First principle study & STM experiment on Dirac nodal-line semimetal ZrGeTe

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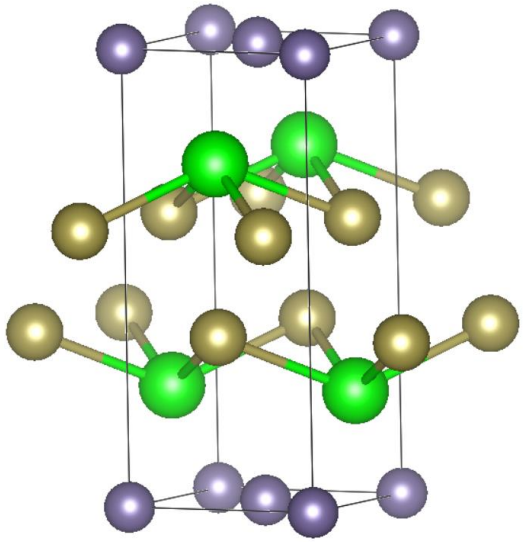
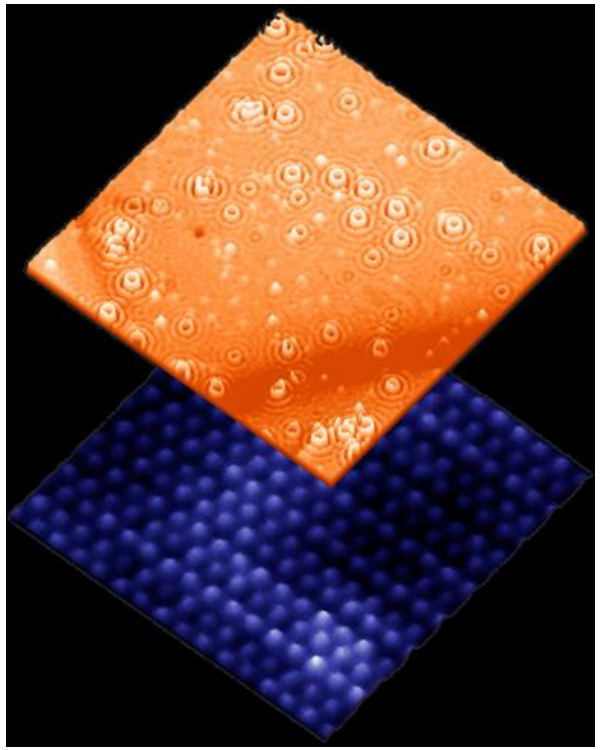
Outline

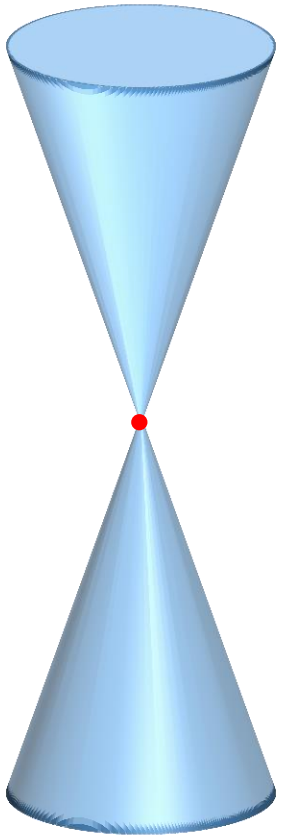
- Introduction
  - Dirac Nodal-line semimetal ZrGeTe
  - Scanning Tunneling Microscope (STM)
  - Quasiparticle interference (QPI)
- STM experiment on ZrGeTe
- First principle study on ZrGeTe
- CEC & QPI fitting
- Conclusions





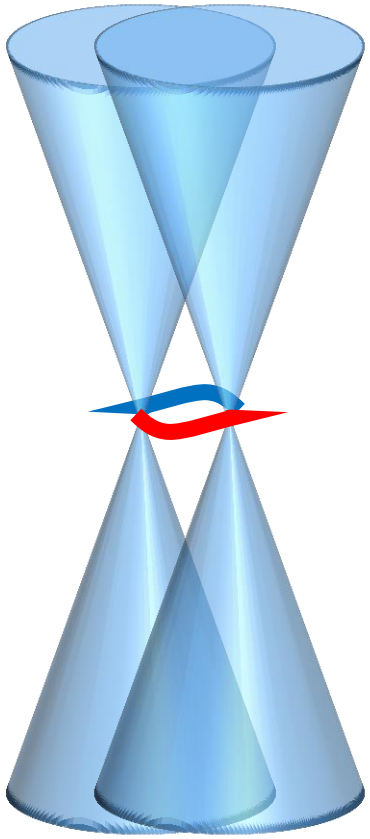
Topological Semimetals

Dirac semimetal



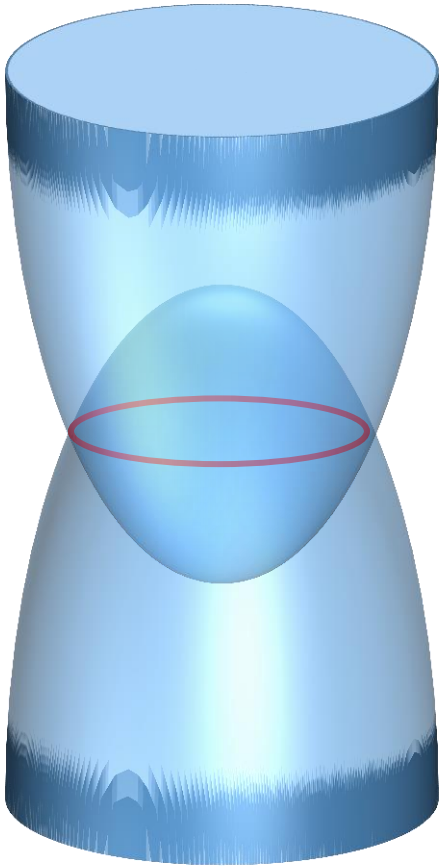
Cd_3As_2, Na_3Bi…

Weyl semimetal



TaAs, NbP…
$MoTe_2$, WTe_2…

Nodal-line semimetal

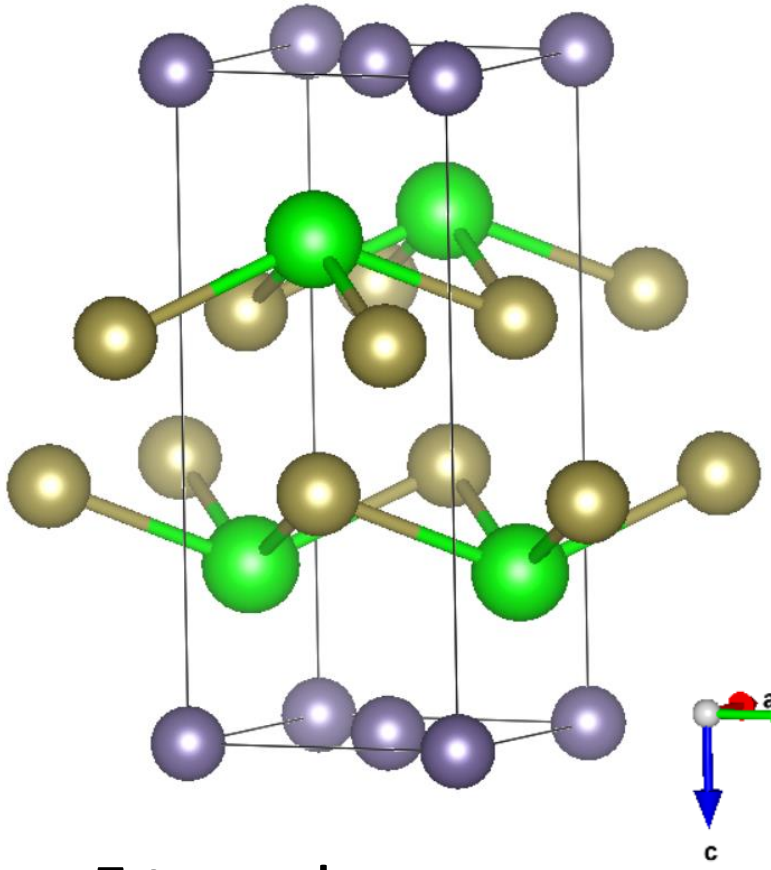


ZrSiS, $PbTaSe_2$, $PtSn_4$…

p.c. Chih-Chuan Su

ZrGeTe

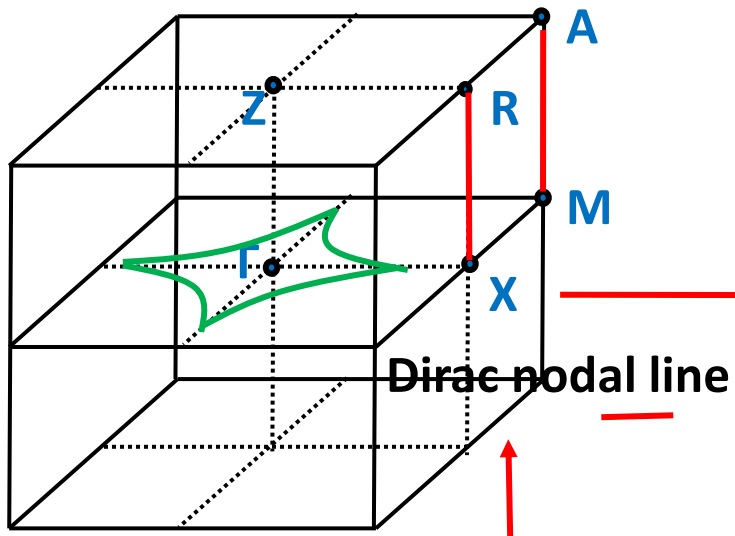
(ZrSiS-family compound)



Tetragonal

P4/nmm (129)

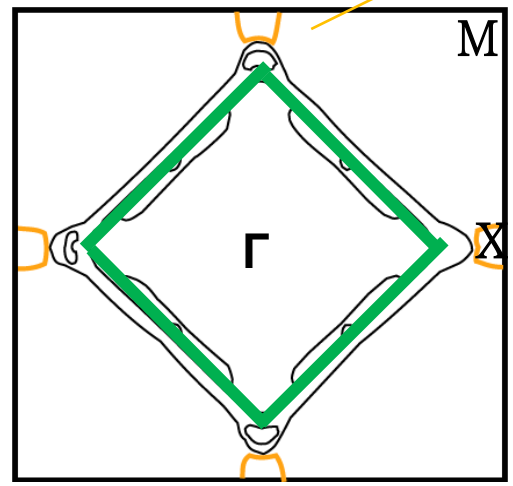
Zr Ge Te



Dirac nodal line

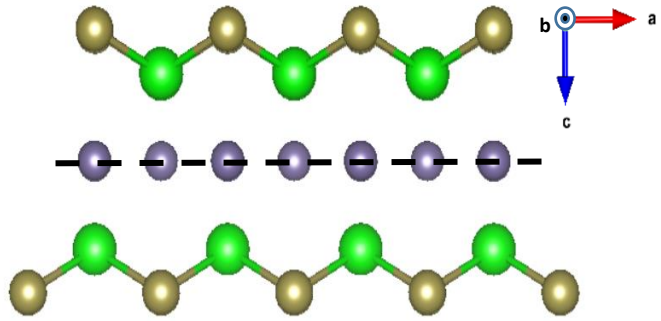
ZrSiS

Surface state

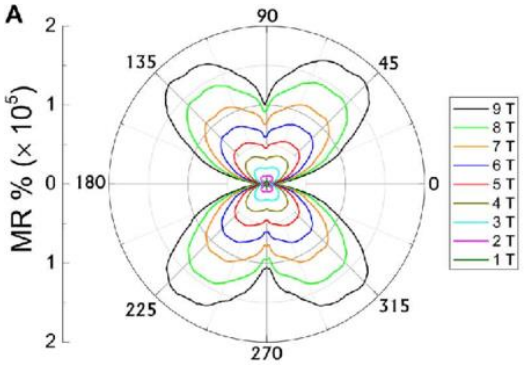


Diamond- shaped Bulk state

Glide-mirror symmetry (nonsymmorphic)



$$M_G:\ (x,y,z) \rightarrow (x,y,-z) + \mathbf{a}_1/2,$$



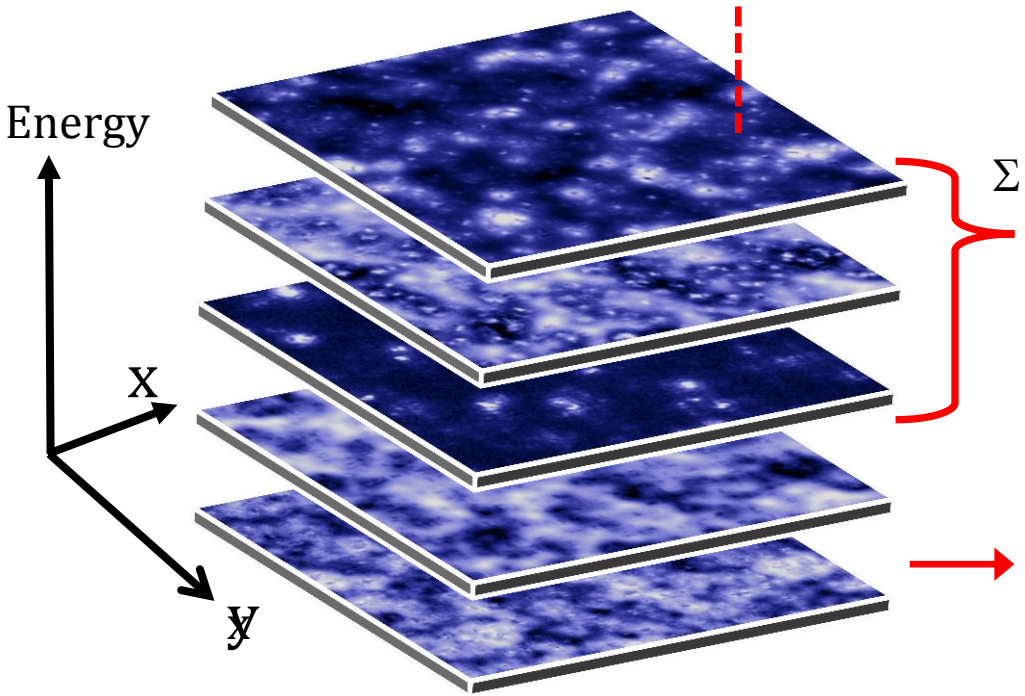
Butterfly MR (Anisotropic)

Possible application!

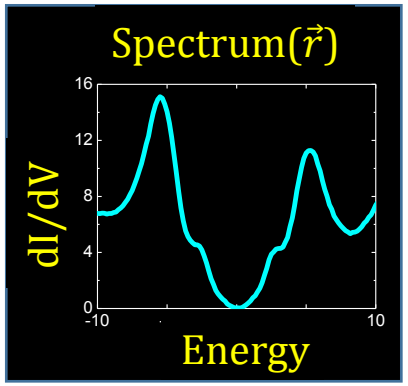
Ali, Mazhar N., et al. *Science advances* 2.12 (2016): e1601742.

Scanning Tunneling Microscope (STM)

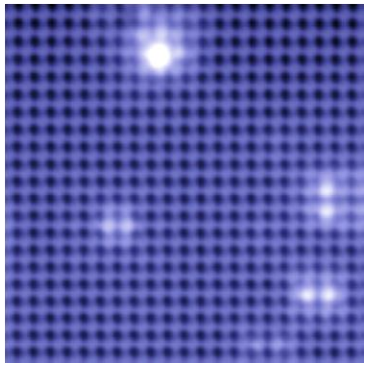
$$\frac{dI}{dV}(\vec{r},V) \propto LDOS(\vec{r},E)$$



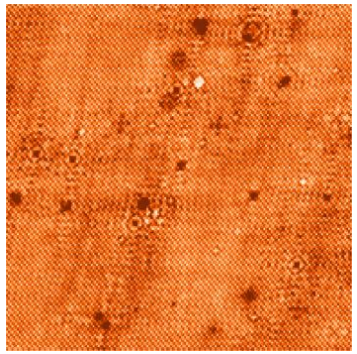
Σ



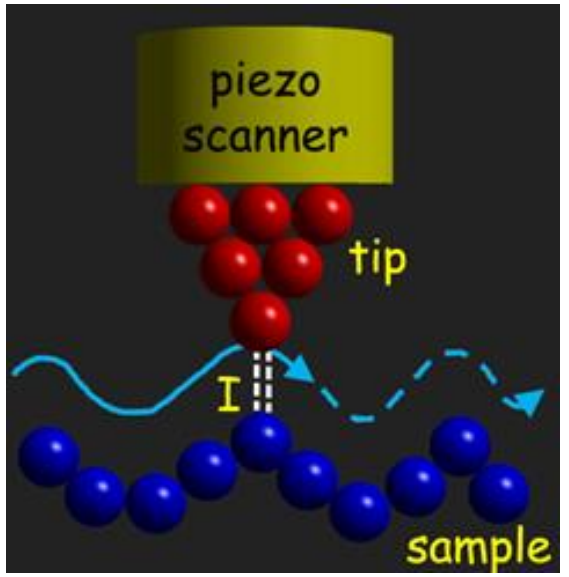
Topography(E)



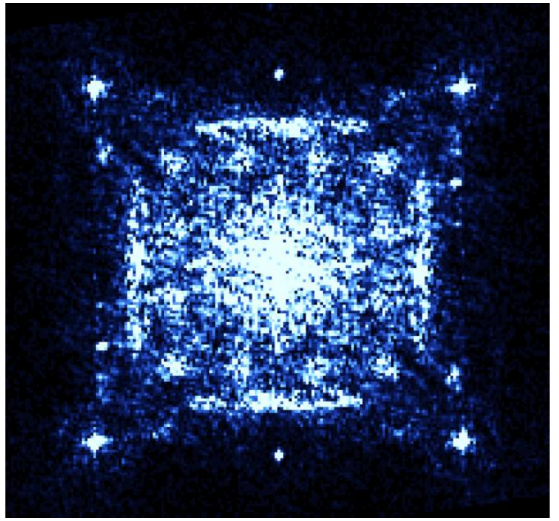
$LDOS(\vec{r},E)$



FFT



$LDOS(\vec{q},E)$

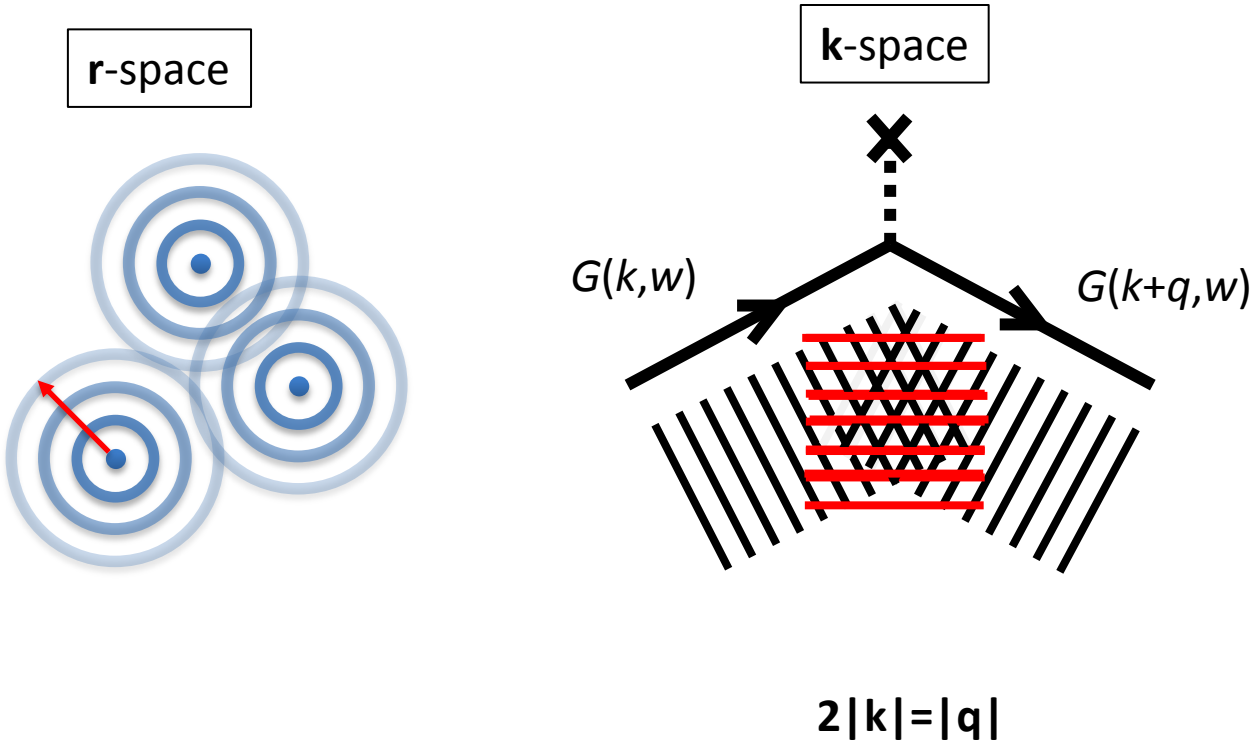


Quasiparticle Interference (QPI)

When scatters are introduced,

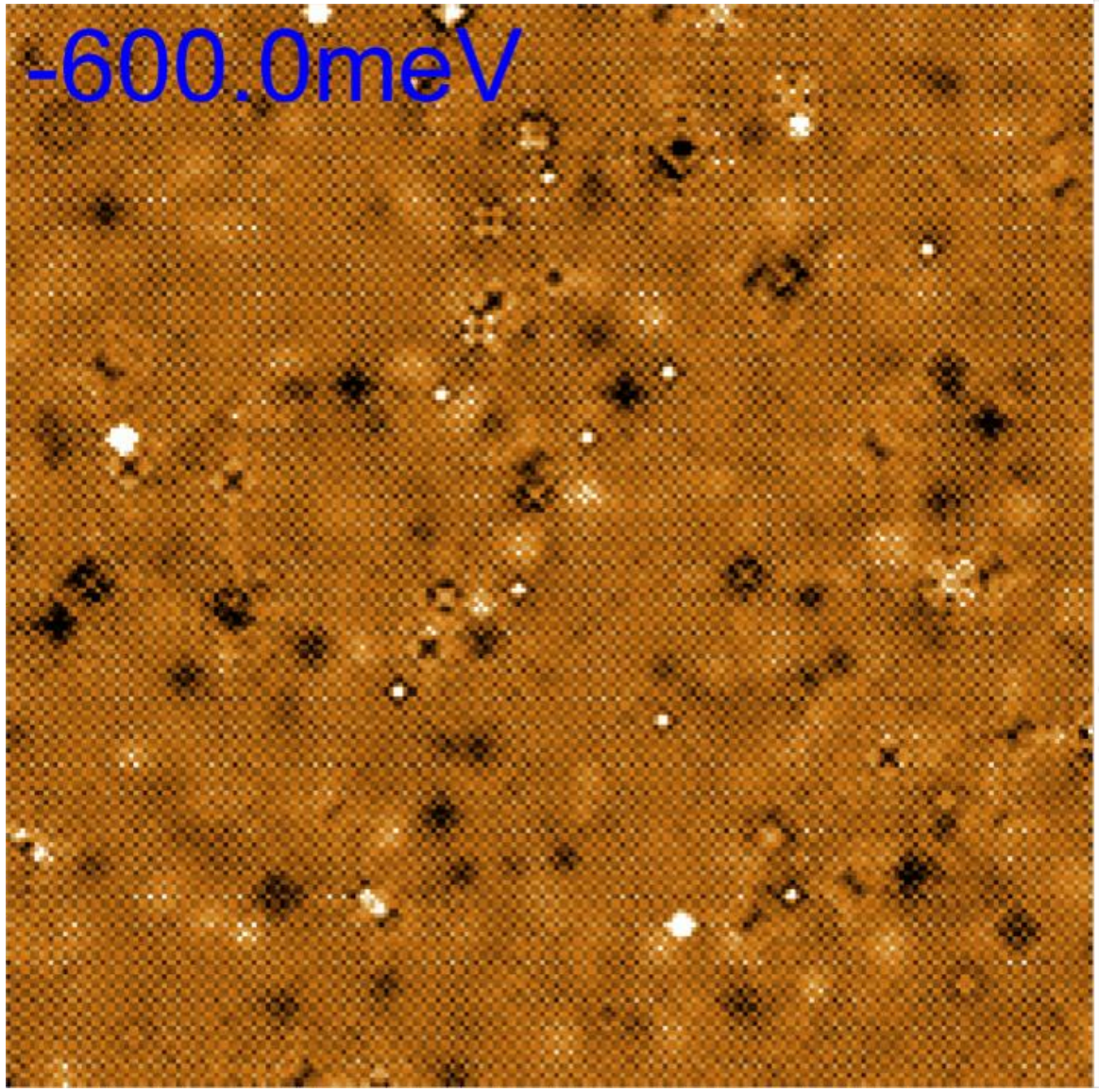
- The impurity breaks the translational invariance of the electronic liquid

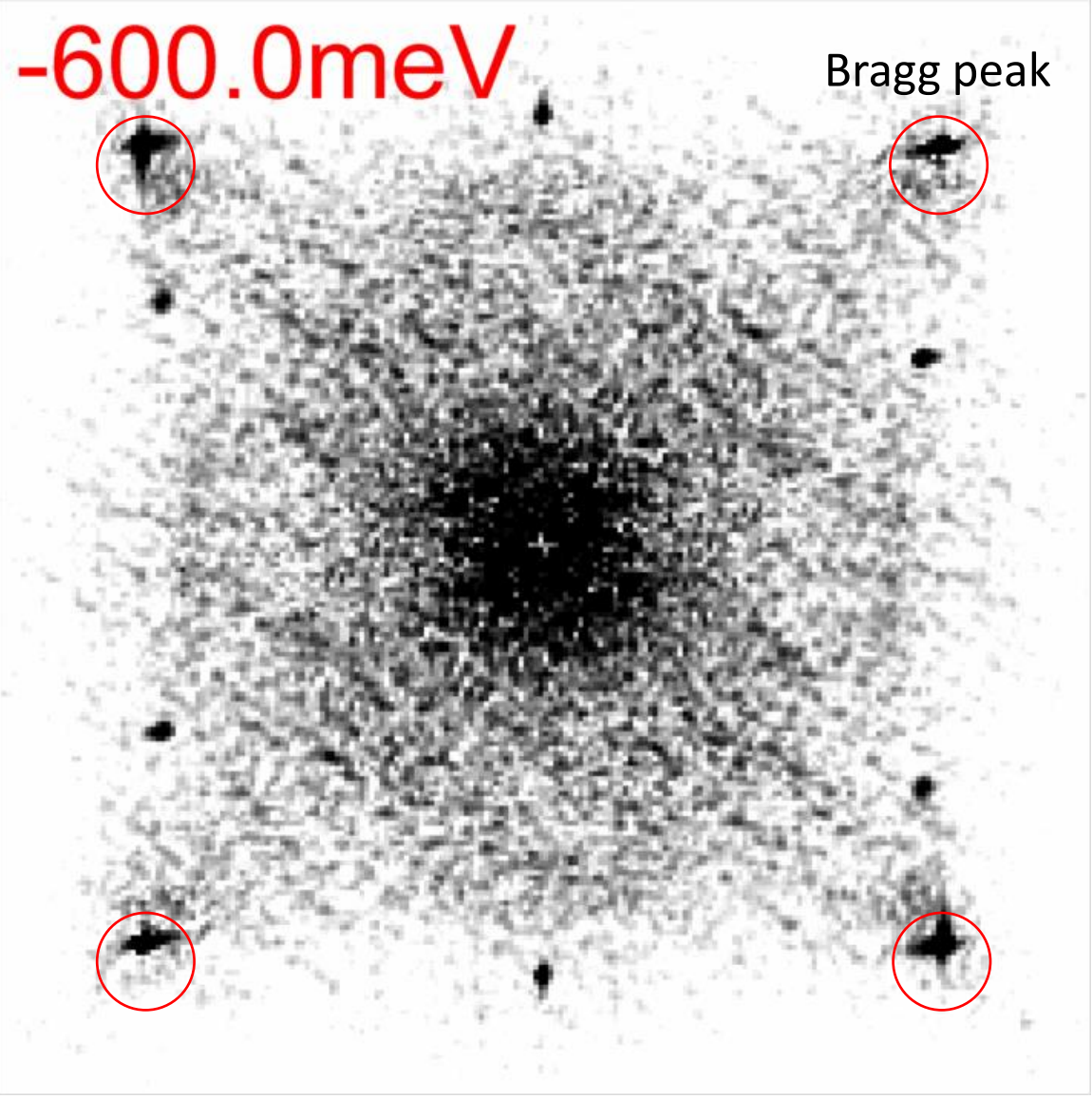
- This allows in first order for mixing of different momentum states.



Q.-H. Wang and D.-H. Lee, PRB 67, 020511 (2003)

Quasiparticle Interference (QPI)





36X36nm

T=4K

First Principle study on ZrGeTe

Calculation Details

- The electronic band structure is carried within the **Density Functional Theory (DFT)** with **PAW_PBE potential** as exchange-correlation.

- Vienna Ab-initio Simulation Package (VASP) (WIEN2k/QuantumEspresso for double check)

Bulk calculation (w/wo SOC)	**9-Layer Slab calculation (w SOC) (20Å vaccum layer)**
ENCUT = 400 eV	ENCUT = 400 eV
25 x 25 x 25 Monkhorst-Pack k-mesh	40 x 40 x 1 Monkhorst-Pack k-mesh
Zr_sV/Ge_d/Te	Zr_sV/Ge_d/Te

POTCAR (PAW_PBE)	NELECT	VRHFIN
Zr	4	5s4d5p
Zr_sV	12	4s4p5s4d
Te	6	s2p4
Ge	4	s2p2
Ge_d	14	3d4s49

[1] J. P. Perdew, K. Burke, and M. Ernzerhof. Phys. Rev. Lett. 77, 3865 (1997)
[2] G. Kresse and D. Joubert. augmented-wave method. Phys. Rev. B 59, 1758 (1999)

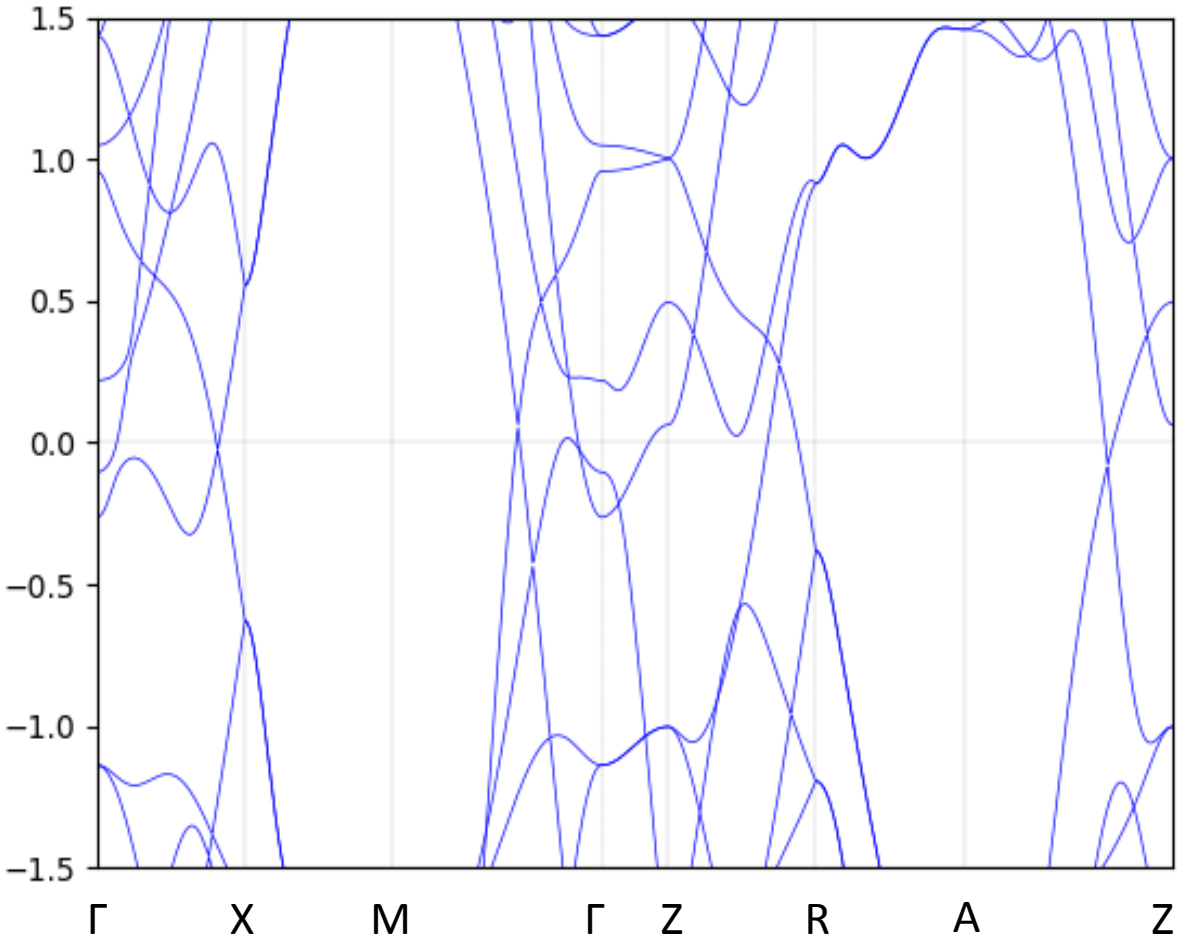
Bulk Band structure

Dirac nodal-line

Dirac crossing protected by crystalline symmetry (Glide mirror symmetry)

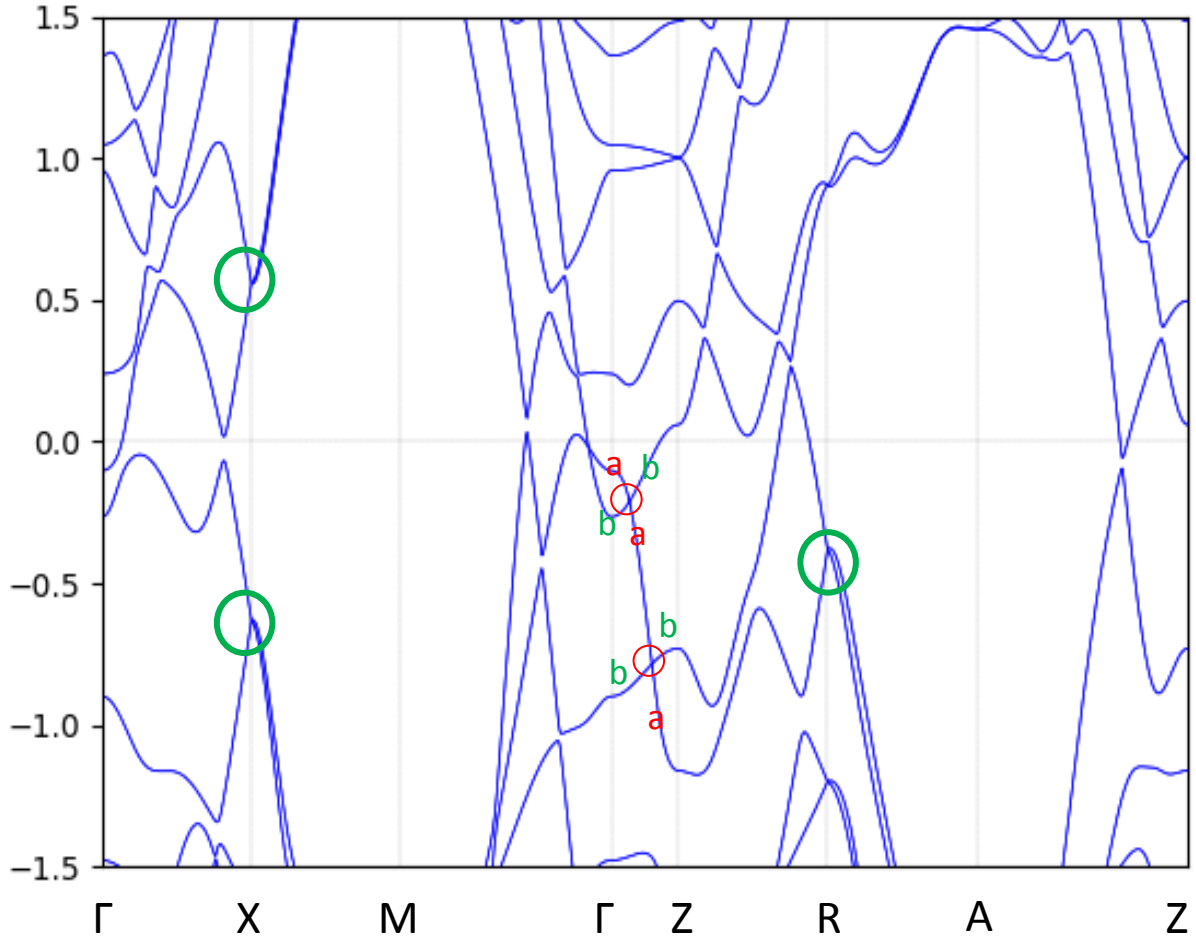
Crossing by band inversion

wo SOC



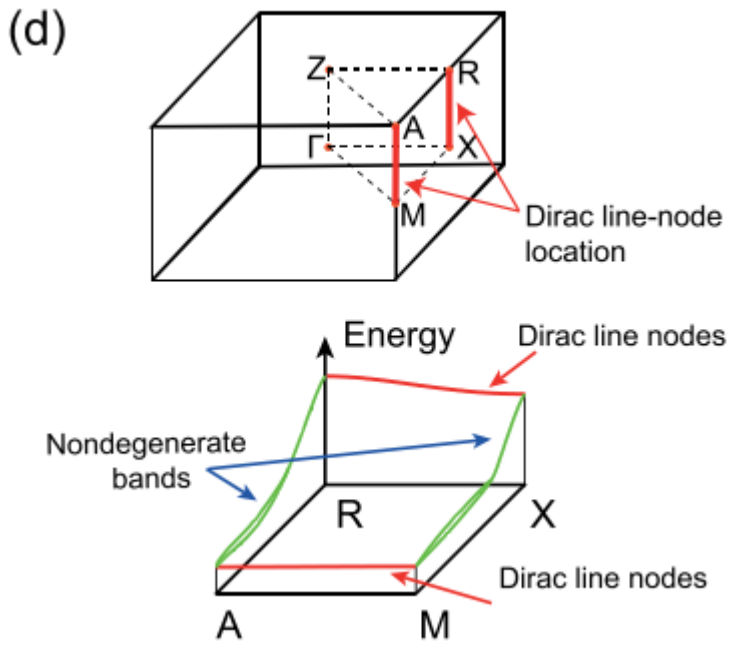
w SOC

a. Γ_6 , M_6 b. Γ_7 , D_7

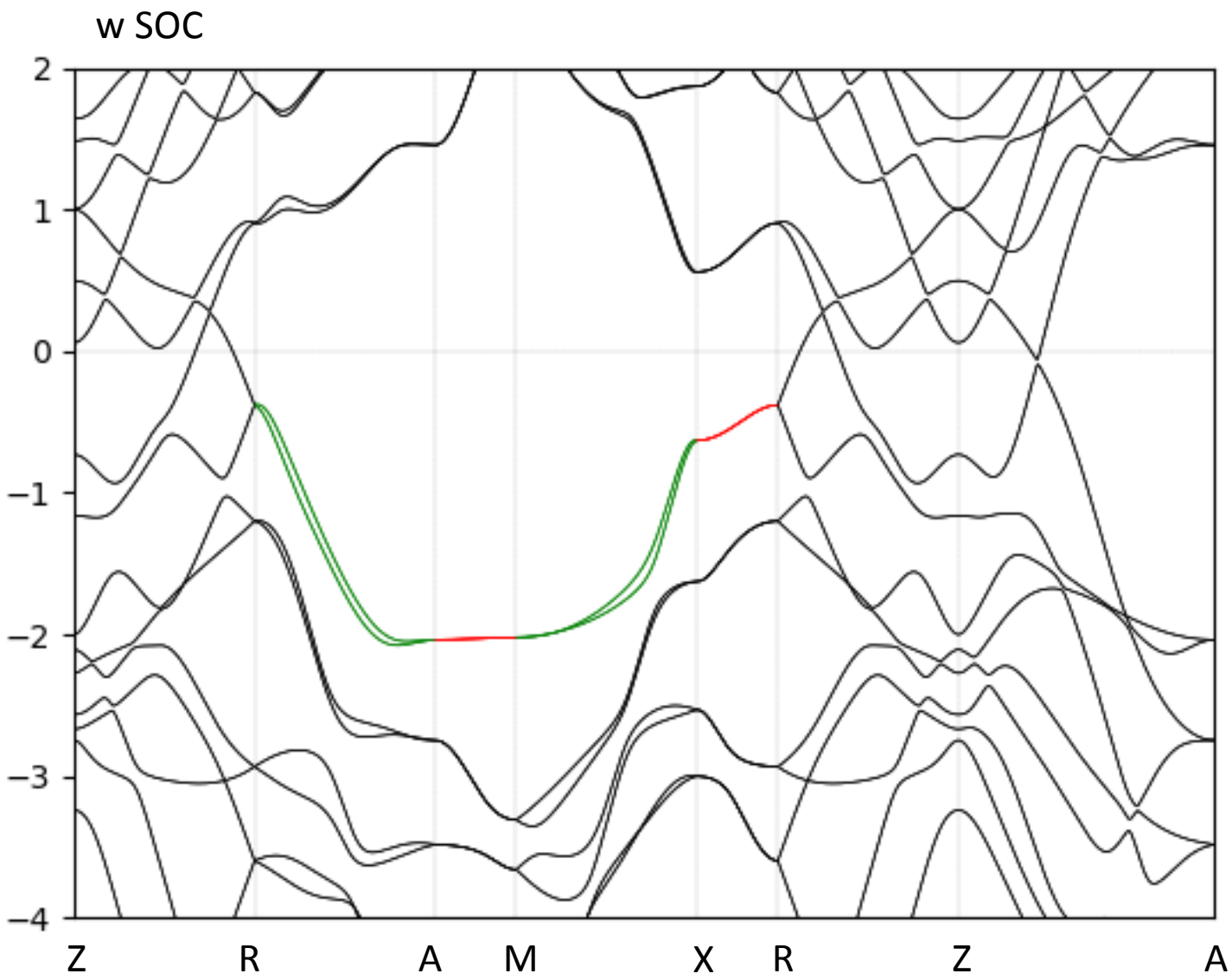


Dirac line-node

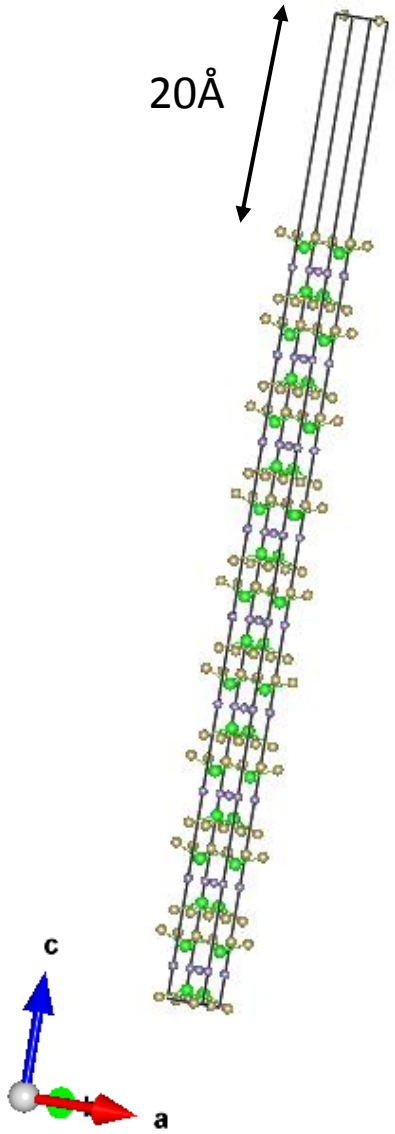
HfSiS/ZrSiS…

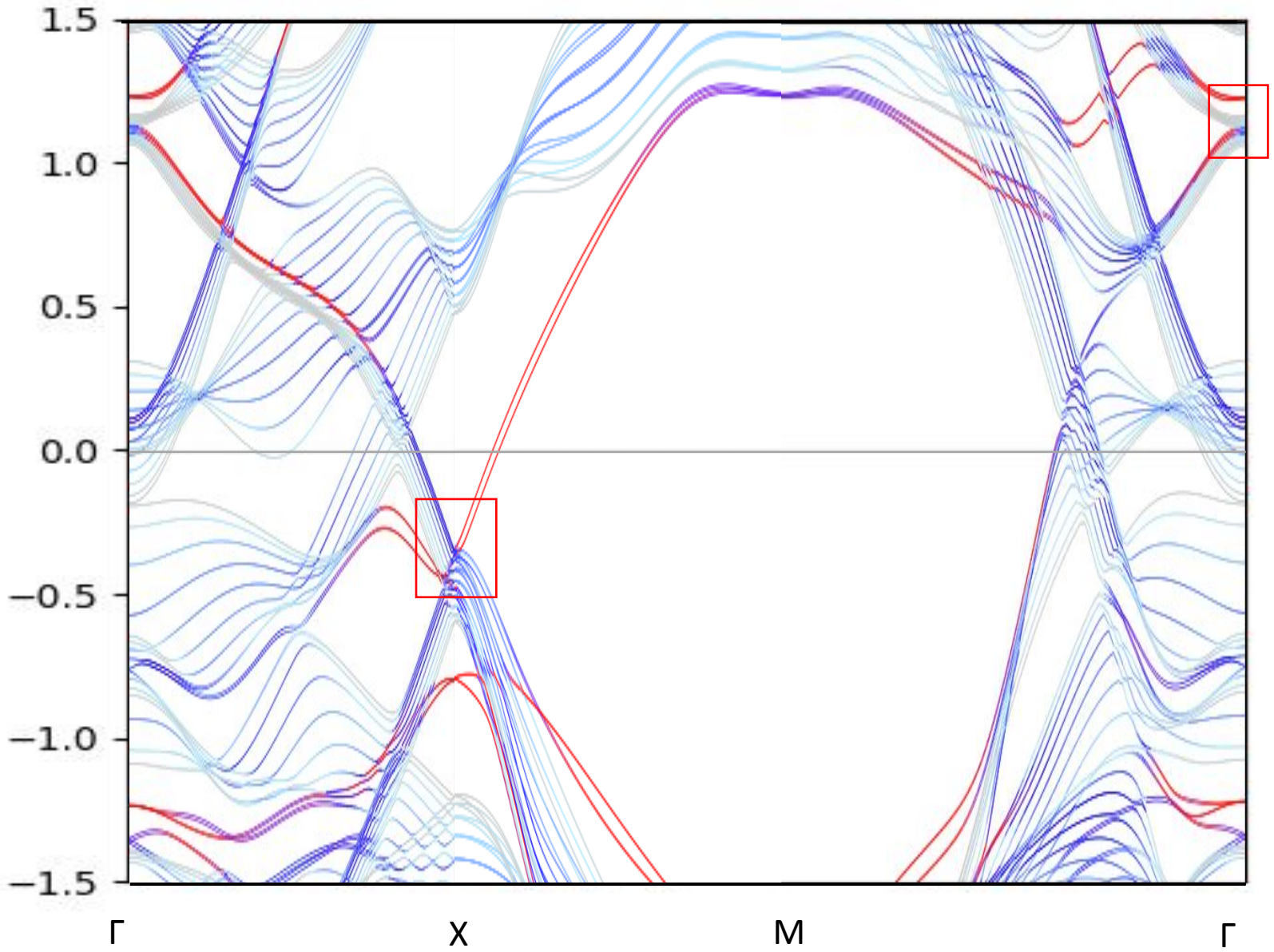


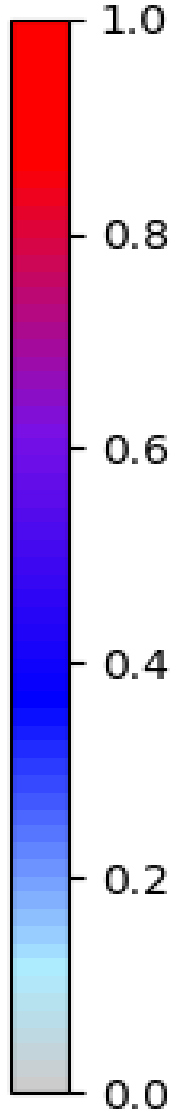
Chen, Cheng, et al. *Physical Review B* 95.12 (2017): 125126.



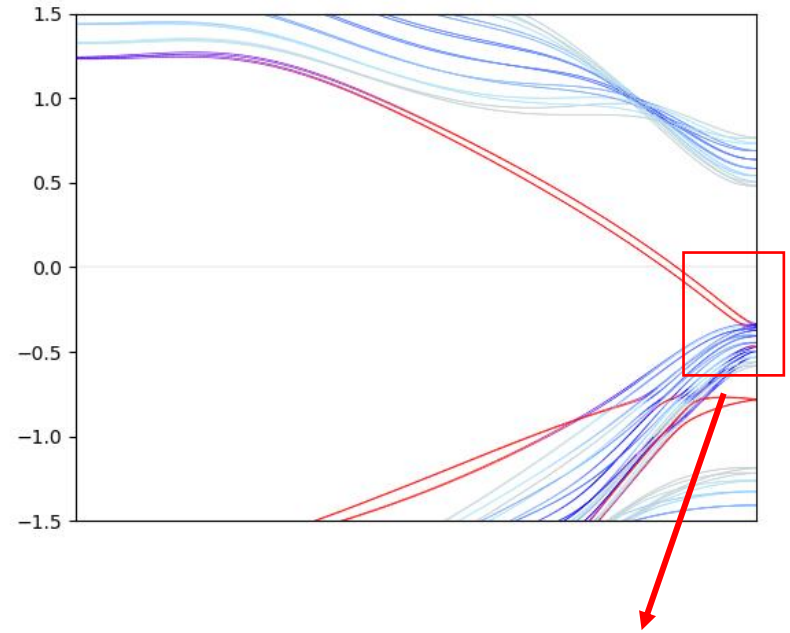
9-Layer slab band structure

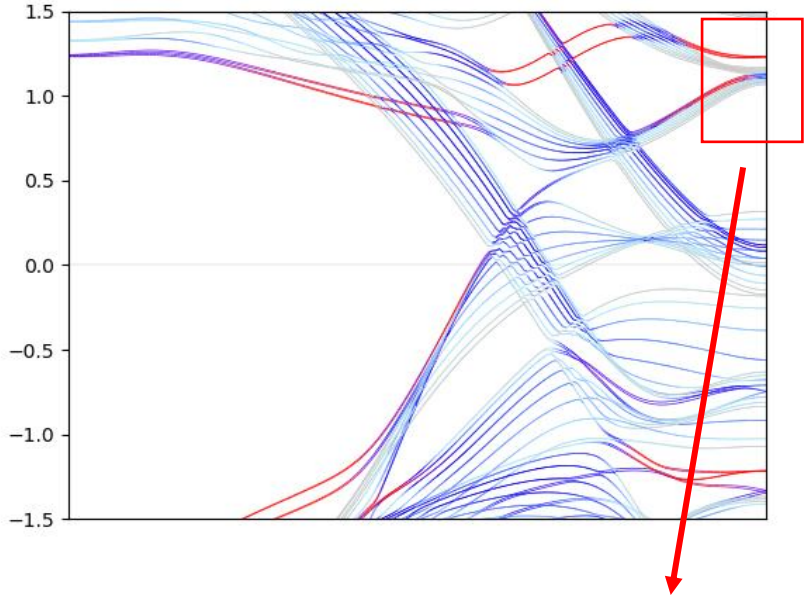


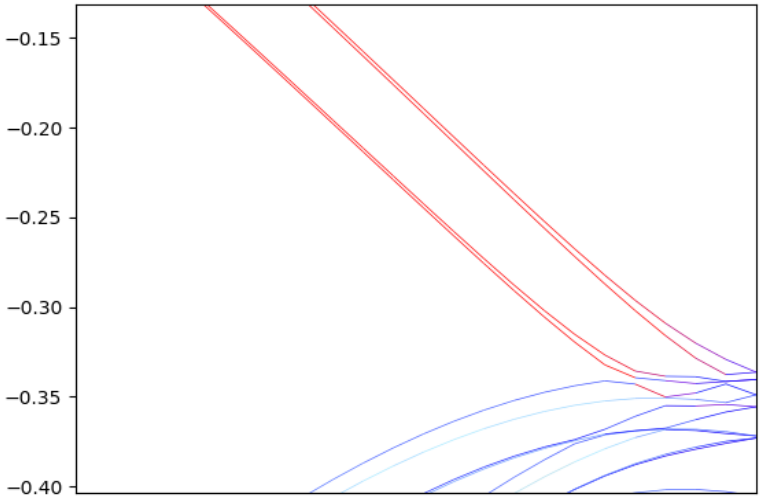


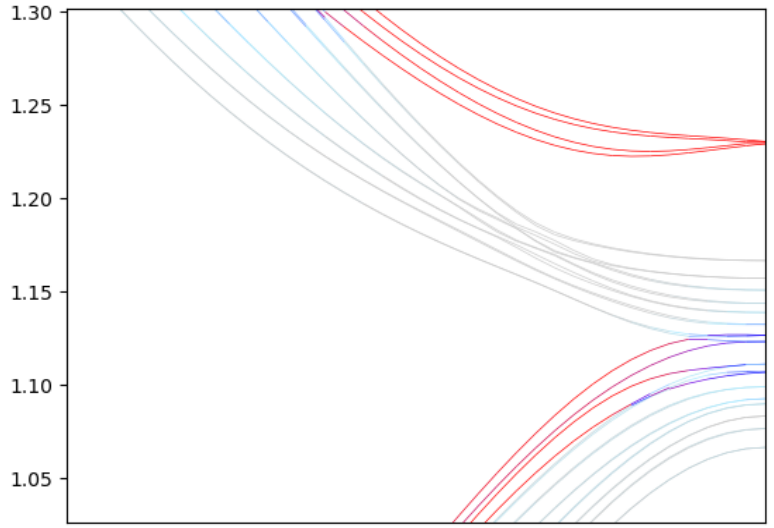


Gapless between **Surface state** and **Bulk-projection state** !

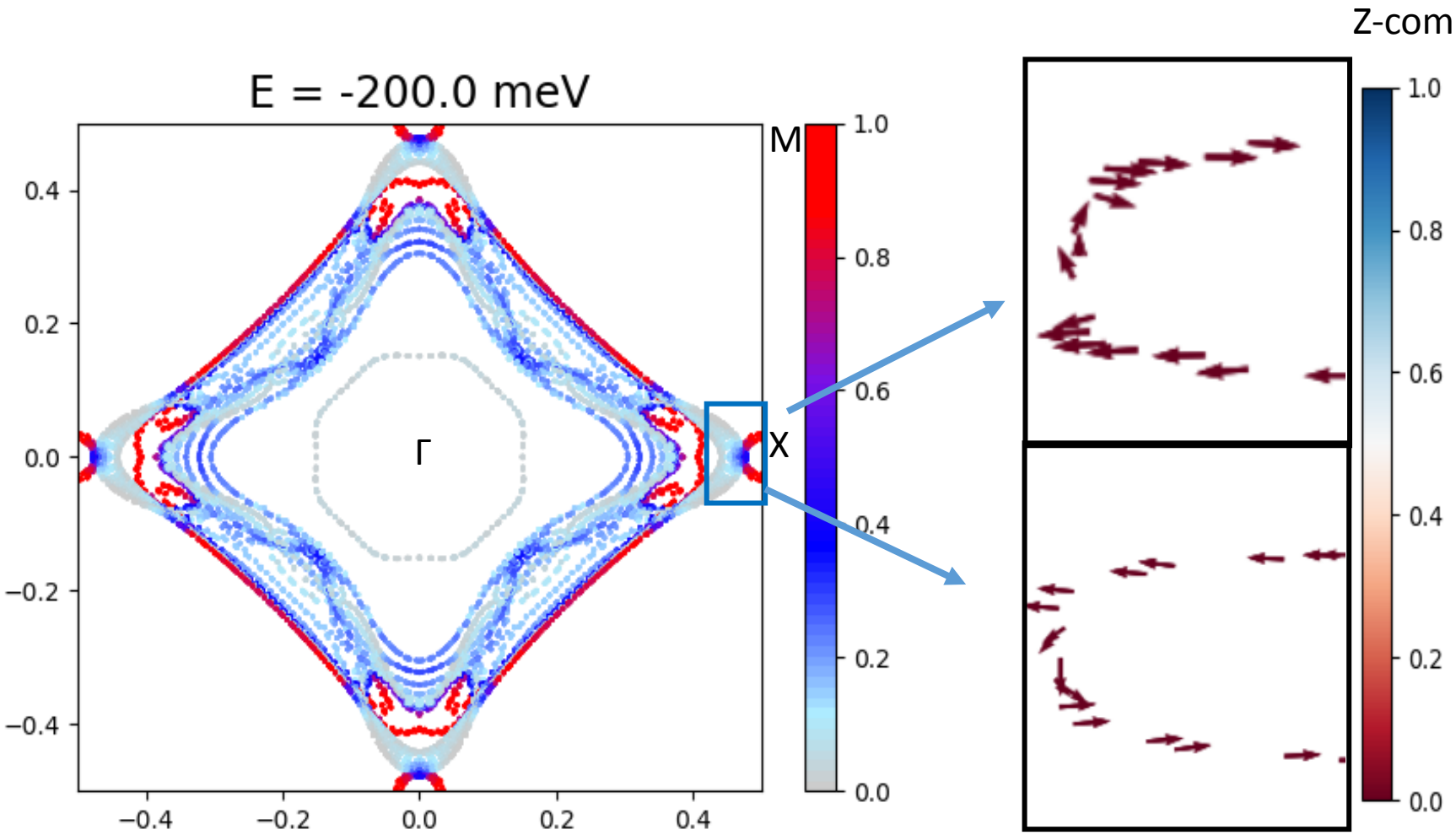


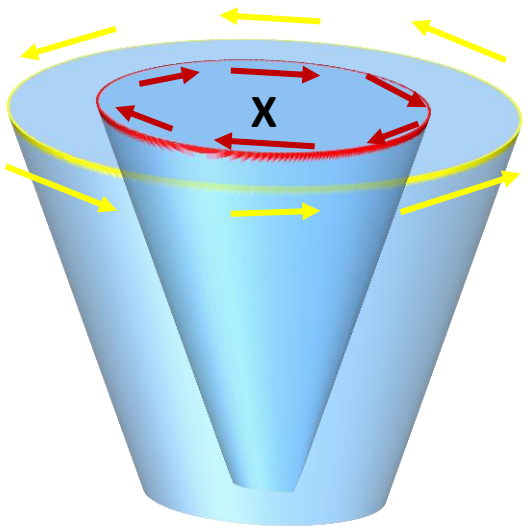






Rashba-splitting helical spin-texture surface state

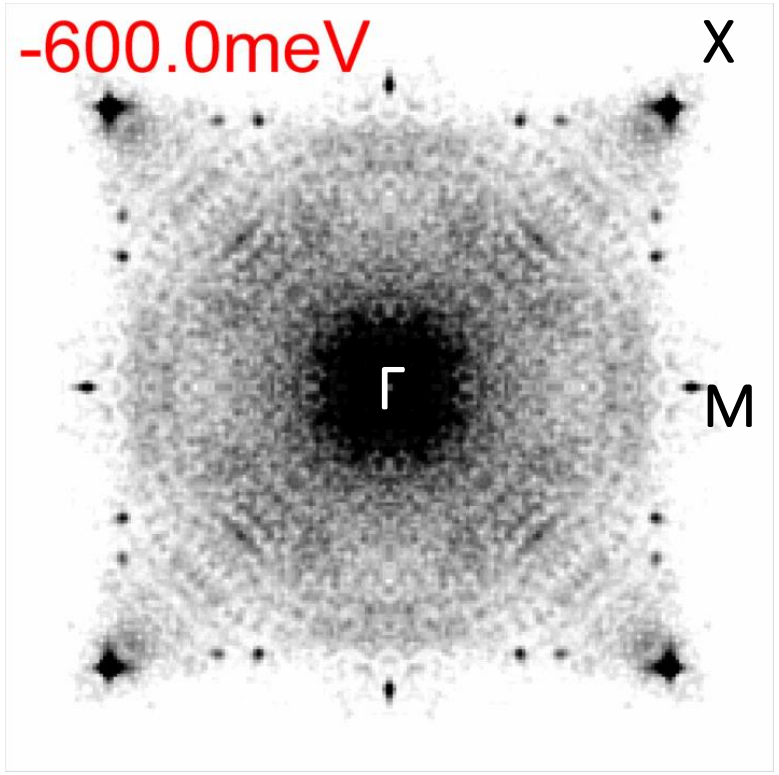


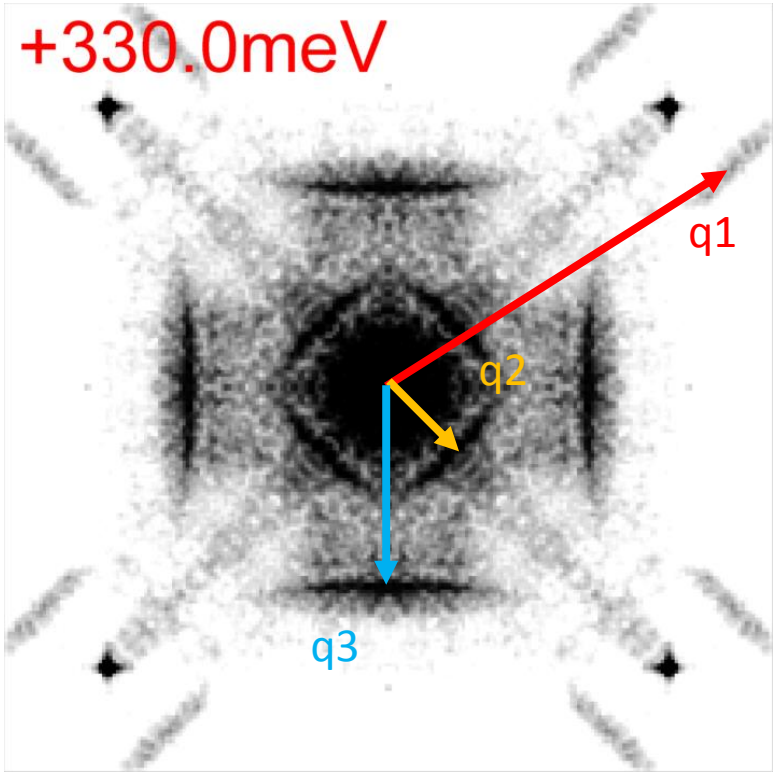


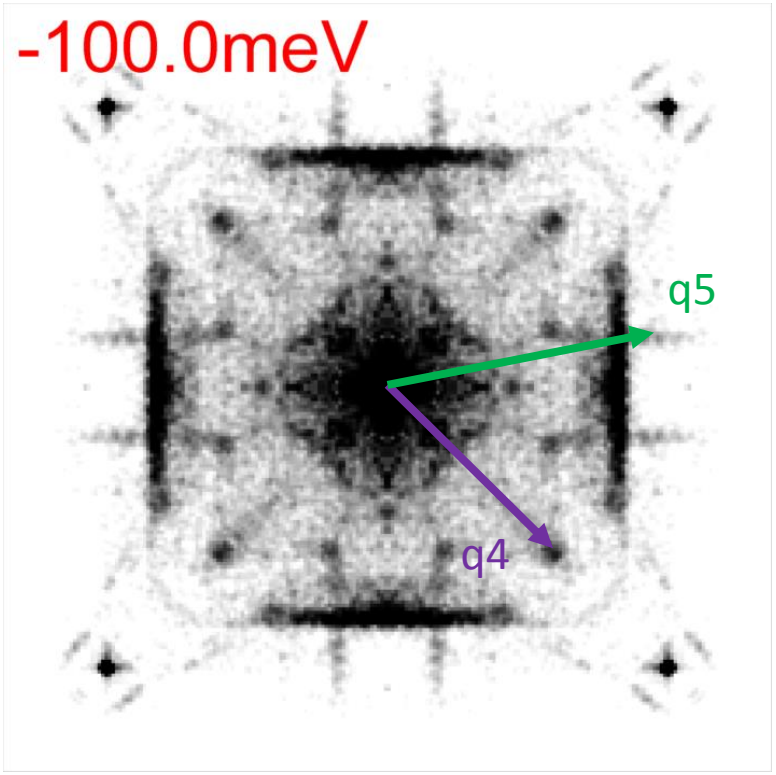
In-Plane Spin texture!

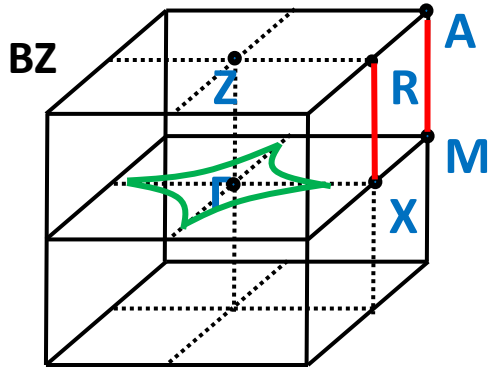
Constant Energy Contour (CEC) & QPI fitting

QPI q-vectors





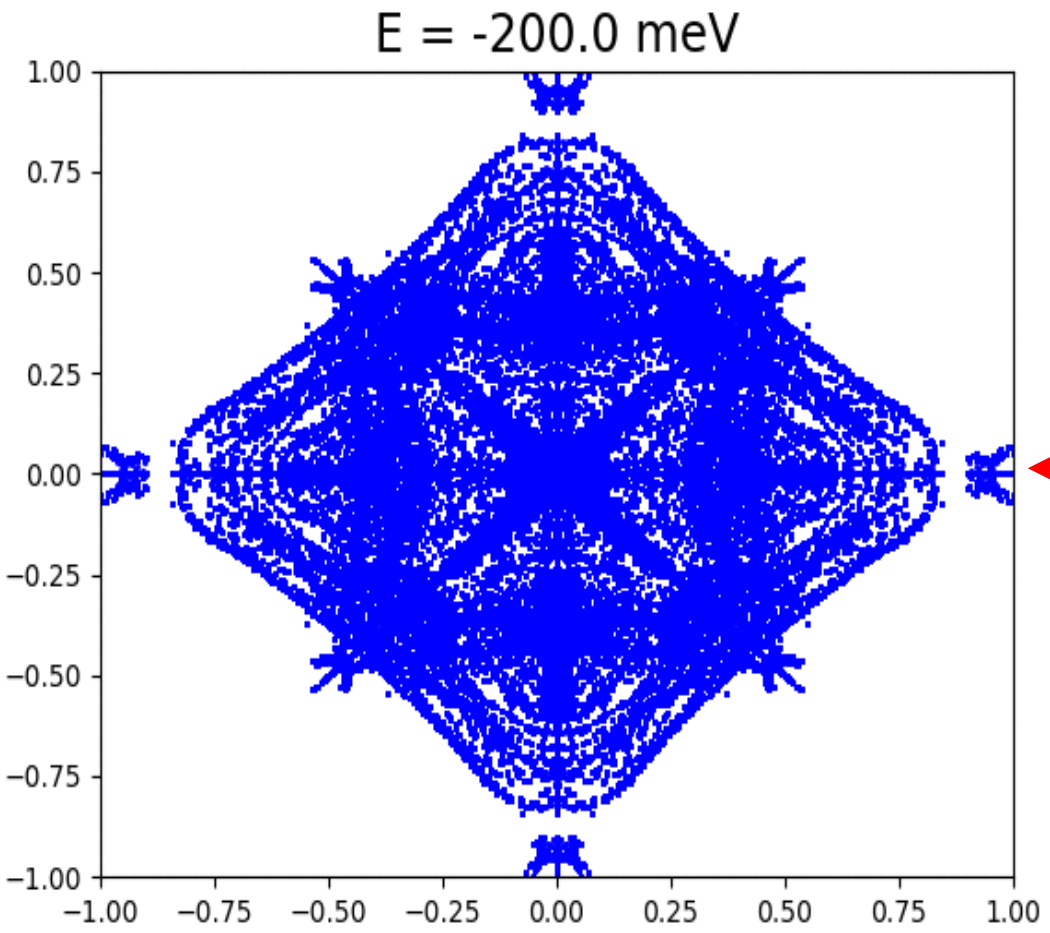


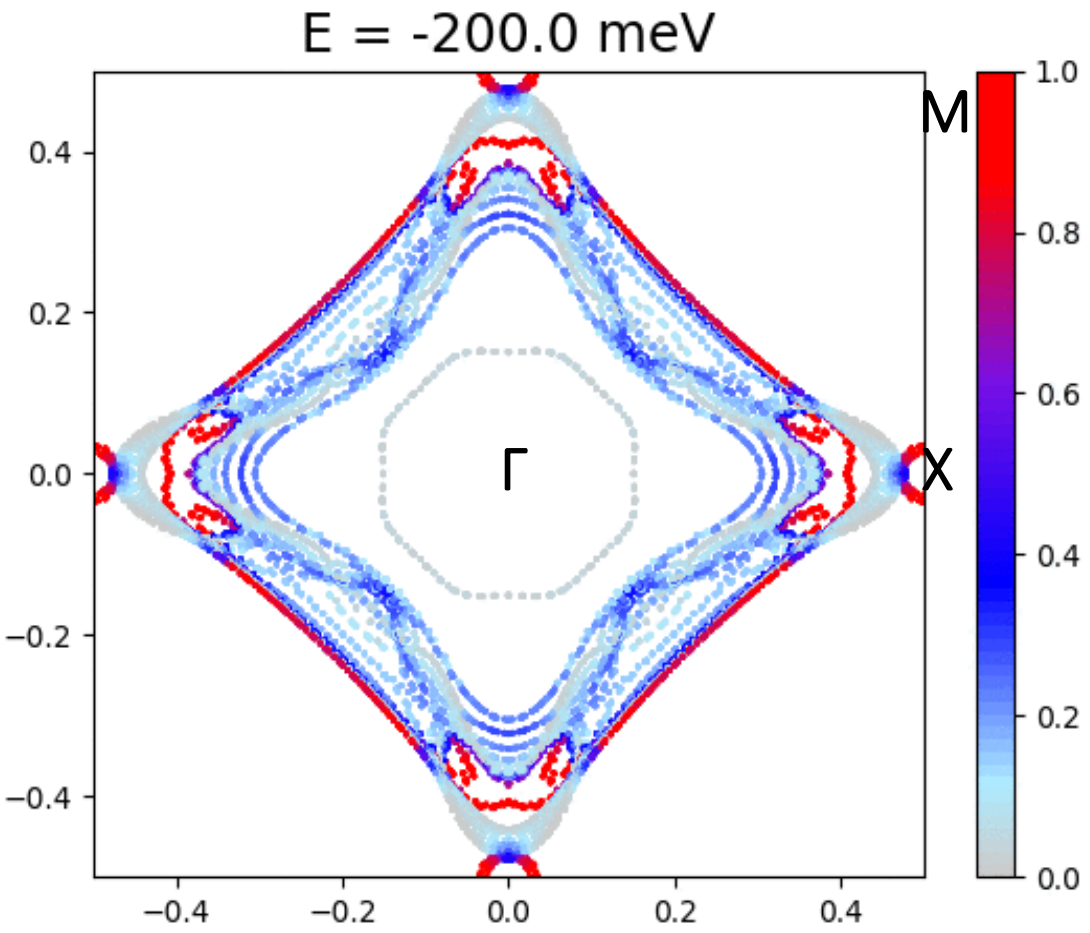


All q-vectors can be identified with JDOS calculation

P.S. After some energy shift:

STM energy = DFT energy + 50 meV

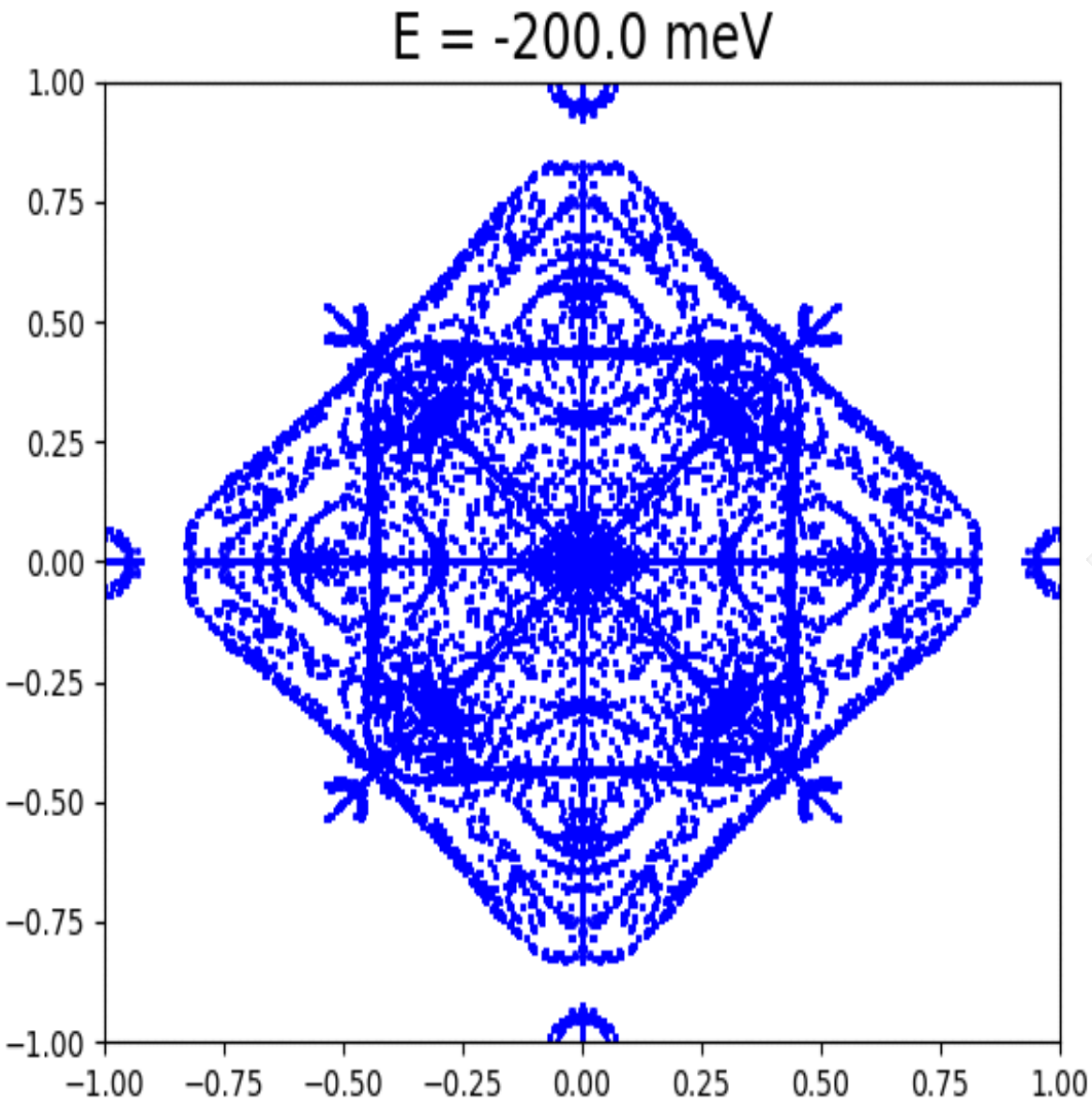




Joint Density of States
(JDOS)
(NO Umklapp scattering)

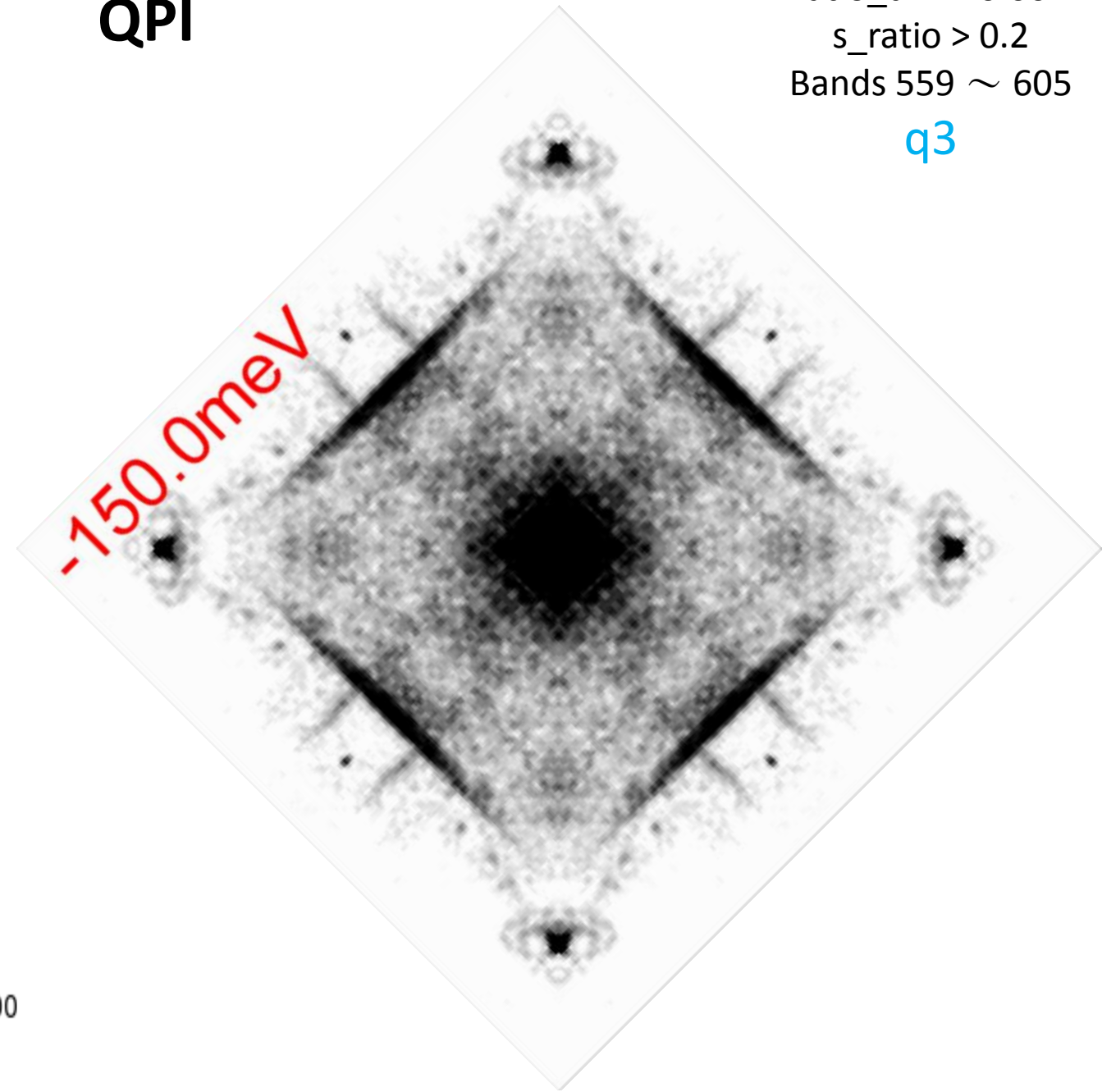
Constant Energy Contour (CEC)
60 x 60 k-mesh with interpolation

JDOS



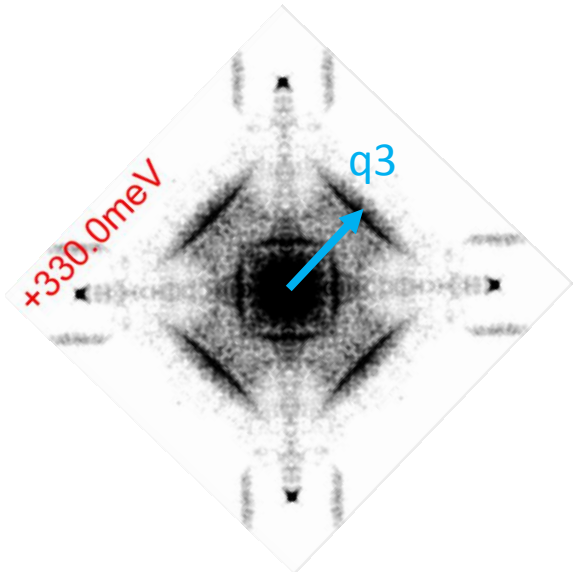
QPI

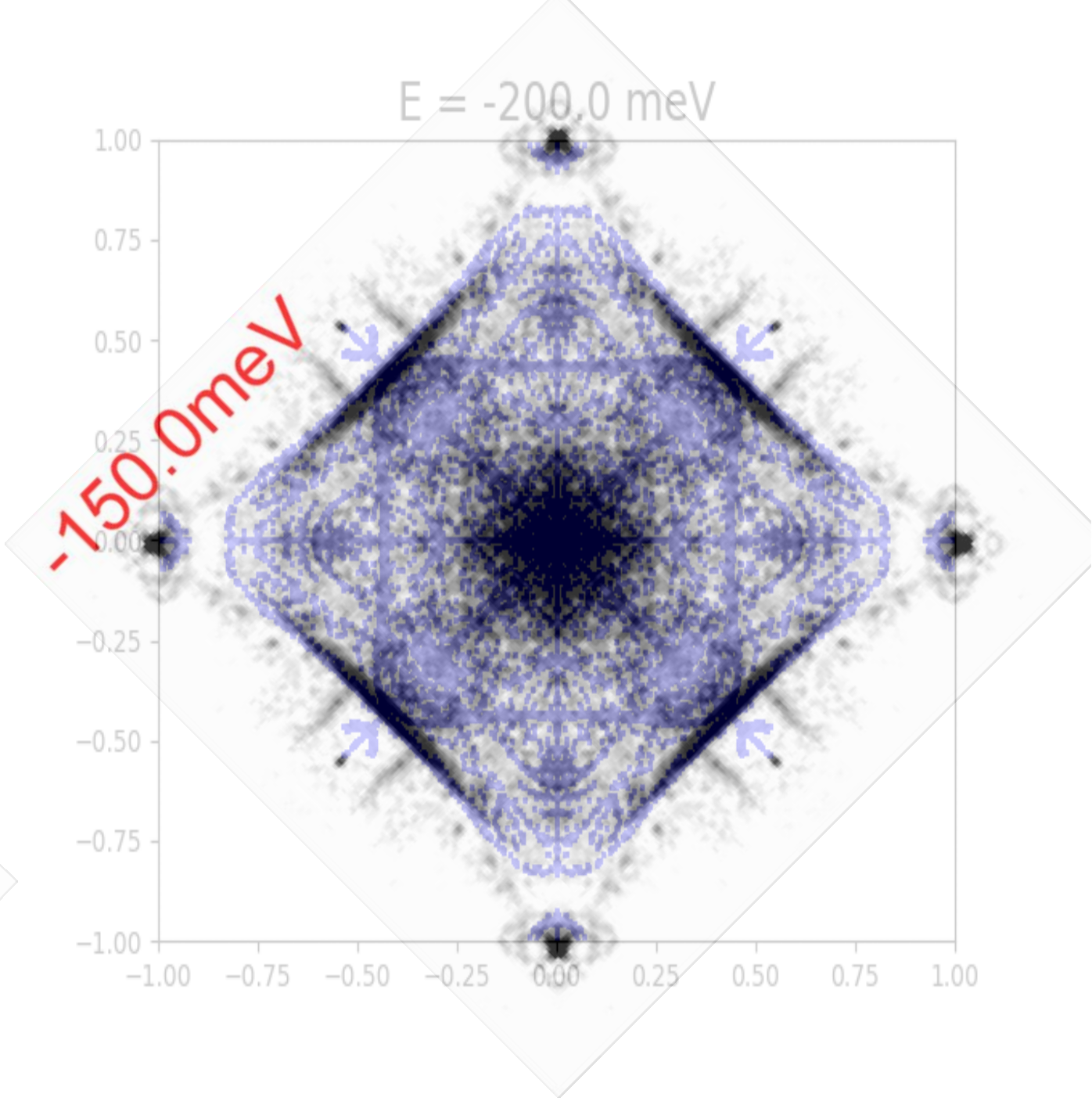
ratio_diff < 0.001
s_ratio > 0.2
Bands 559 ∼ 605
q3

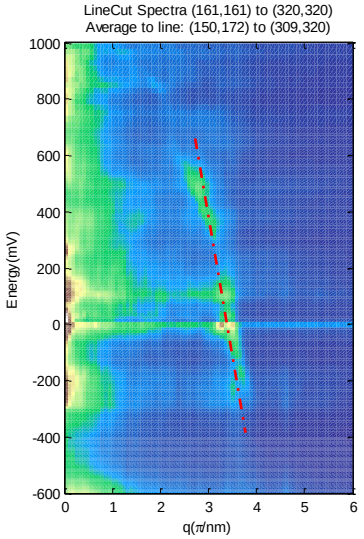


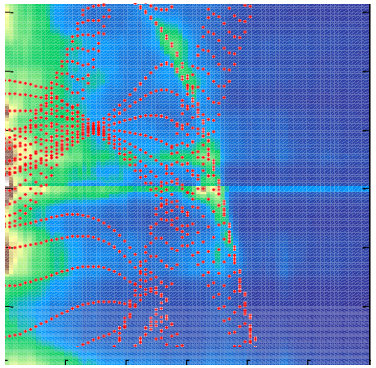
ratio_diff < 0.001
s_ratio > 0.2
Bands 559 ～ 605

q3



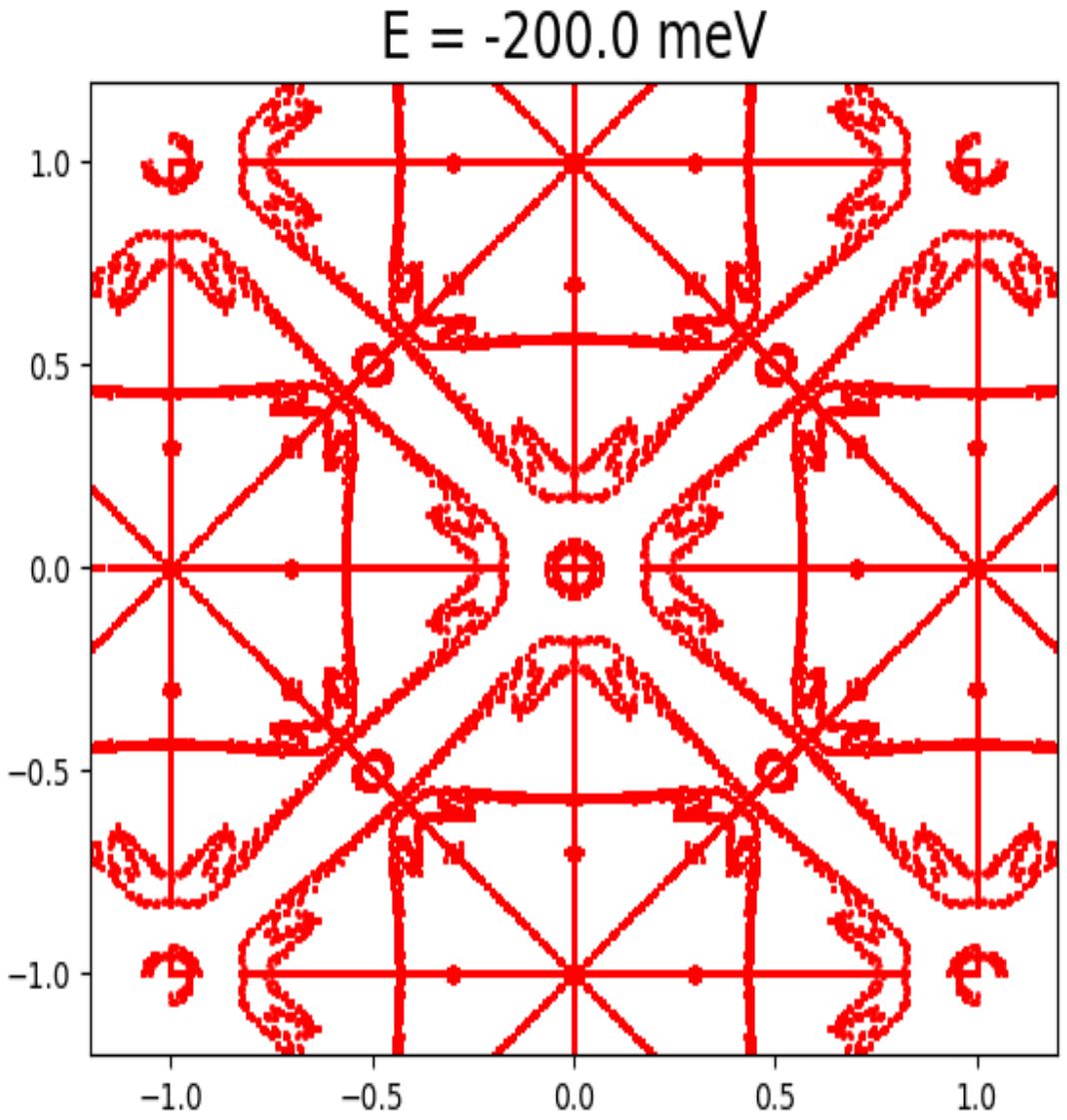






DFT calculation

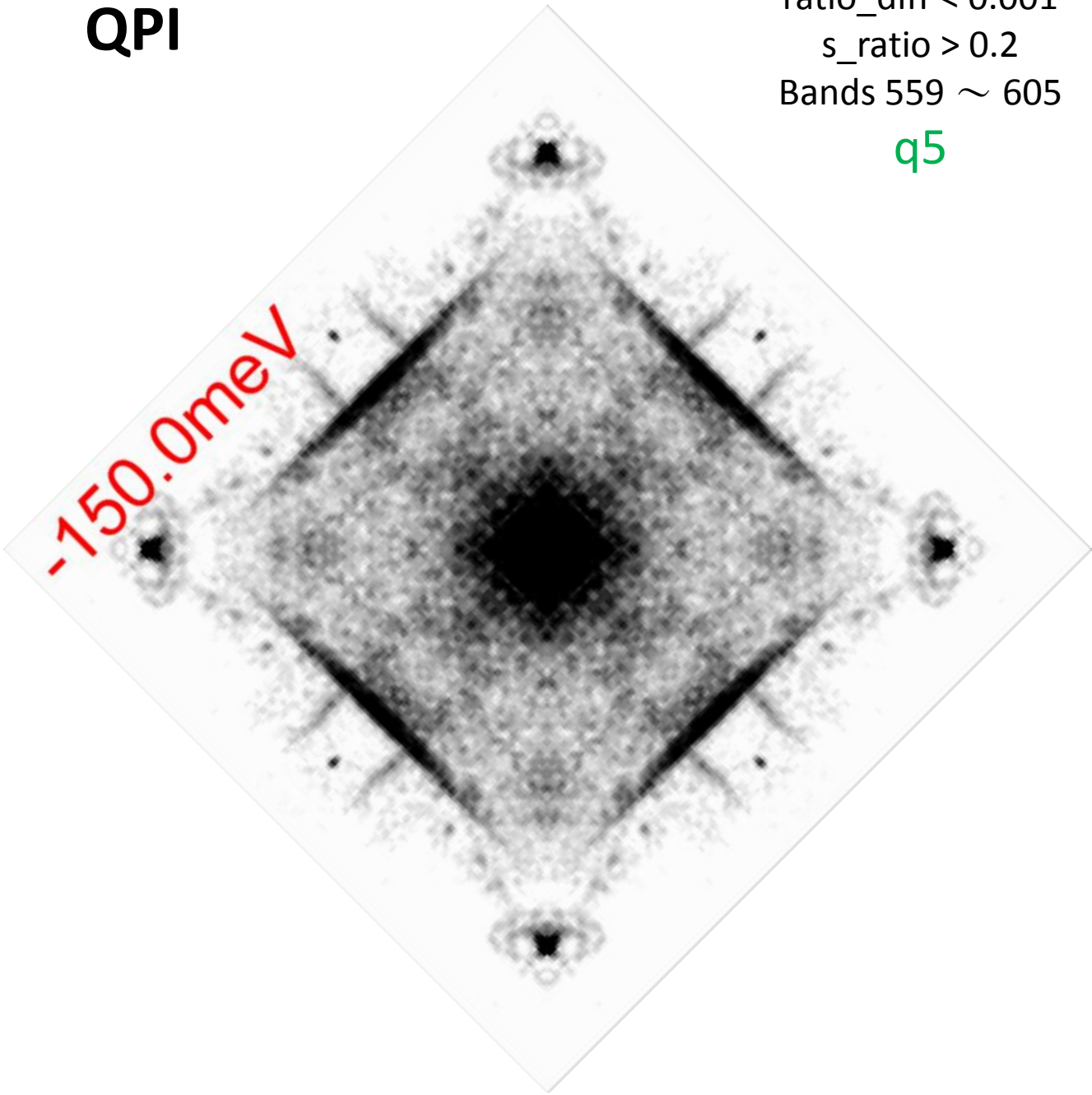
JDOS



QPI

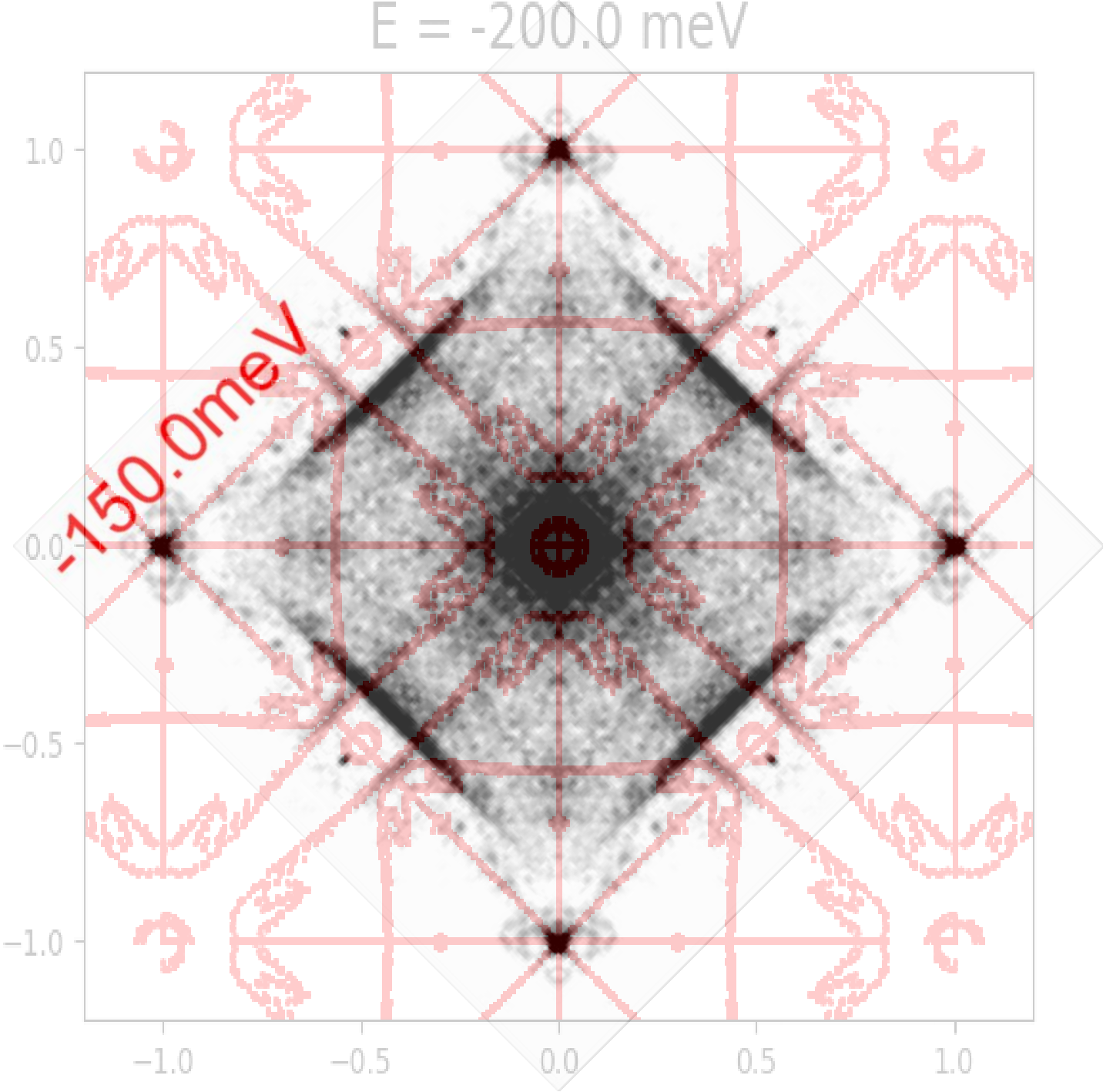
ratio_diff < 0.001
s_ratio > 0.2
Bands 559 ～ 605

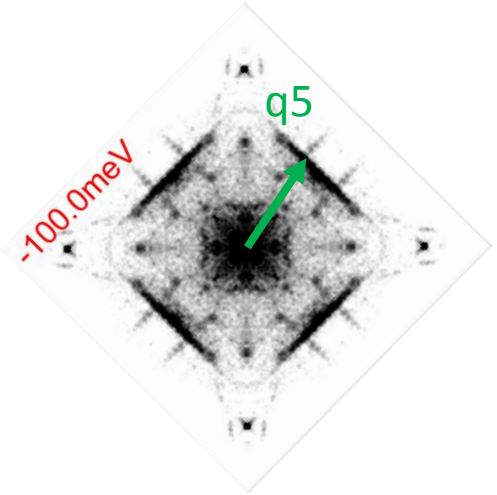
q5



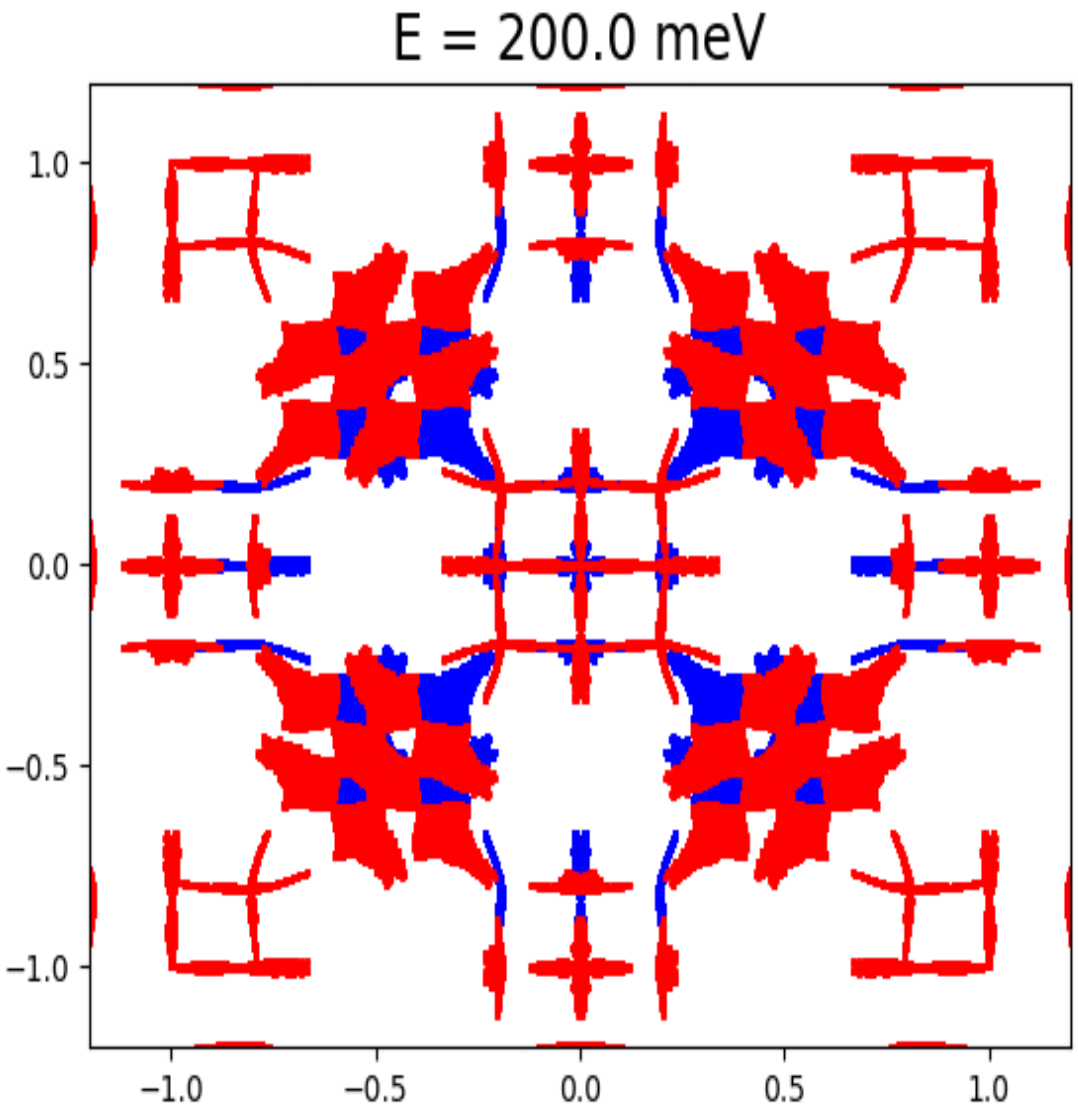
ratio_diff < 0.001
s_ratio > 0.2
Bands 559 ∼ 605
q5

NOT SEEN BEFORE
In other system!



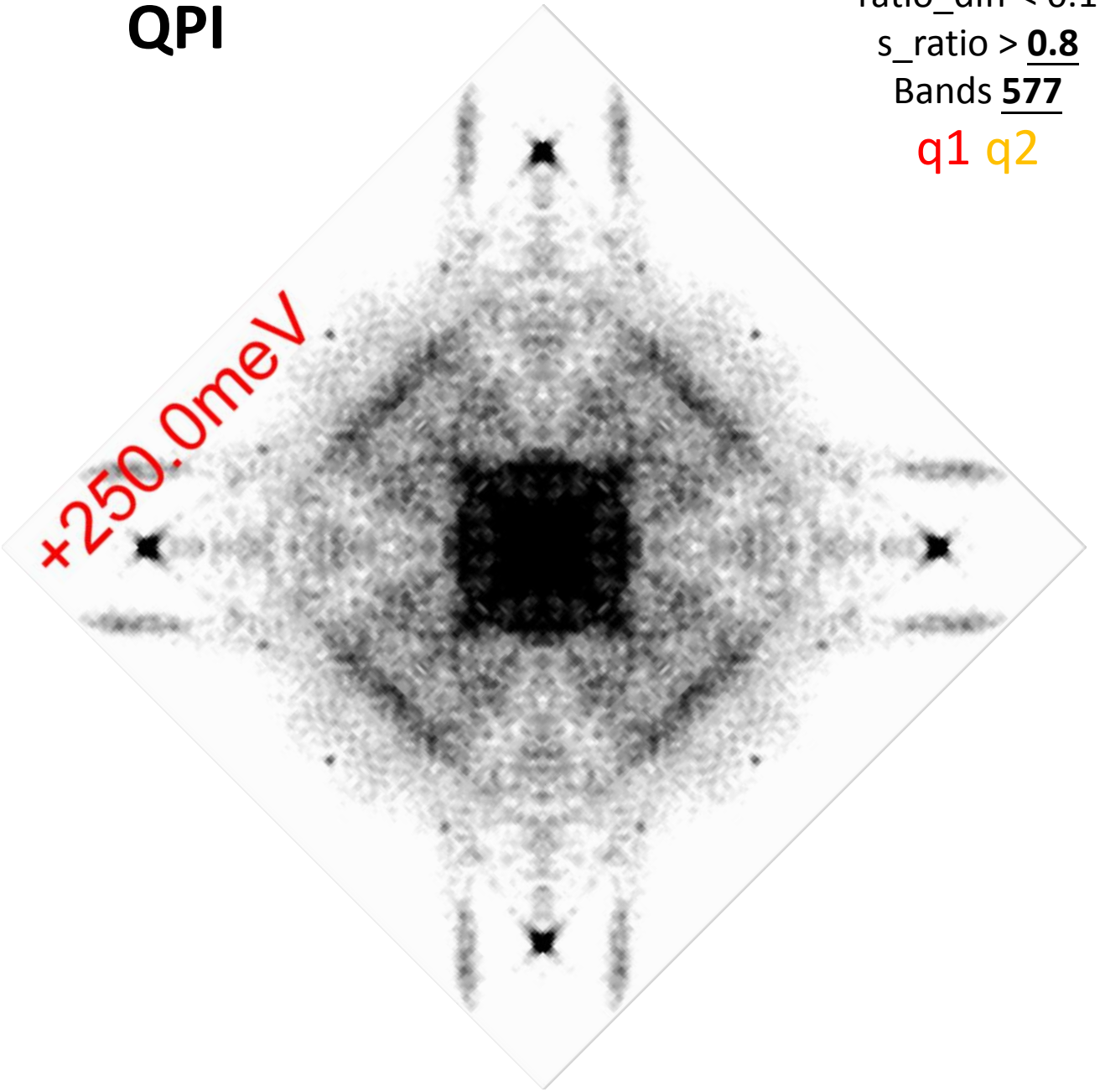


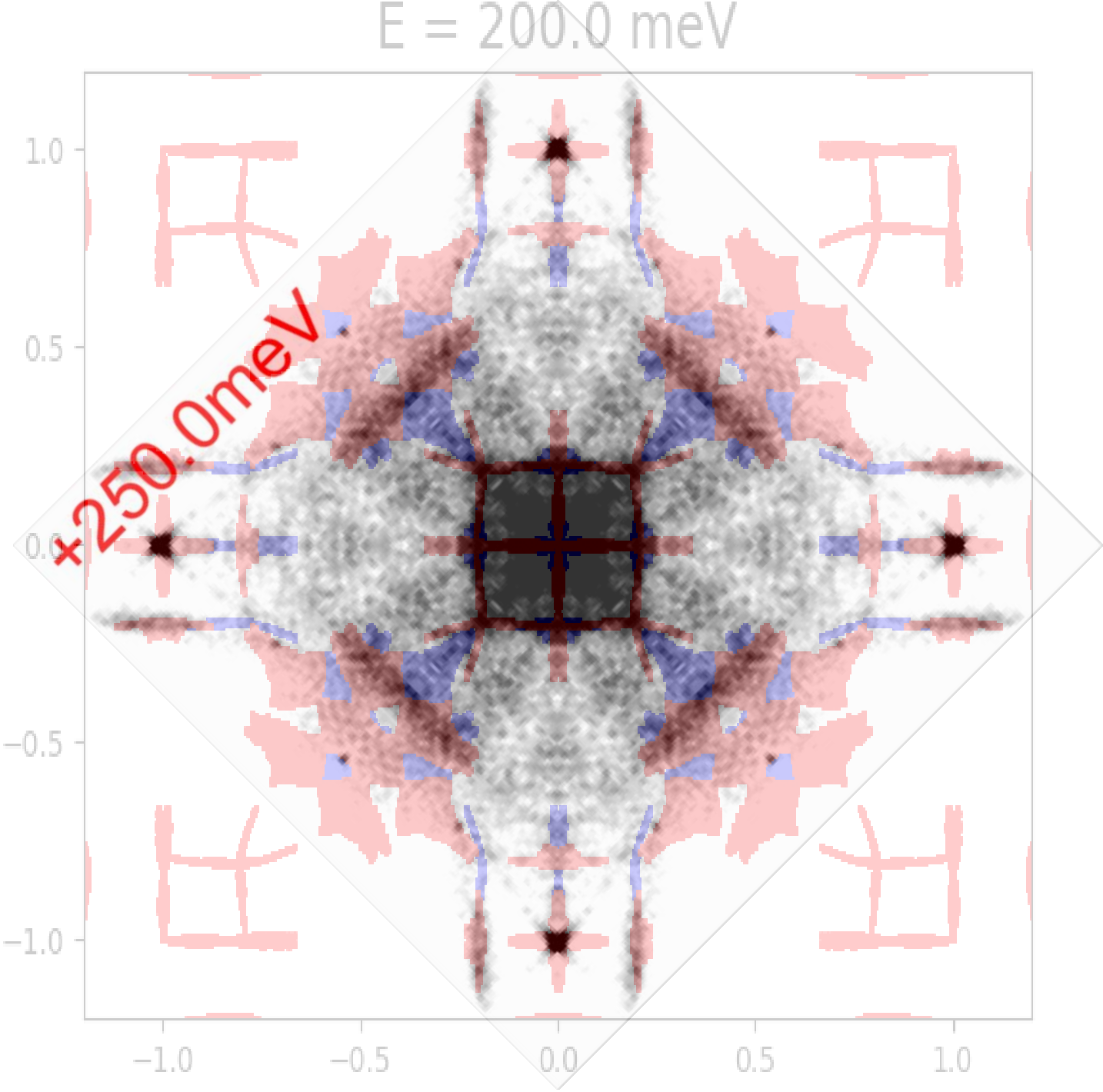
JDOS

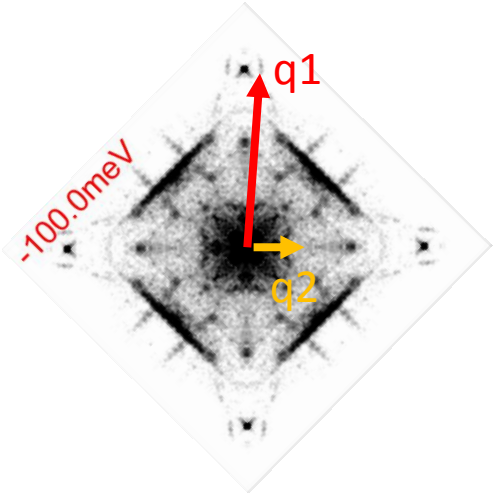


QPI

ratio_diff < 0.1
s_ratio > **0.8**
Bands **577**
q1 q2







ratio_diff < 0.1

s_ratio > **0.8**

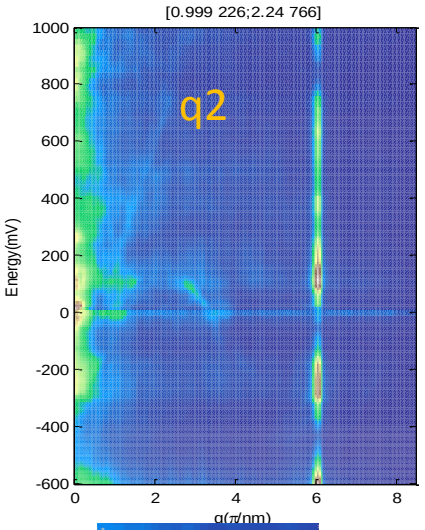
Bands **577**

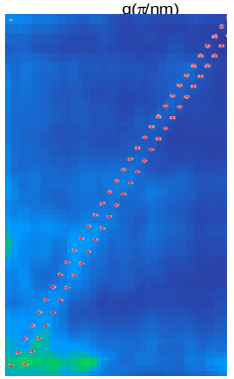
q1 q2

Red (Umklapp)

Blue

QPI line-cut





DFT calculation

q1 ⟶

Umklapp scattering of q2.

q2 ⟶

scattering between X-point surface states.

q3 ⟶

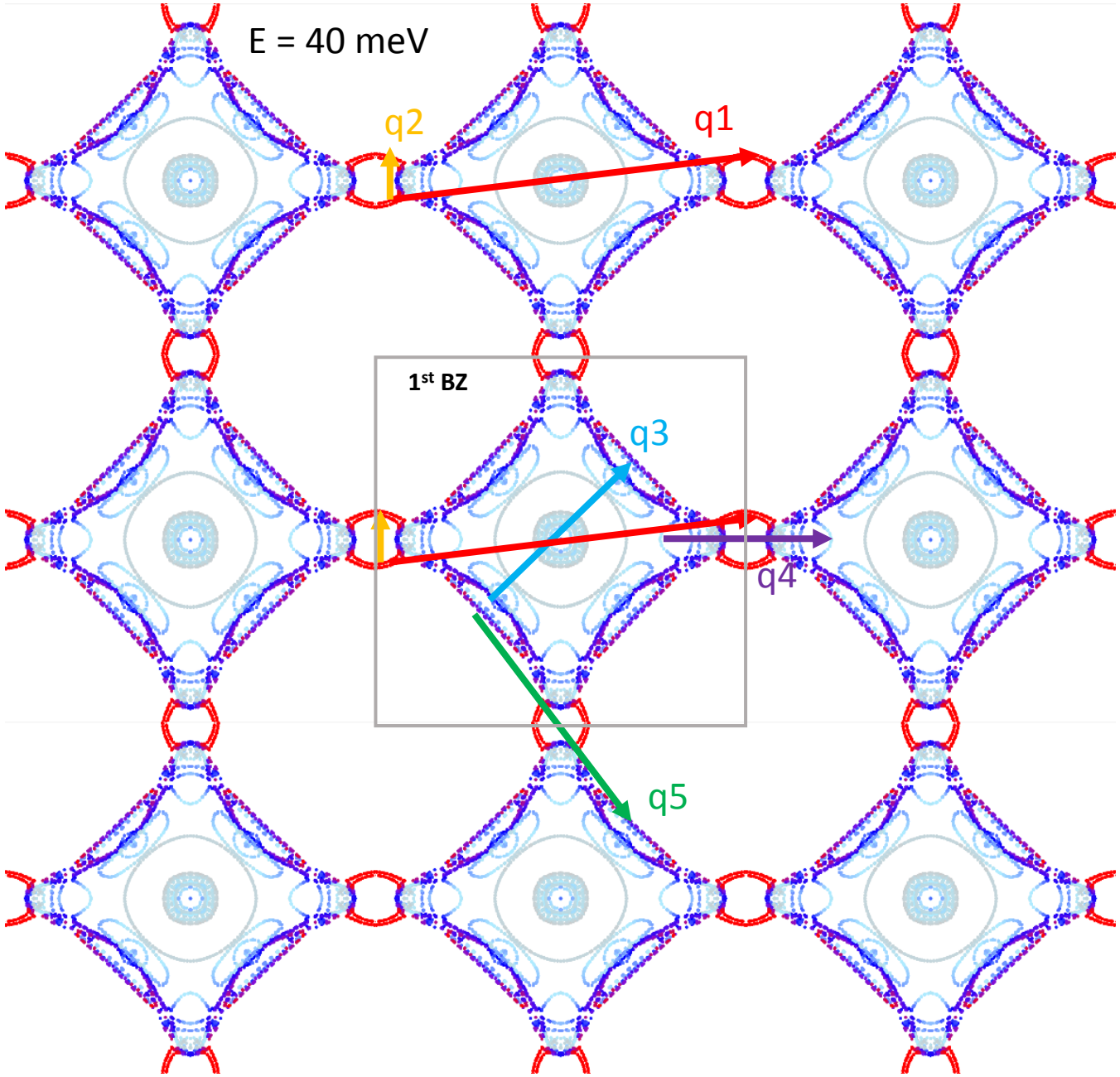
scattering between diamond-shape bands.

q4 ⟶

Umklapp scattering between bulk-projection pockets (Z-R)

q5 ⟶

Umklapp scattering of q3.

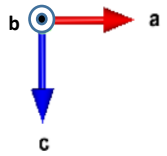


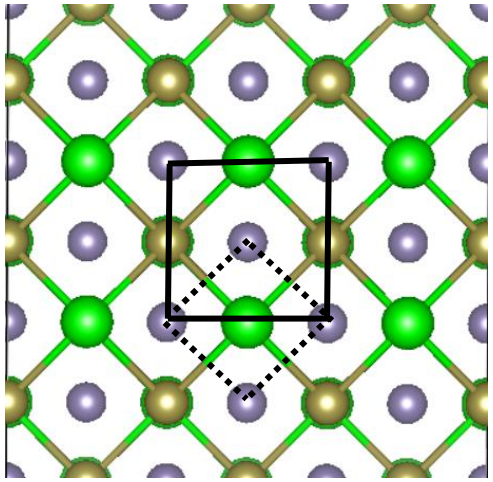
Possible Scenario :
P4/nmm Nonsymmorphic zone folding

$$M_G : (x, y, z) \rightarrow (x, y, -z) + \mathbf{a}_1/2,$$

Zr
Ge
Te

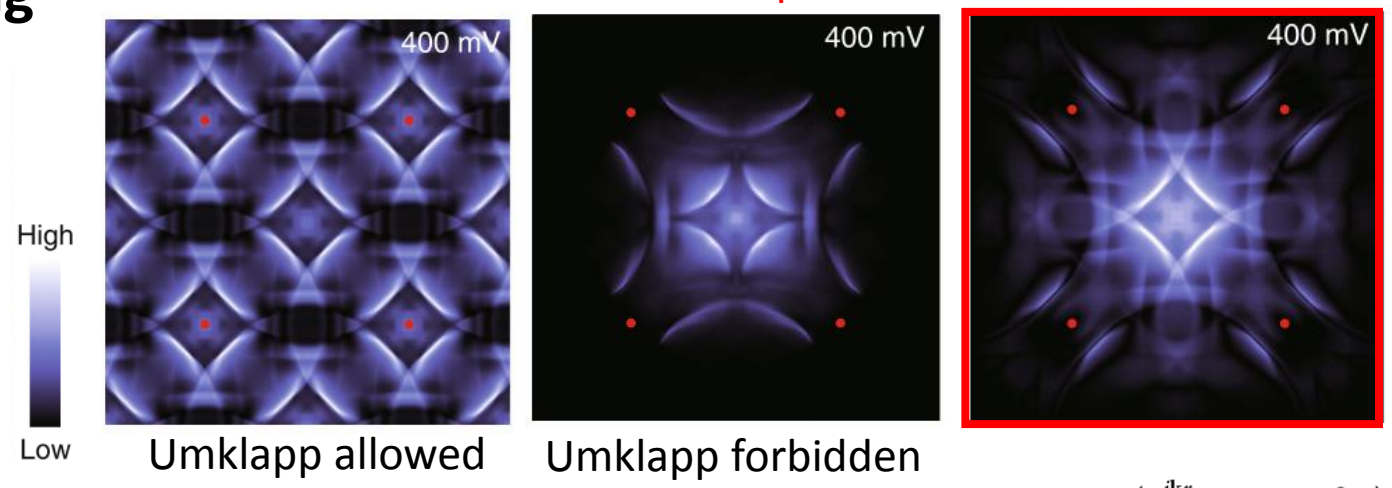
Mirror Plane





ZrSiSe T-matrix simulated QPI

Consider phase difference between sites

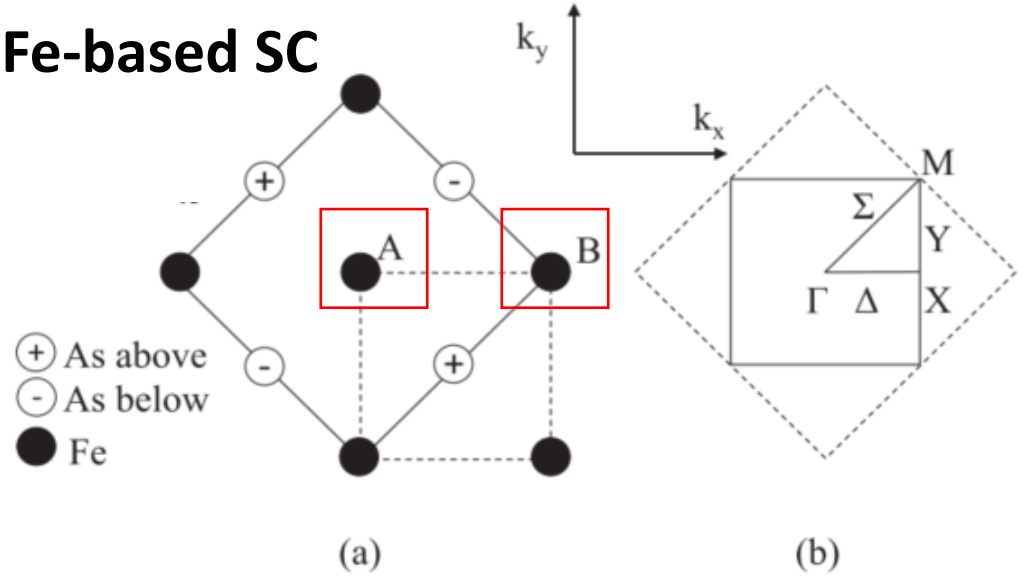


Umklapp allowed Umklapp forbidden

Zhu, Zhen, et al. *Nature communications* 9.1 (2018): 4153.

$$\mathrm{U}(\mathbf{k}) = \begin{pmatrix} e^{i\mathbf{k}r_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & e^{i\mathbf{k}r_n} \end{pmatrix}$$

Fe-based SC



Nica, Emilian M., Rong Yu, and Qimiao Si. *Physical Review B* 92.17 (2015): 174520.

FORBIDDEN!

q1 ⟶

Umklapp scattering of q2.

q2 ⟶

scattering between X-point surface states.

q3 ⟶

scattering between diamond-shape bands.

q4 ⟶

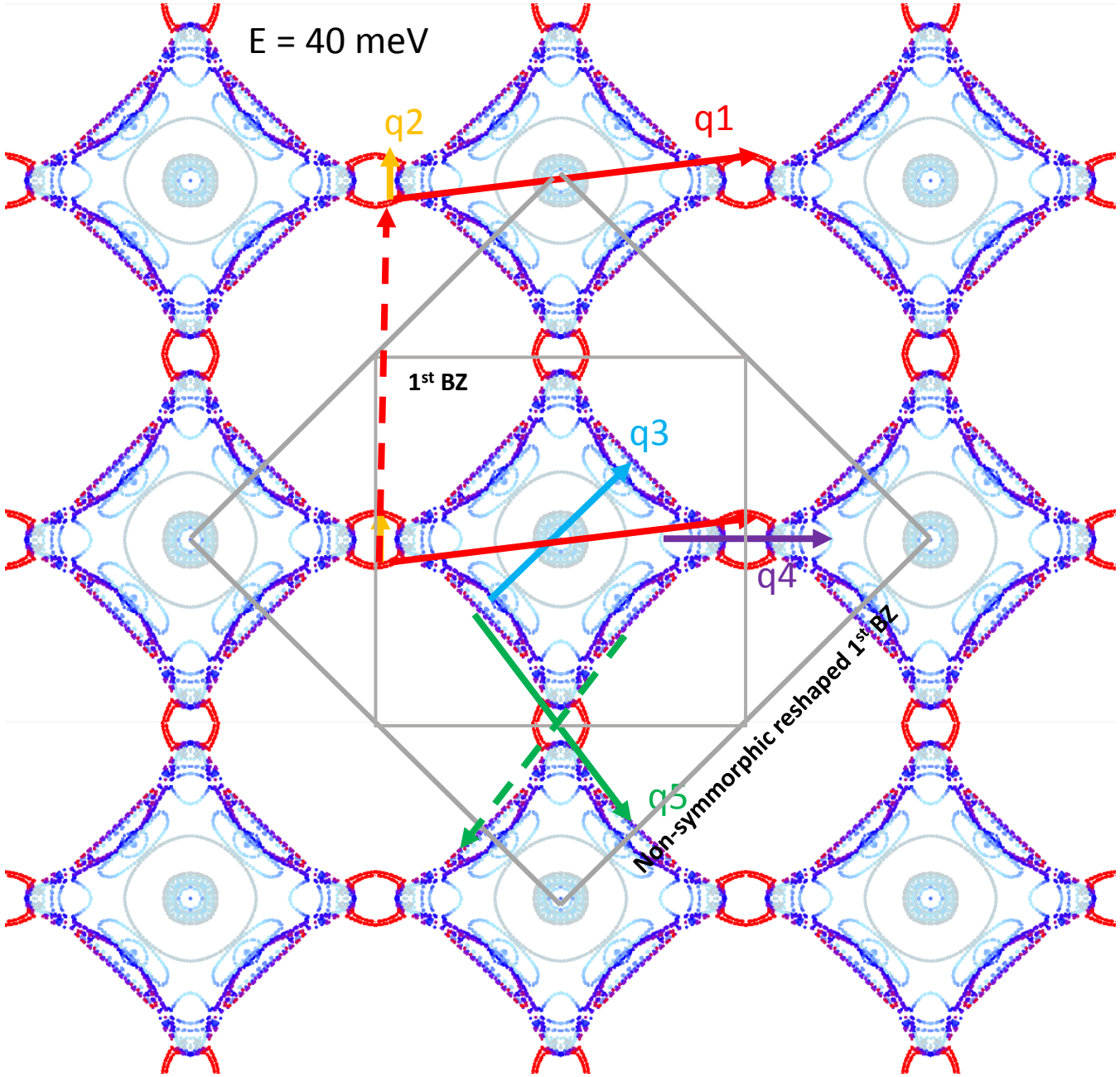
Umklapp scattering between bulk-projection pocket (Z-R)

q5 ⟶

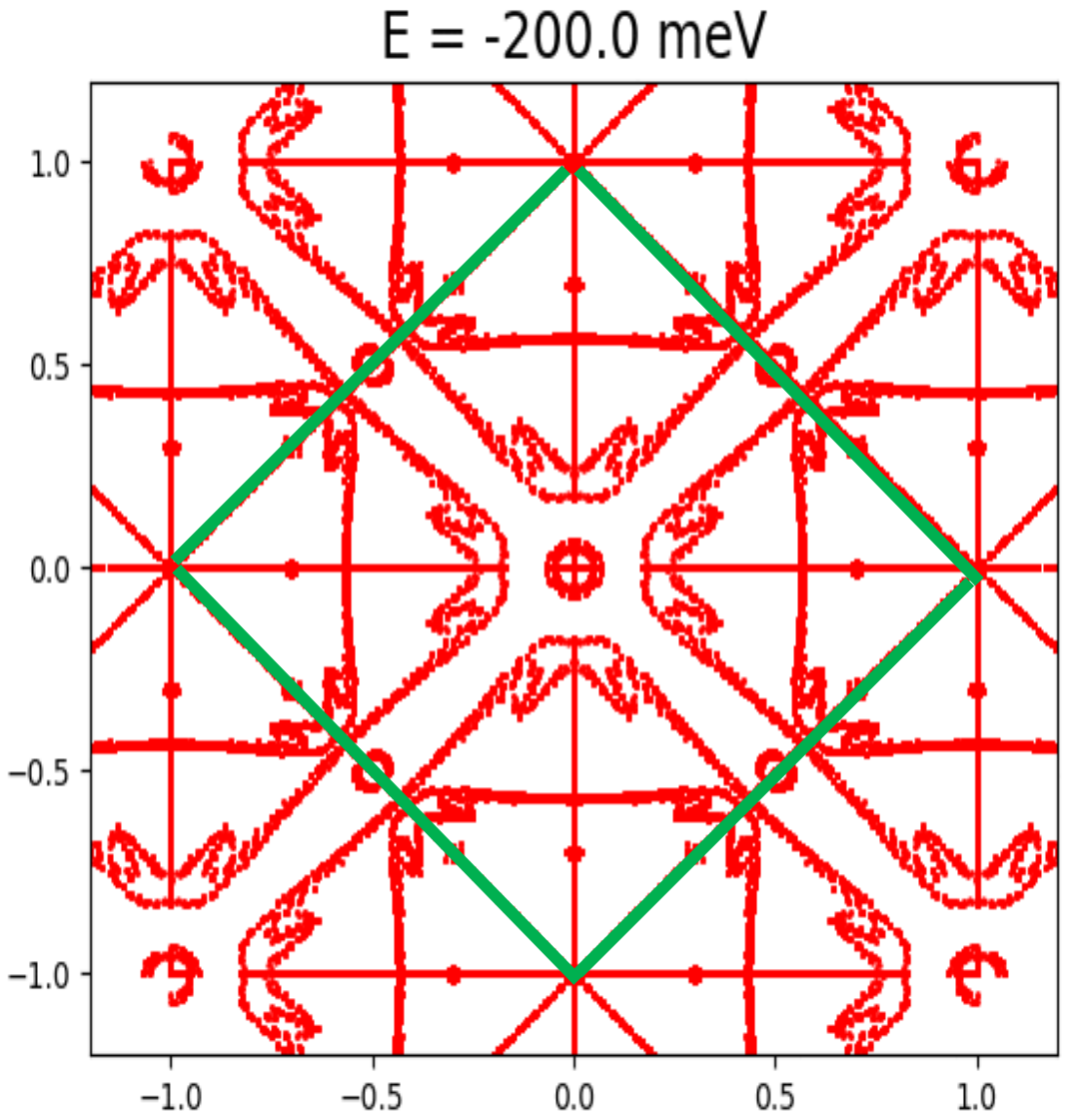
Umklapp scattering of q3.

ALL 5 q-vectors are within

non-symmorphic reshaped 1st BZ



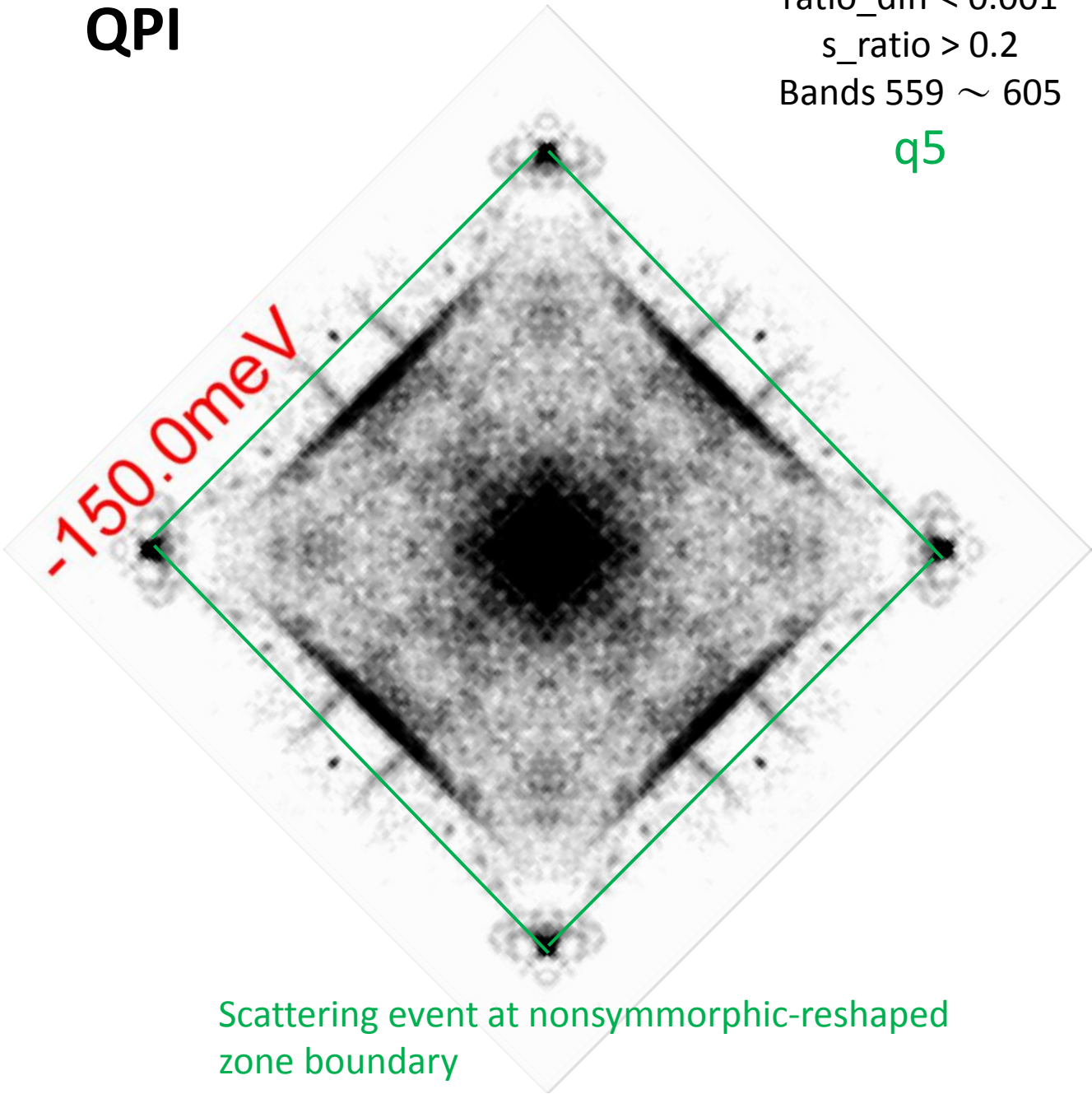
JDOS



QPI

ratio_diff < 0.001
s_ratio > 0.2
Bands 559 ～ 605

q5



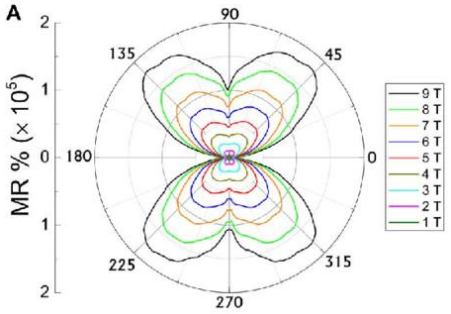
Scattering event at nonsymmorphic-reshaped zone boundary

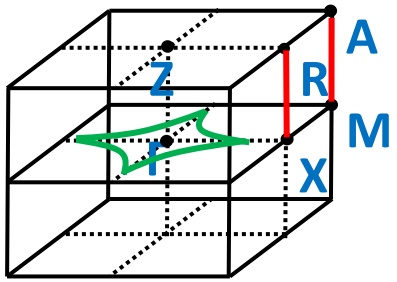
Conclusions & Future works

- ZrGeTe is a platform that host interplay between several interesting exotic quantum phases, including **Dirac Semimetal (DSM) , Dirac nodal line , Weak TI/TCI… etc.**

Zhang, Tiantian, et al. *Nature* 566.7745 (2019): 475.

- Our bulk calculation confirms the **Dirac line node** on the BZ-boundary, and the similar diamond-shaped bulk Fermi surface as ZrSiS family, which might possess useful properties such as large anisotropic MR.



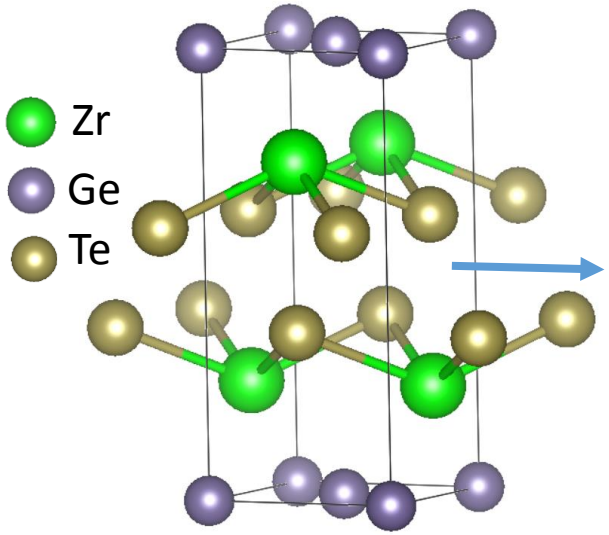


- All the STM QPI signals can be identified with 9-layer slab calculation. Also, the **nonsymmorpic effect possibly plays a role in the QPI patterns like ZrSiSe**.

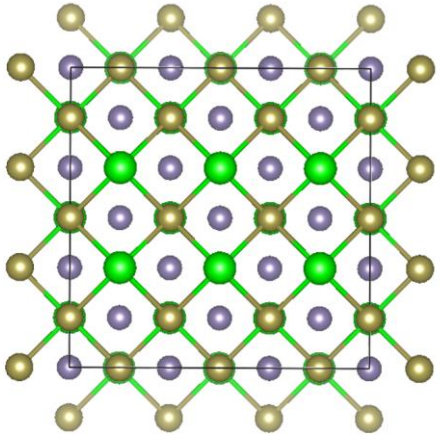
Hosen, M. Mofazzel, et al. *Physical Review B* 97.12 (2018): 121103
Ali, Mazhar N., et al. *Science advances* 2.12 (2016): e1601742.

Thanks for your attention!

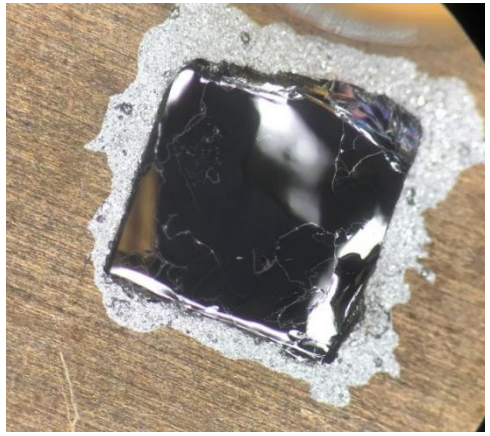
ZrGeTe STM Topography

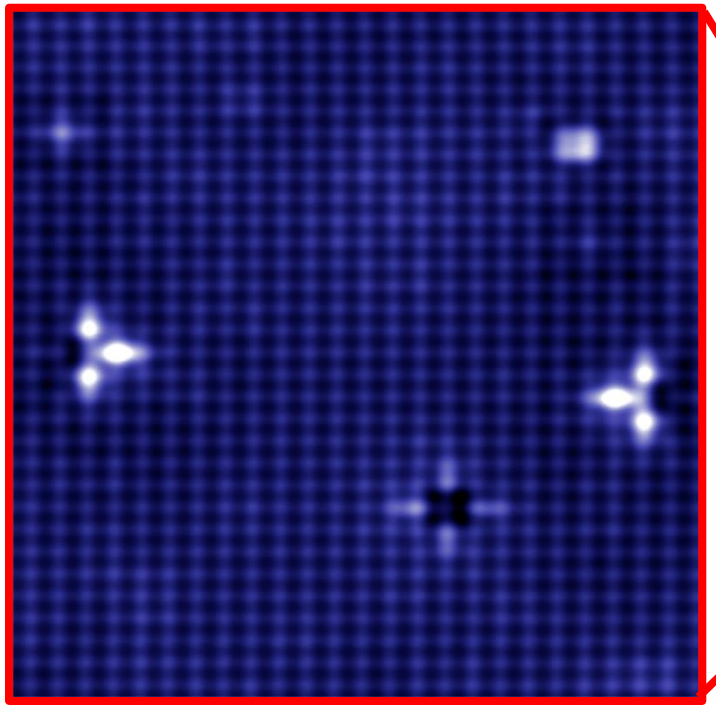


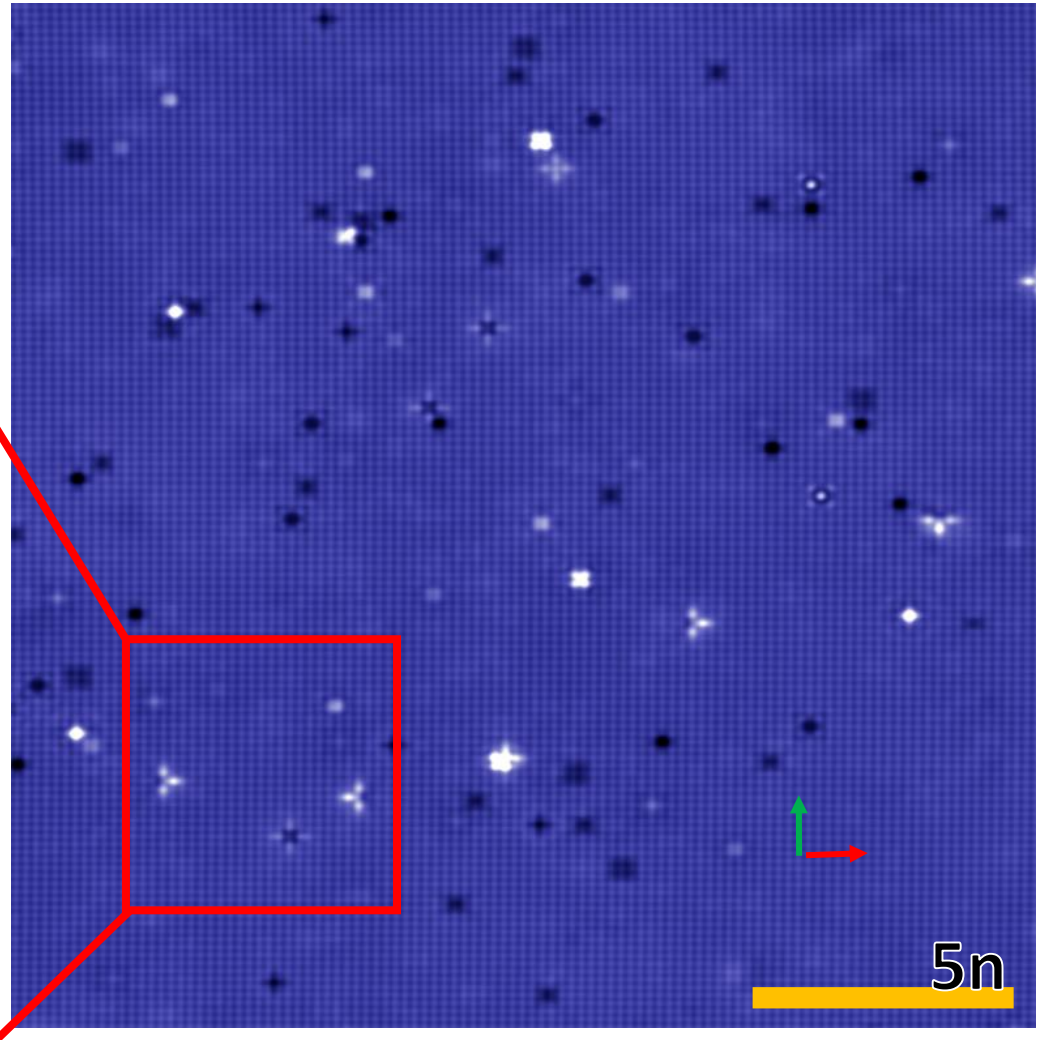
Cleavage plane



Tetragonal
P4/nmm (129)

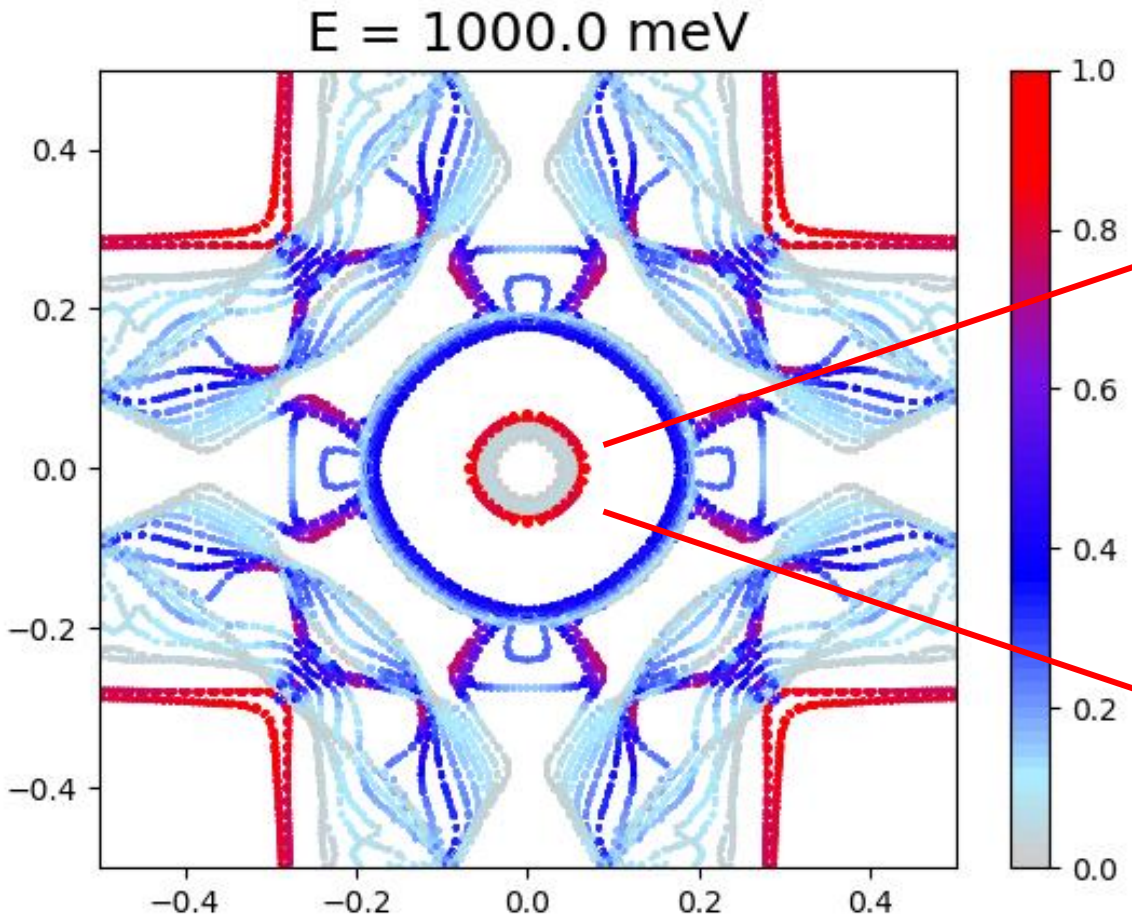


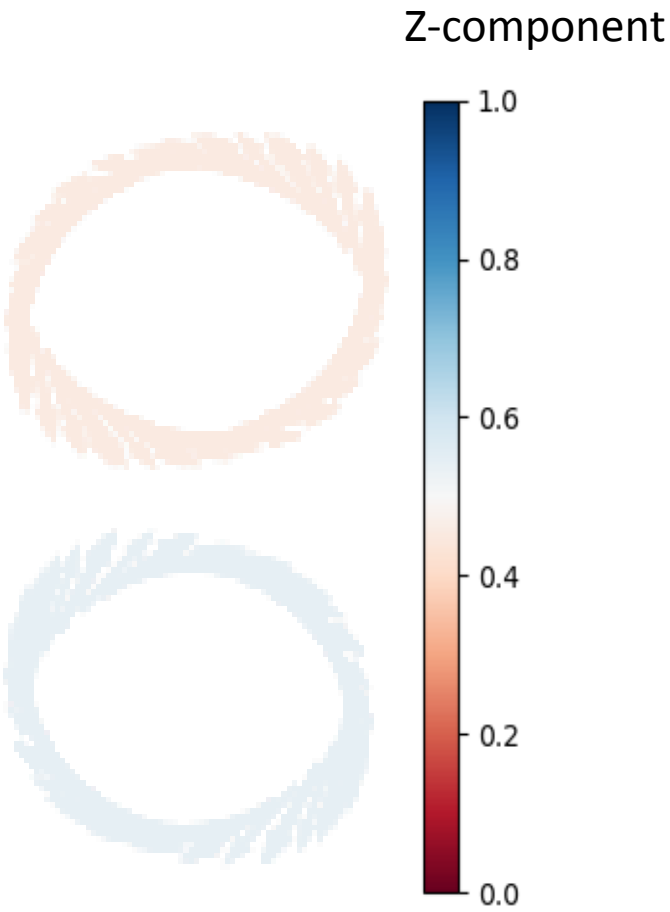




T=4.4K

Rashba-splitting helical spin-texture surface state

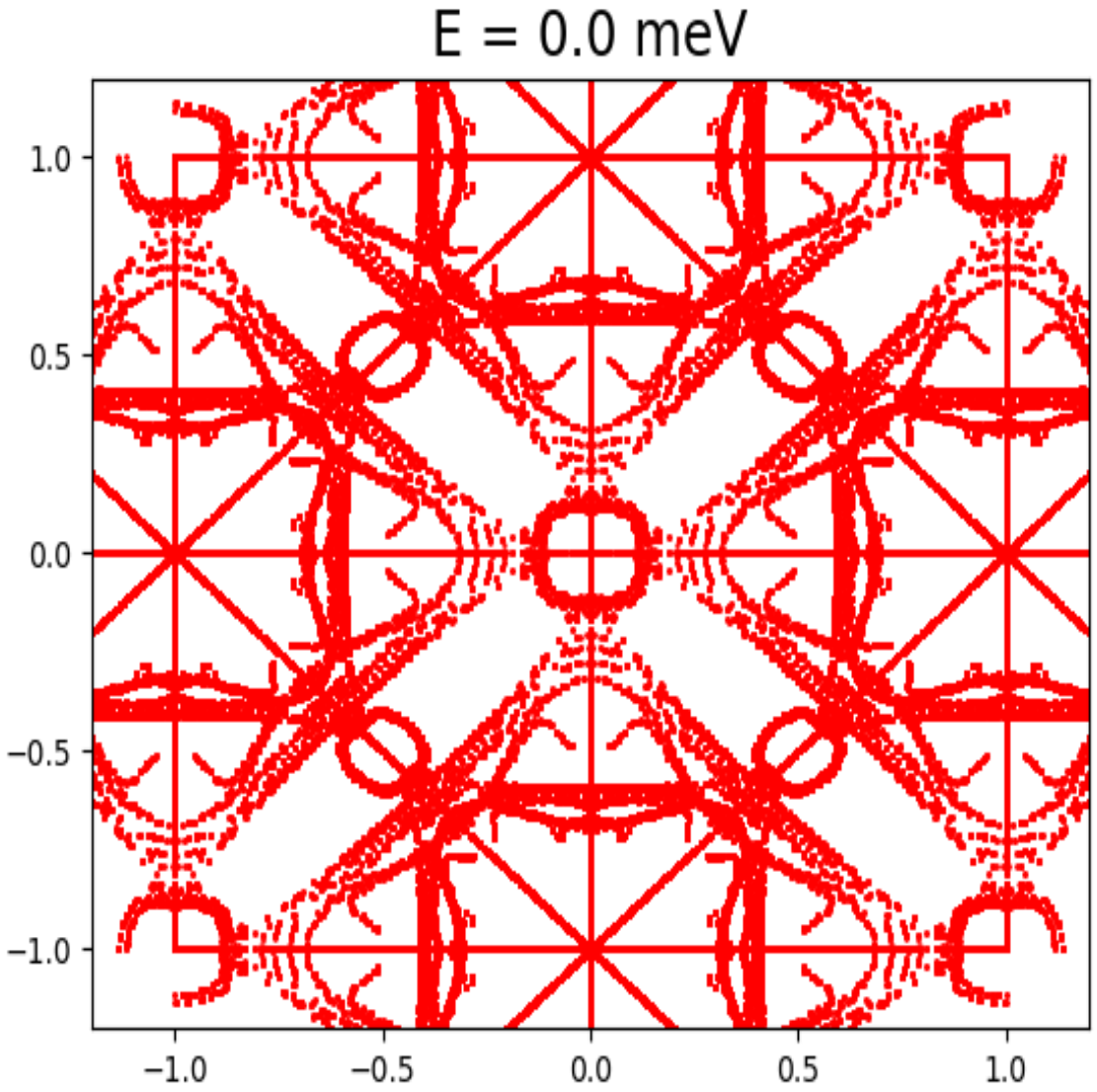


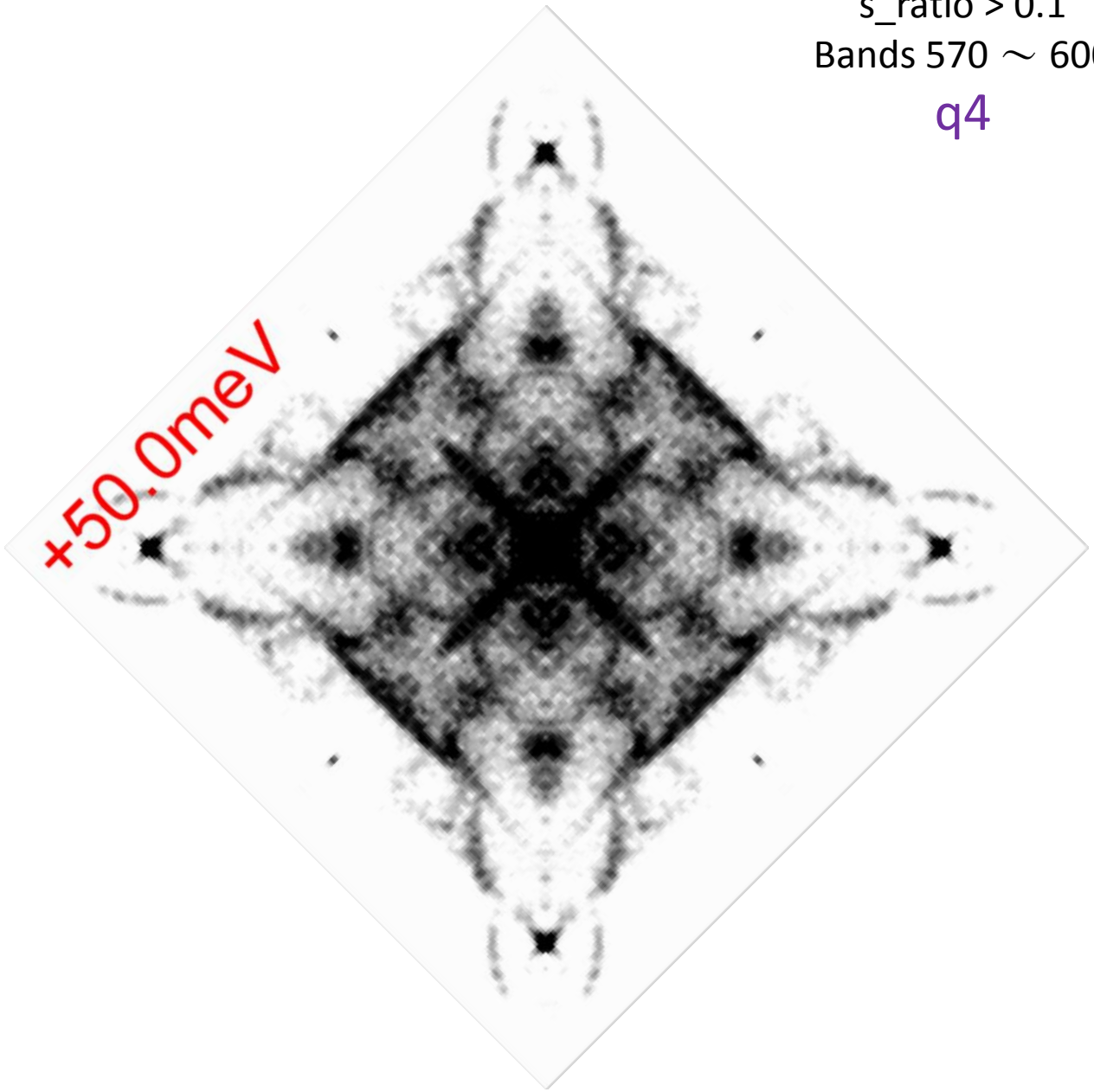


Out-of Plane Spin texture

ratio_diff = 0.0
s_ratio > 0.1
Bands 570 ∼ 600

q4

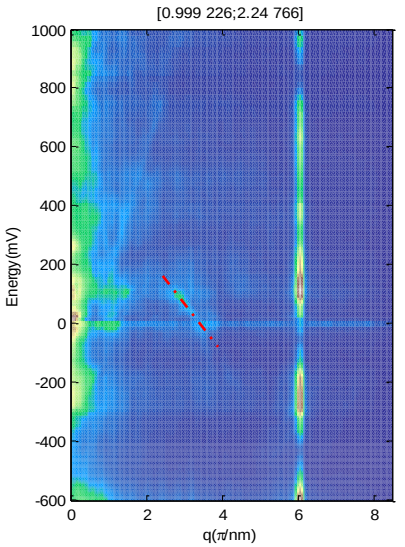


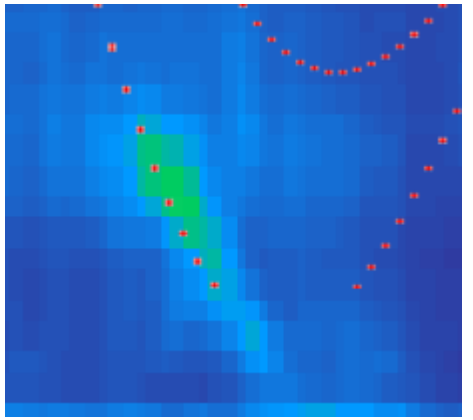


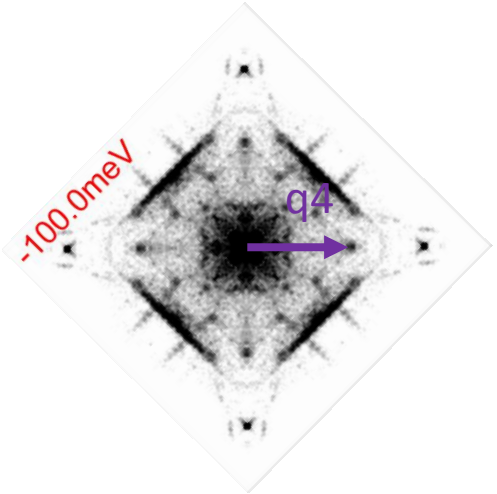
ratio_diff = 0.0
s_ratio > 0.1
Bands 570 ∼ 600

q4

QPI line-cut







E = 0.0 meV

+50.0meV

DFT calculation

ratio_diff < 0.1
s_ratio > **0.8**
Bands **577**
q1 q2