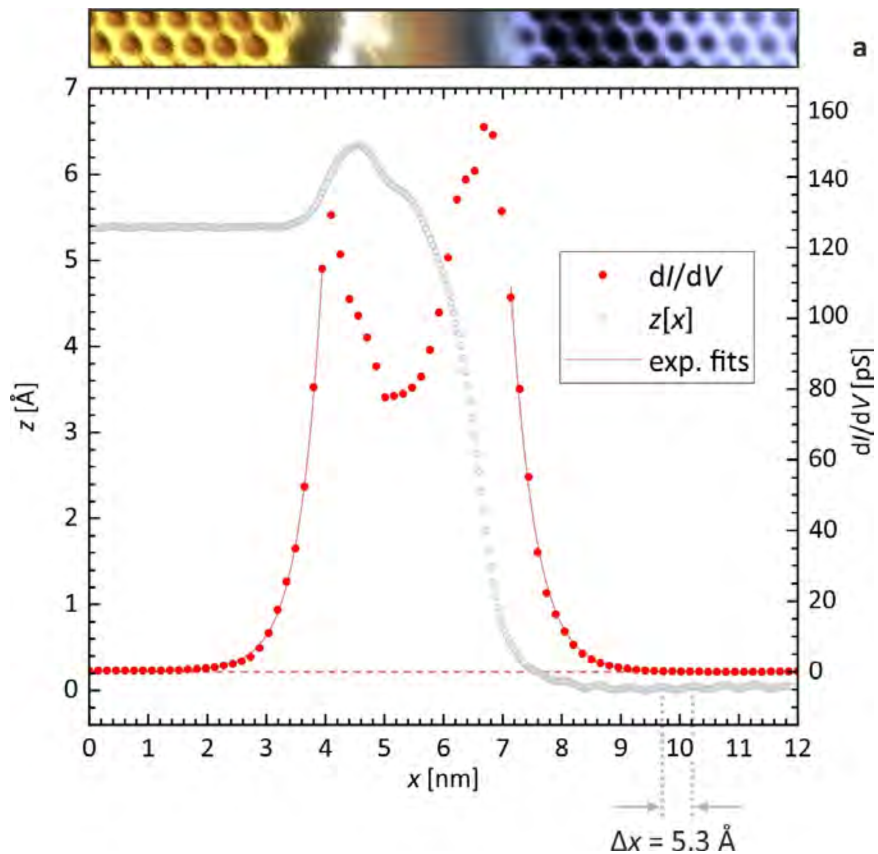
overlay DFT/STM



arXiv:1608.00812

Bismuthene on SiC(0001): edge state spectroscopy

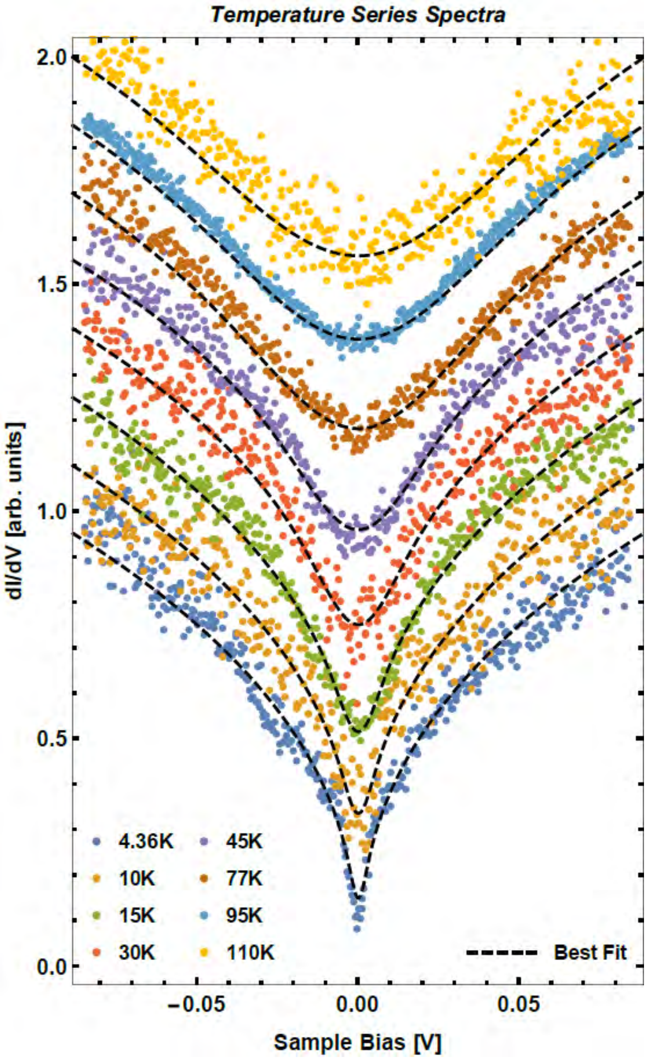


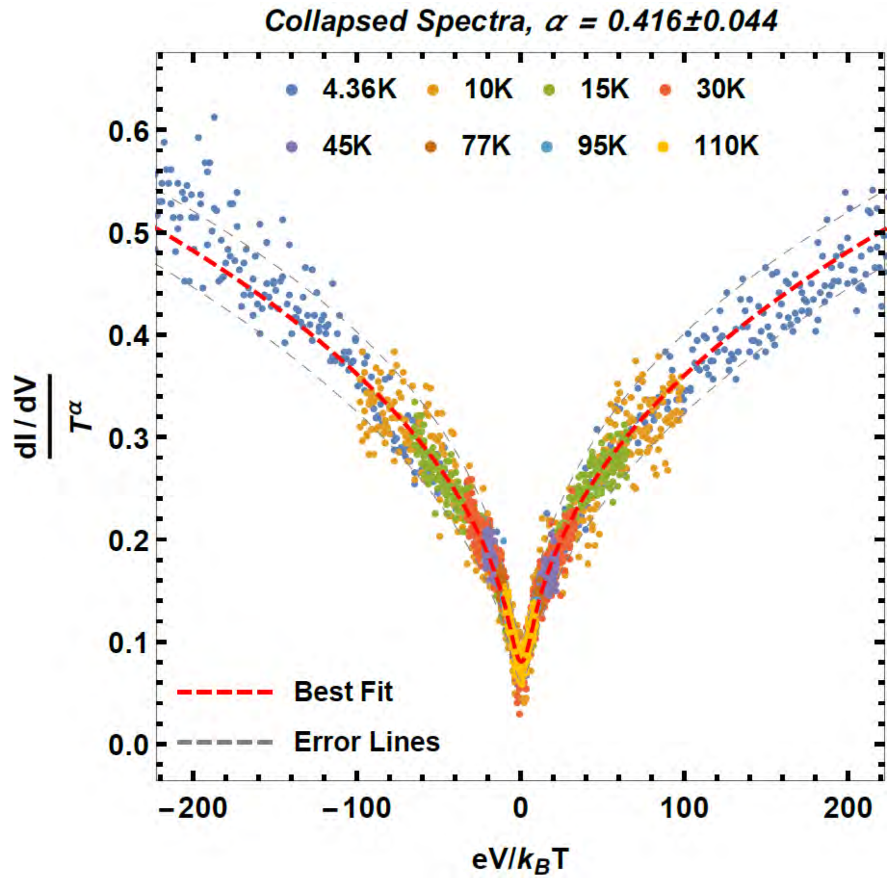


- **metallic edge states in bulk gap**
- **zero bias anomaly @ E_F**
  → Tomonaga-Luttinger liquid behavior ?
- **exponential decay into bulk**
  quantitatively consistent with theory

arXiv:1608.00812

Bismuthene on SiC(0001): edge state zero bias anomaly



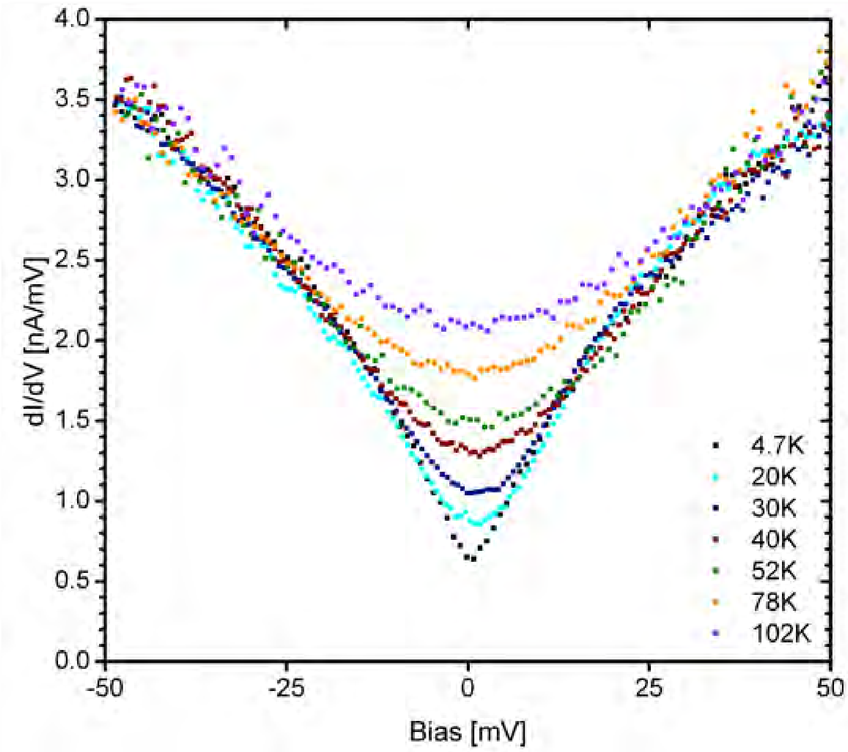


- power law behavior in E and T
- scaling behavior

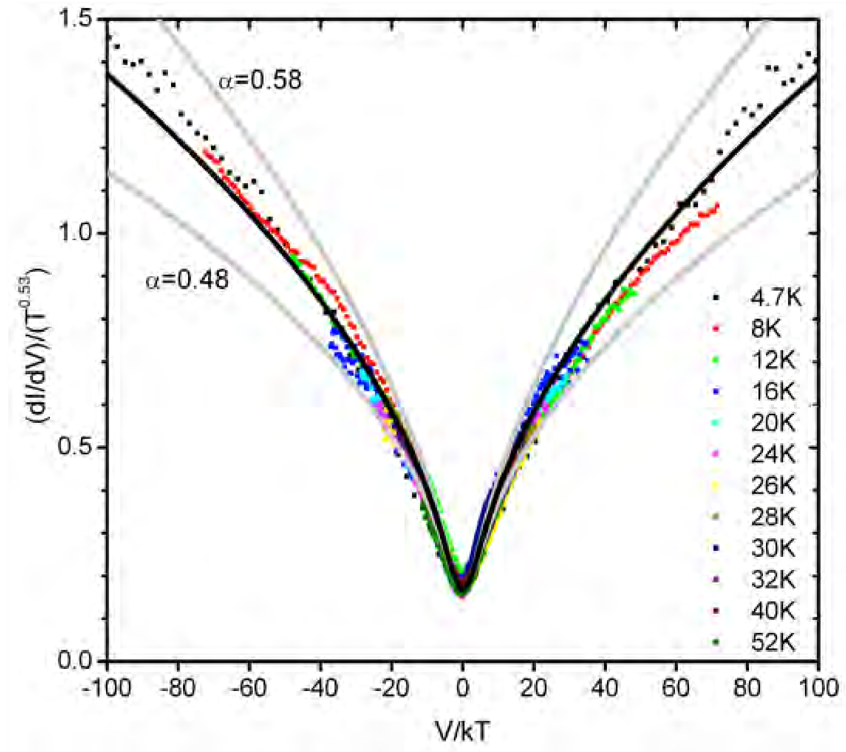
→ **hallmarks of 1D physics: Tomonaga-Luttinger liquid**

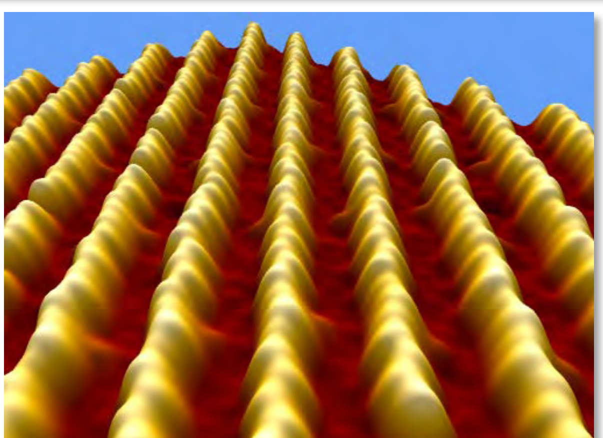
TLL behavior in atomic nanowires: Au/Ge(100)

differential tunneling conductivity



scaled conductivity





TLL scaling behavior:

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

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

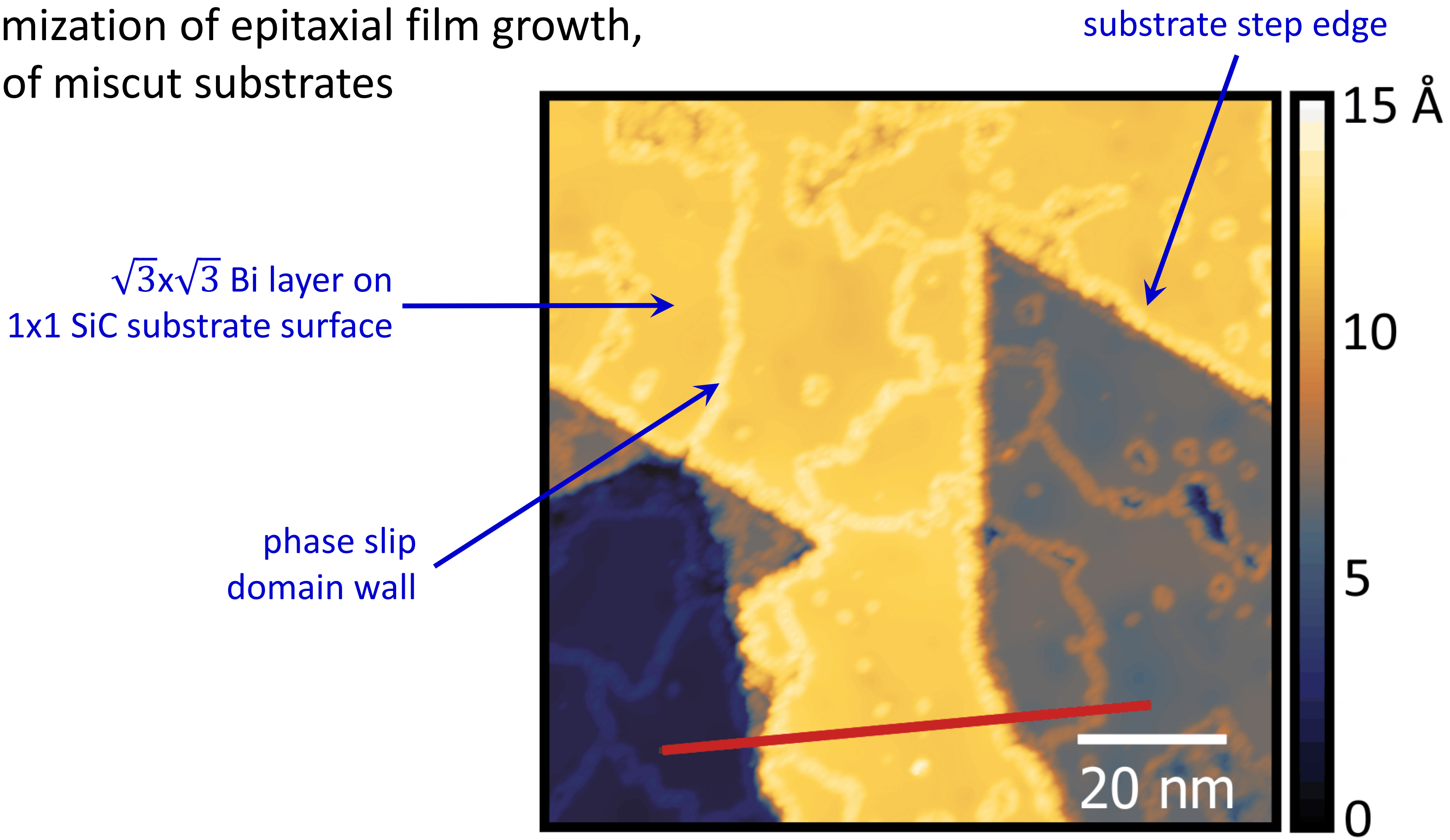
Bismuthene on SiC(0001): remaining challenge

experimental verification of topological character of 1D edge states !

→ *e.g.*, by demonstrating QSHE or by spin-resolved ARPES

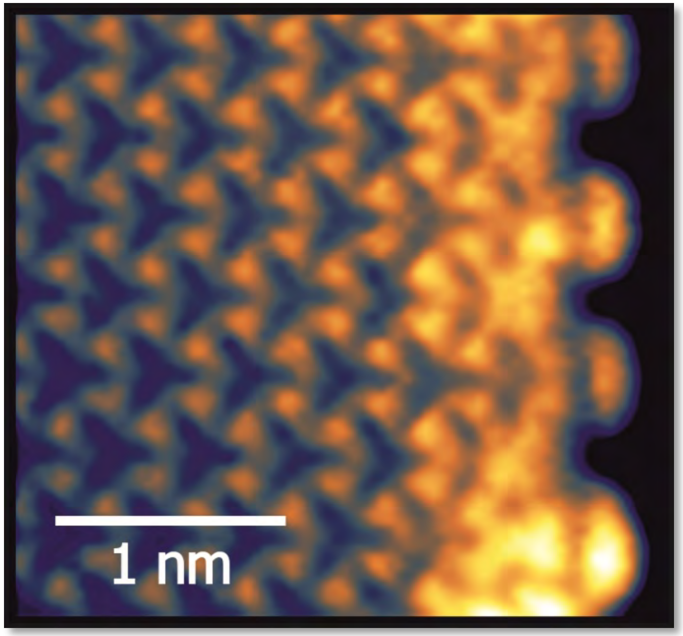
→ requires larger structural domains ($\sqrt{3}$x$\sqrt{3}$ superstructure)

→ optimization of epitaxial film growth,
use of miscut substrates



Summary: Bismuthene on SiC(0001)

- candidate material for a **new QSH mechanism**
- **active role of substrate**:
  orbital "filtering" and full exploitation
  of *atomic* SOC
- **large bulk band gap** (~0.8 eV),
  also SiC substrate (3.2 eV)
  → room-temperature compatible!!
- Rashba-split VBM at K,K' (→ **valleytronics**)
- **metallic 1D edge states**
- **helical character** of edge states established from theory,
  experimentally still to be demonstrated !



F. Reis et al., arXiv:1608.00812