The 4th OpenMX developer's meeting

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Quantum spin Hall states of WTe_2

2023.11.9

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Outline

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1. Background
2. Quantum spin Hall states of WTe_2
   - Electronic properties of the steps in bilayer Td-WTe_2,

     MO, A. Sekine, M. Ohtomo, and K. Kawaguchi,
     Appl. Phys. Express 15, 065004 (2022).
   - Quantum spin Hall states in 2D monolayer WTe_2/$MoTe_2$ lateral heterojunctions for topological quantum computation,

     MO and A. Sekine, ACS Appl. Nano Mater. 6, 2020 (2023).

2D Topological Insulator (TI)

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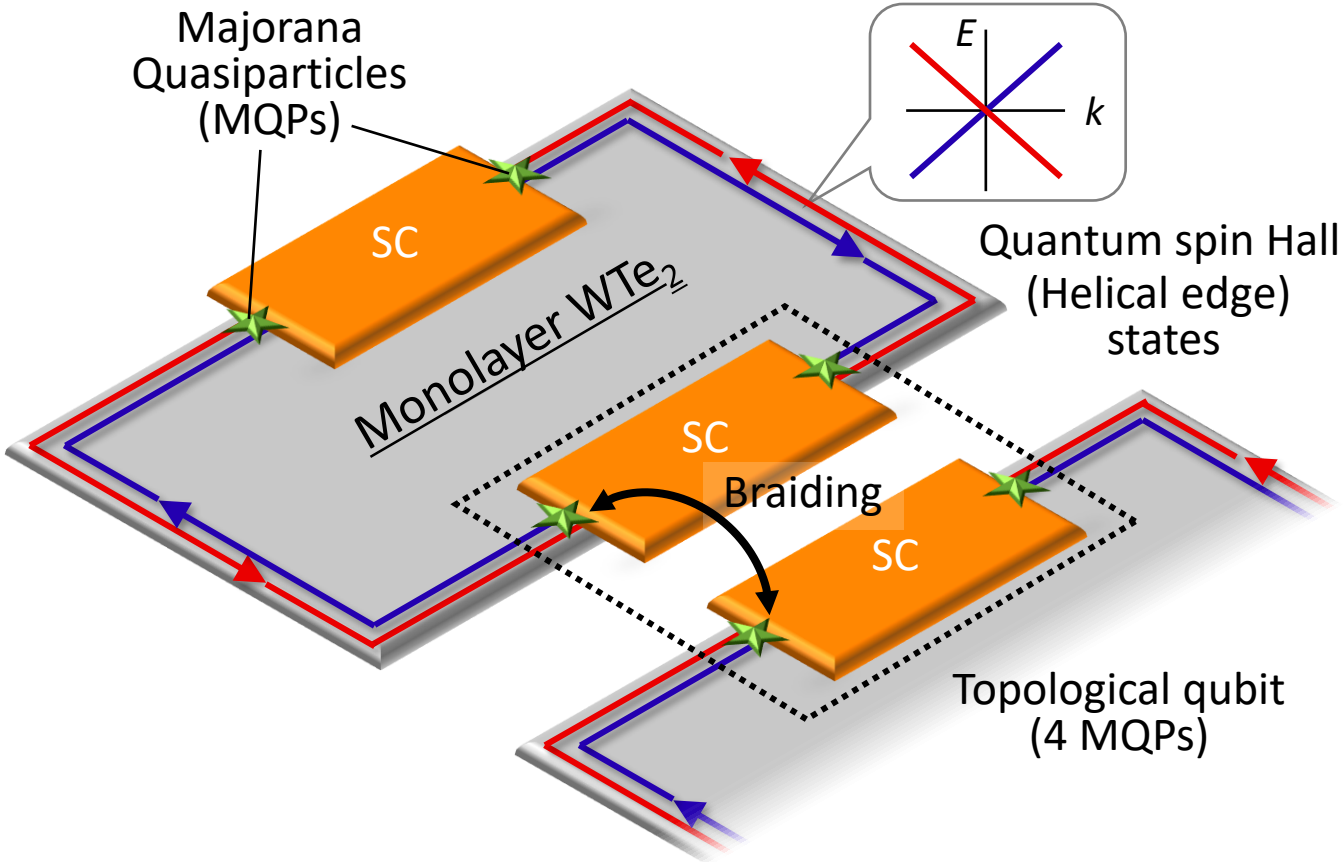
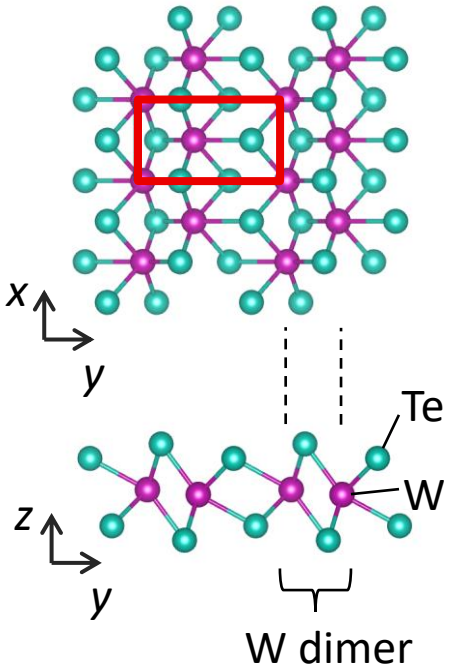


Monolayer WTe_2



Steps in Bilayer WTe_2

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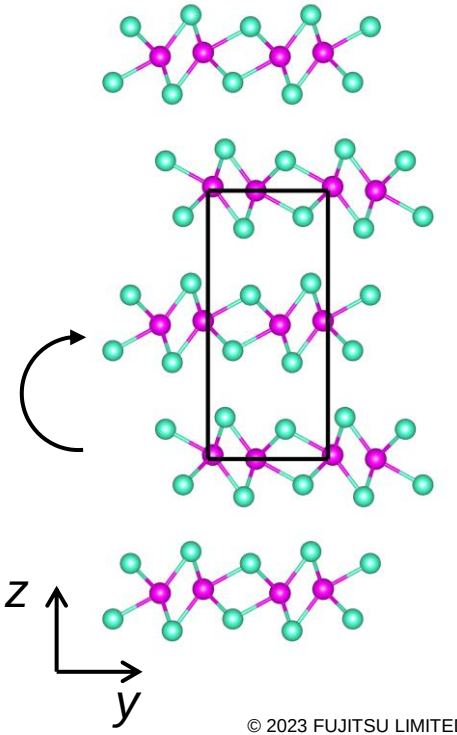
Electronic properties of the steps in bilayer Td-WTe_2,

MO, A. Sekine, M. Ohtomo, and K. Kawaguchi,
Appl. Phys. Express 15, 065004 (2022).

- Handling of monolayer WTe_2 and its edges is very difficult.
- Can we use step edges in few-layer WTe_2?

Use atomic structures as cut out from bulk WTe_2 without any geometry optimization.



Monolayer WTe_2

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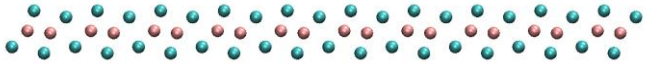
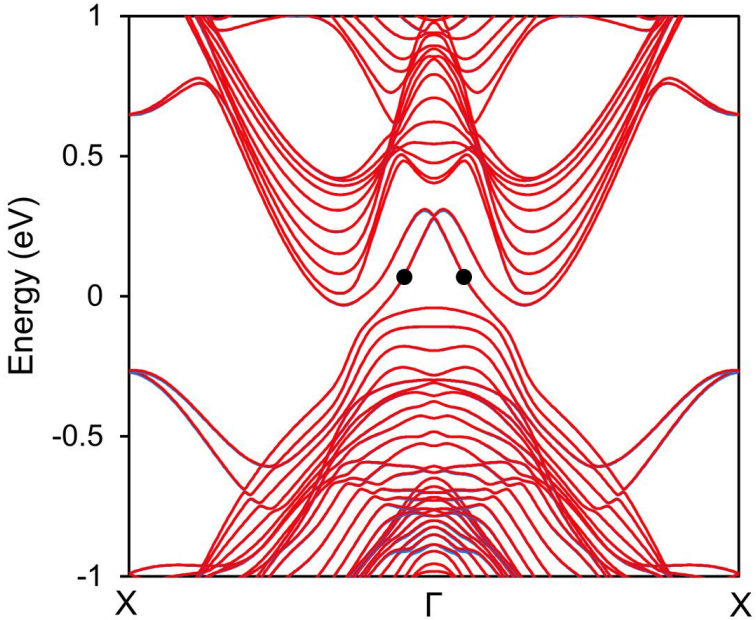
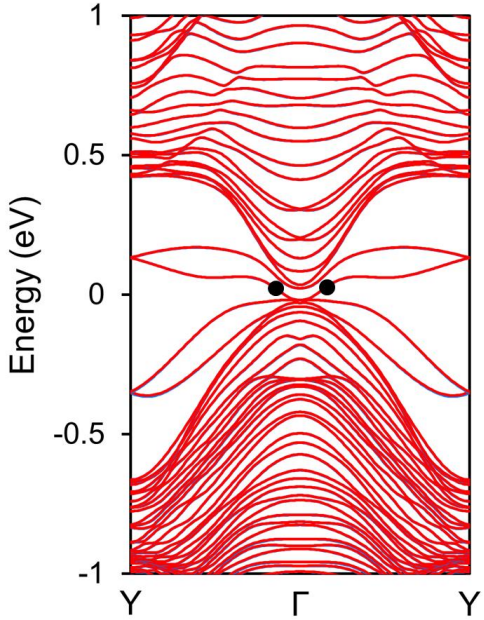
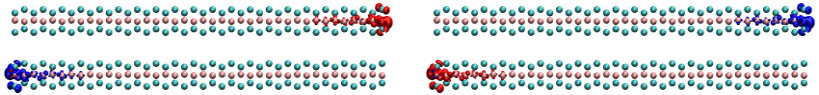
x-stripe 

y-stripe 



Quantum spin Hall
(QSH)
(Helical edge)
state bands





x-steps in Bilayer WTe_2

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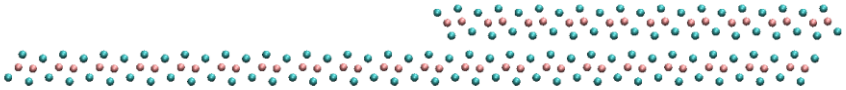
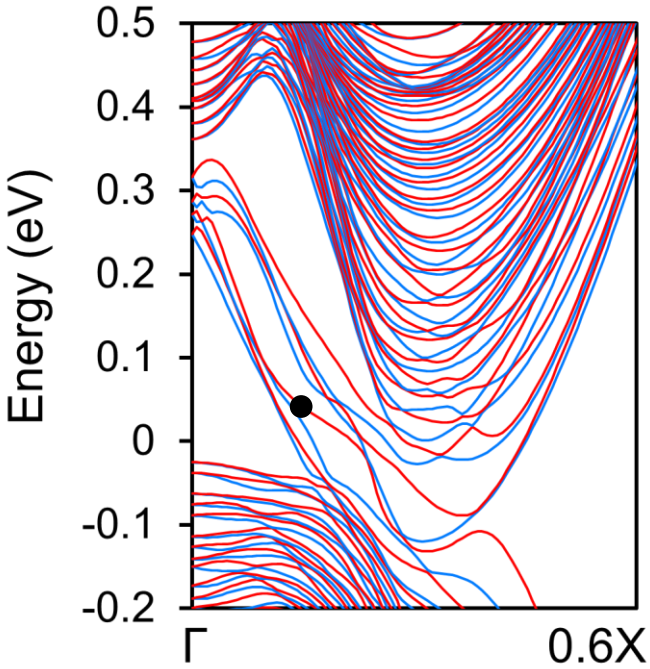
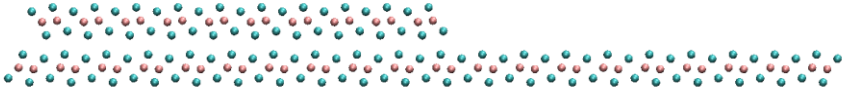
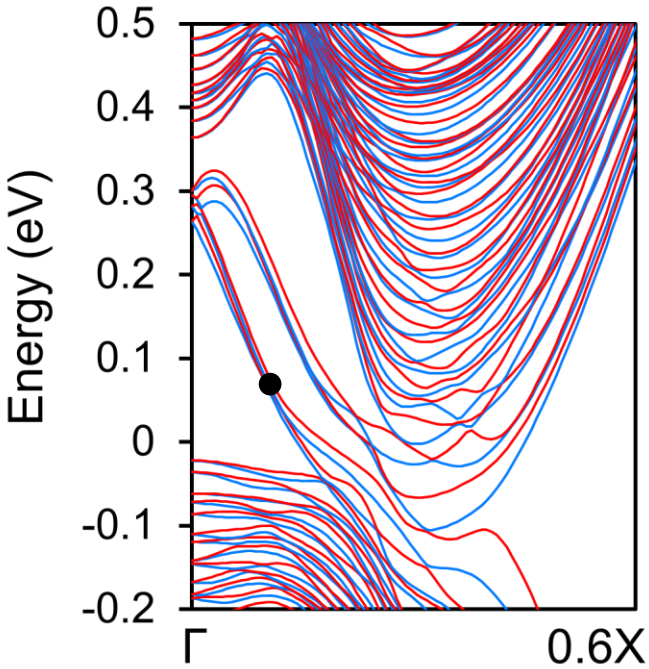
Left step





Right step





x-steps in Bilayer WTe_2

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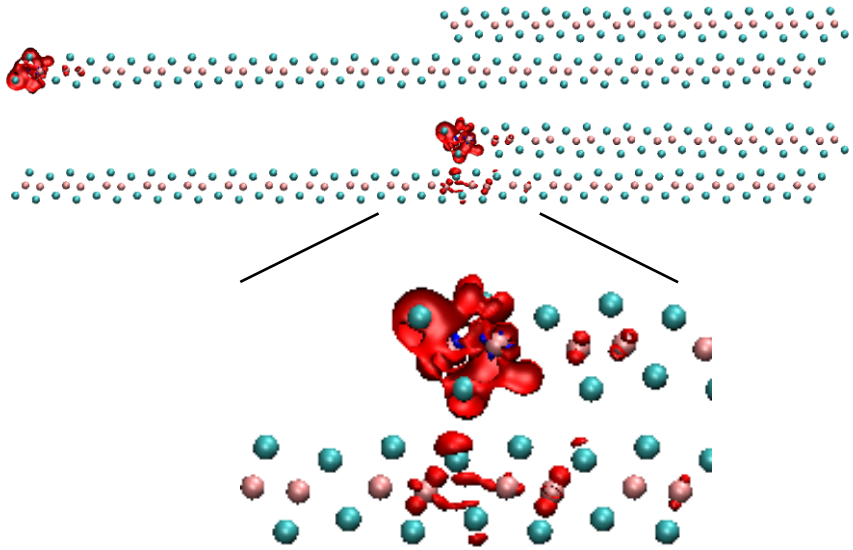
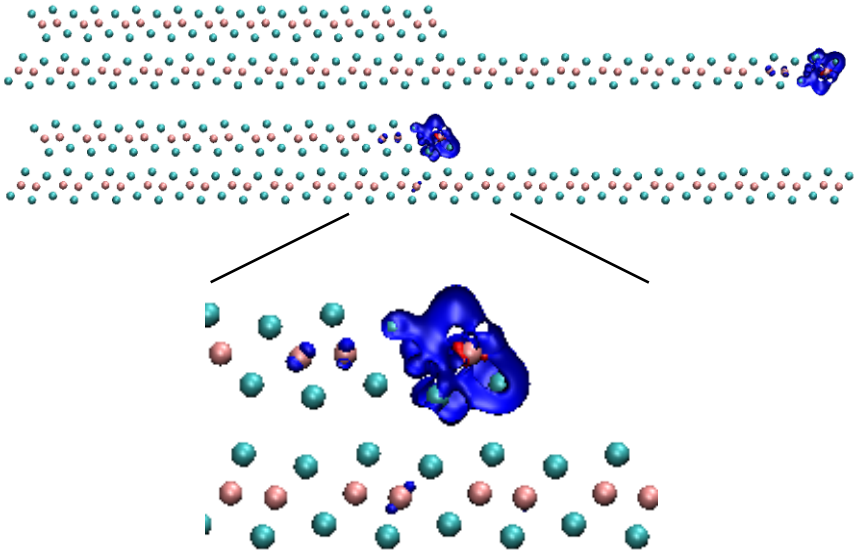
Left step



Right step



Depending on the atomic structure of the step, some edge states may be considered as QSH states.

y-steps in Bilayer WTe_2

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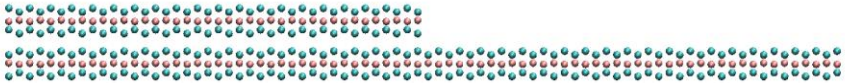
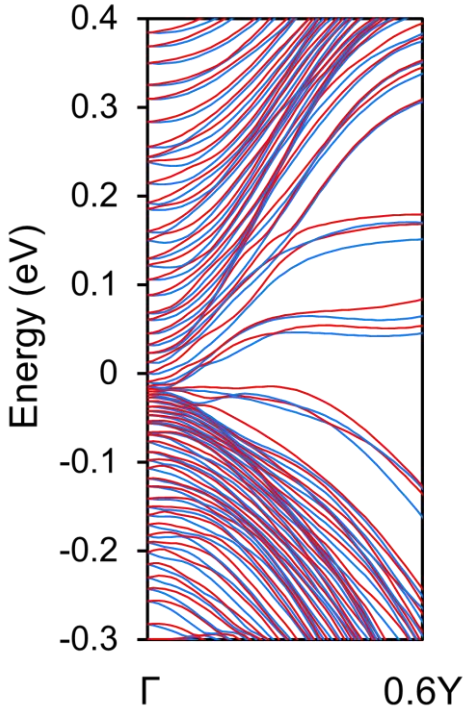
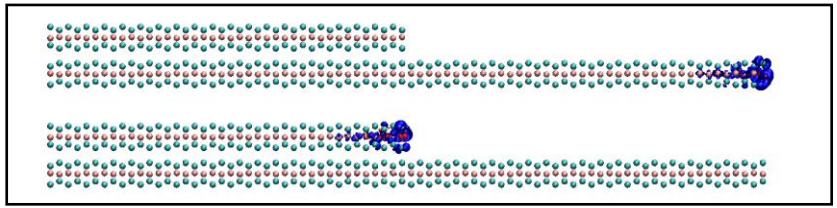
Right step

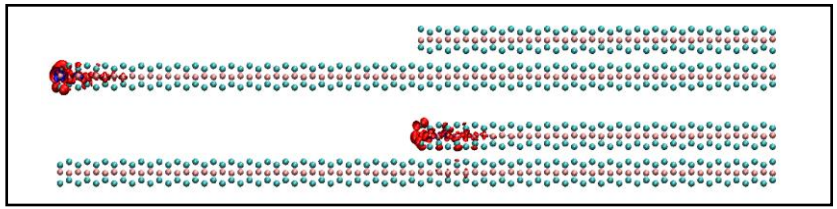




Right step



Left step



In either step, the edge states can be considered as QSH states.

Steps in Bilayer WTe_2

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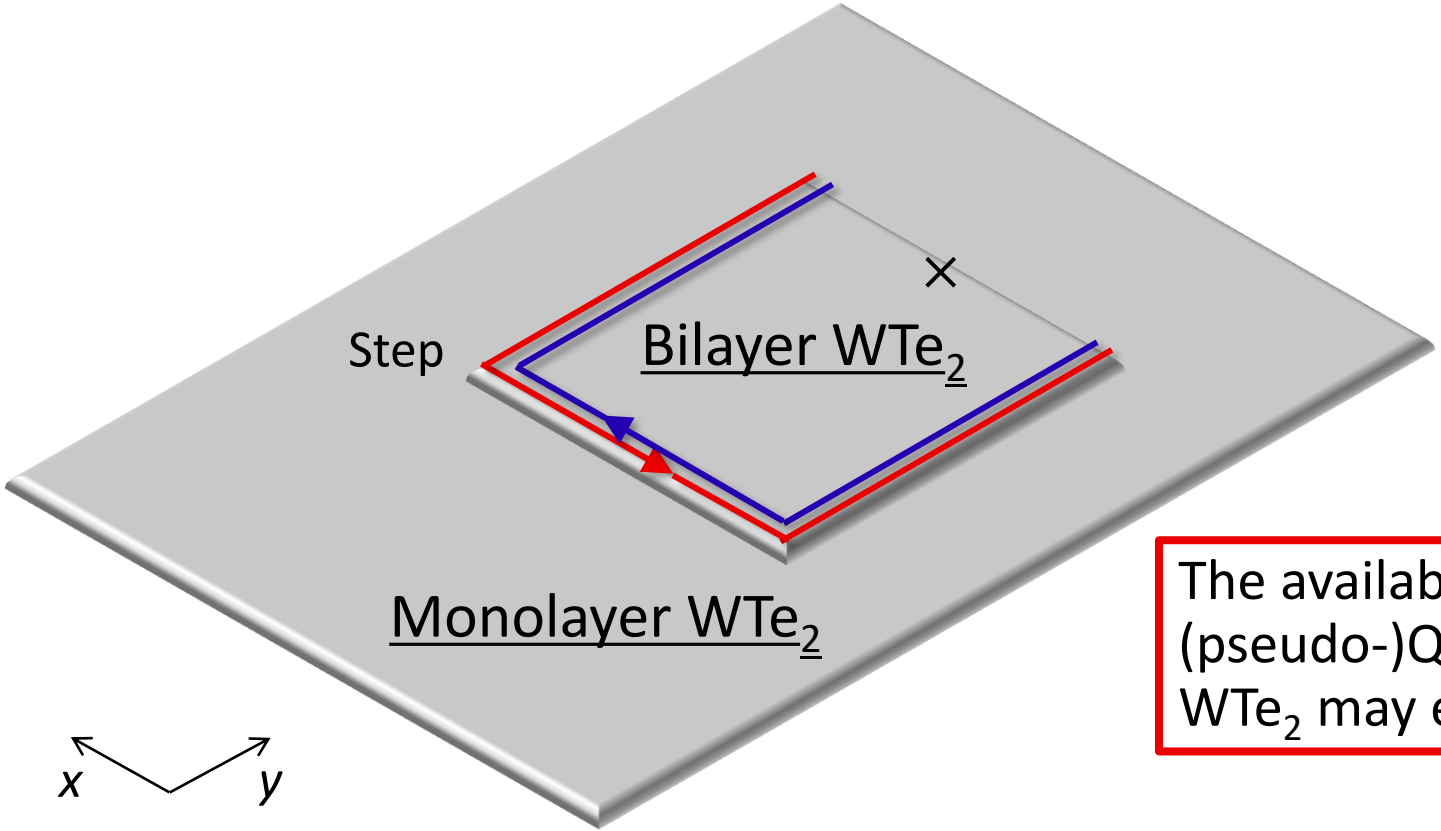

The availability of (pseudo-)QSH states of WTe_2 may expand.

$WTe_2/MoTe_2$ Lateral Heteromonolayer

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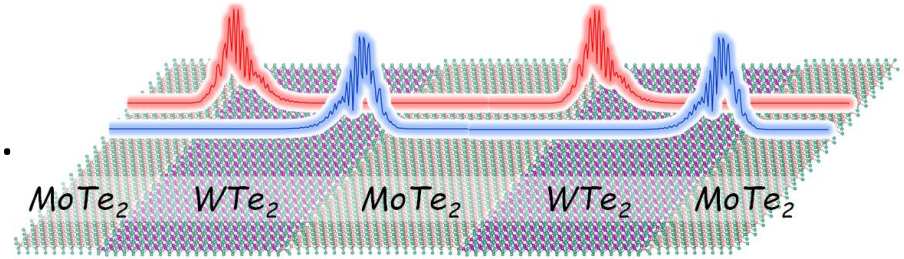
Quantum spin Hall states in 2D monolayer $WTe_2/MoTe_2$ lateral heterojunctions for topological quantum computation,

MO and A. Sekine,

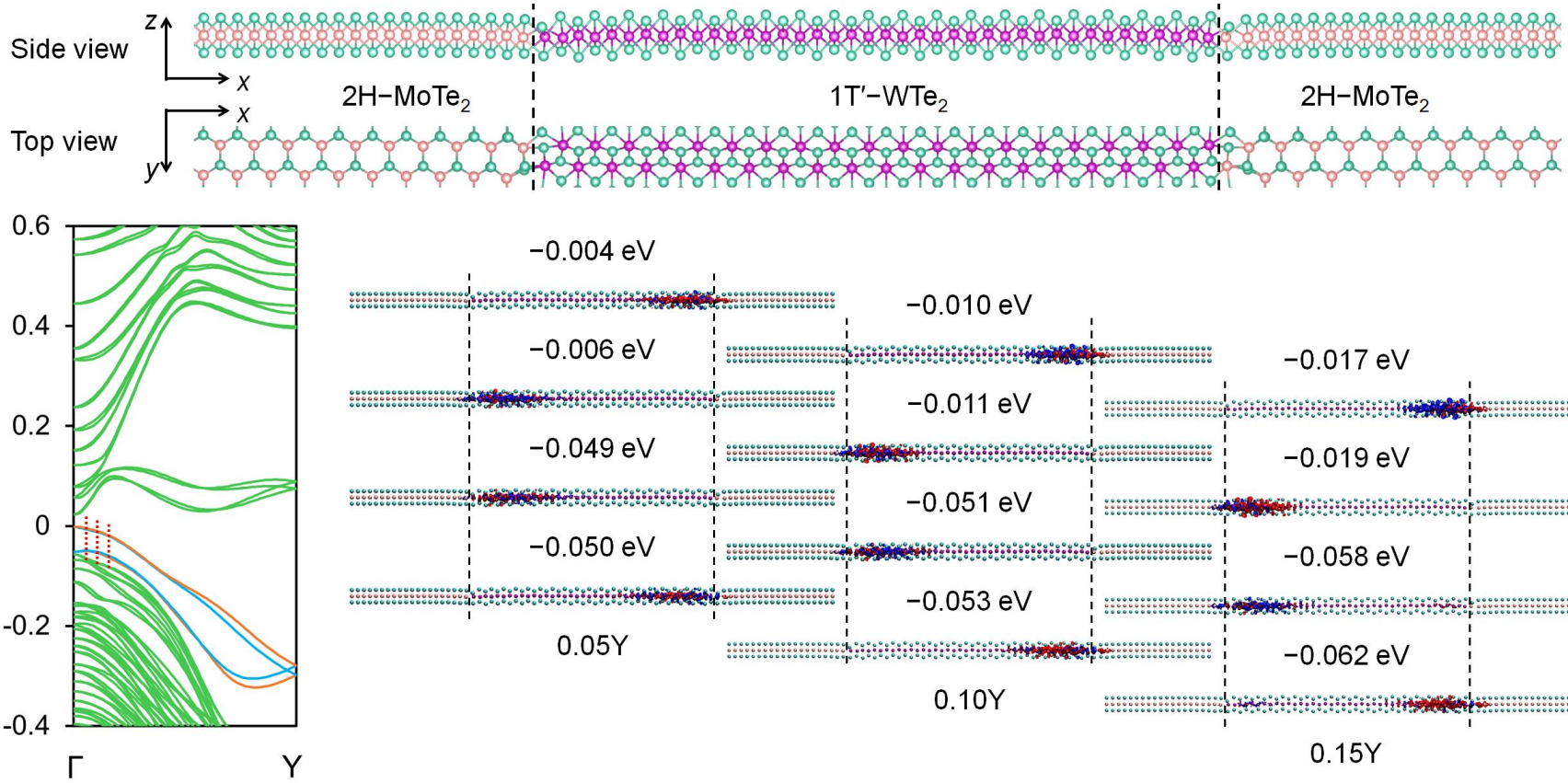
ACS Appl. Nano Mater. 6, 2020 (2023).



- ○ Handling step edges is still difficult.
- ○ The band gap of bilayer WTe_2 is smaller than that of monolayer.

x-heterojunctions:
Low symmetry leads to a potential gradient and various junction-localized state bands.

y-heterojunctions



WTe_2/WTe_2 Lateral Heteromonolayer

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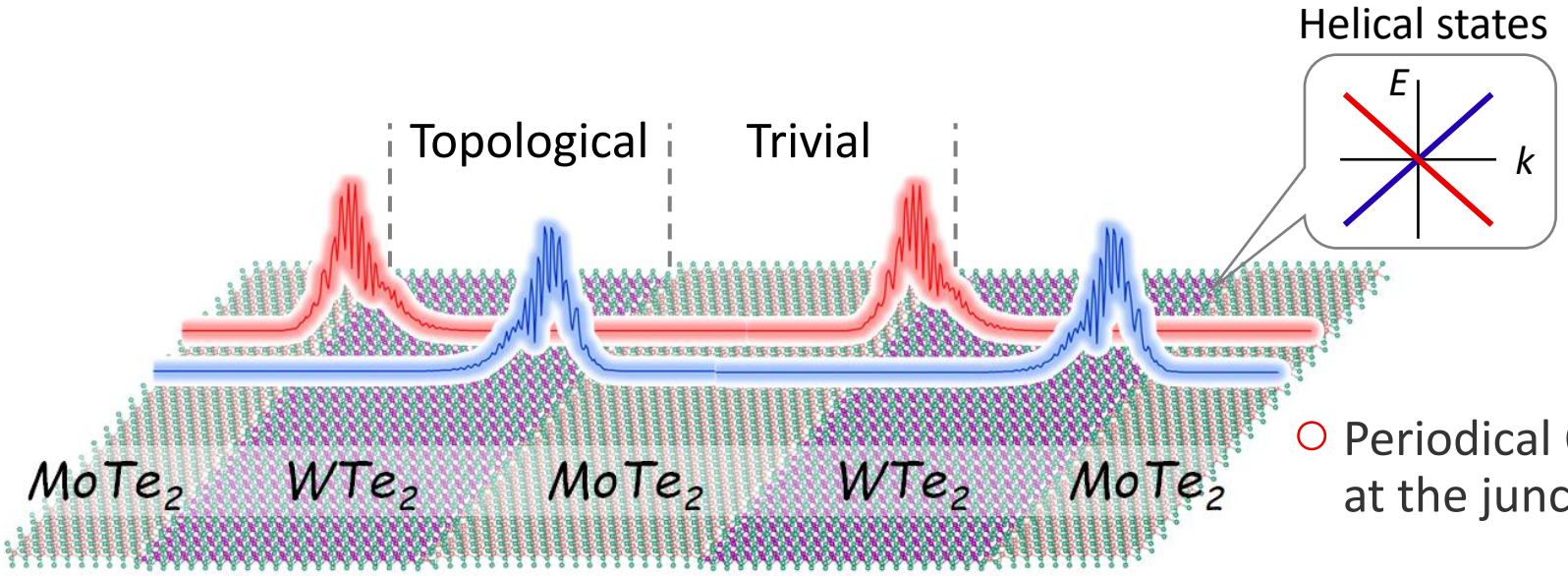
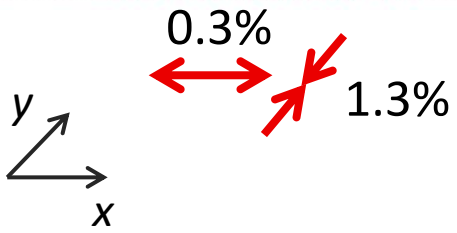
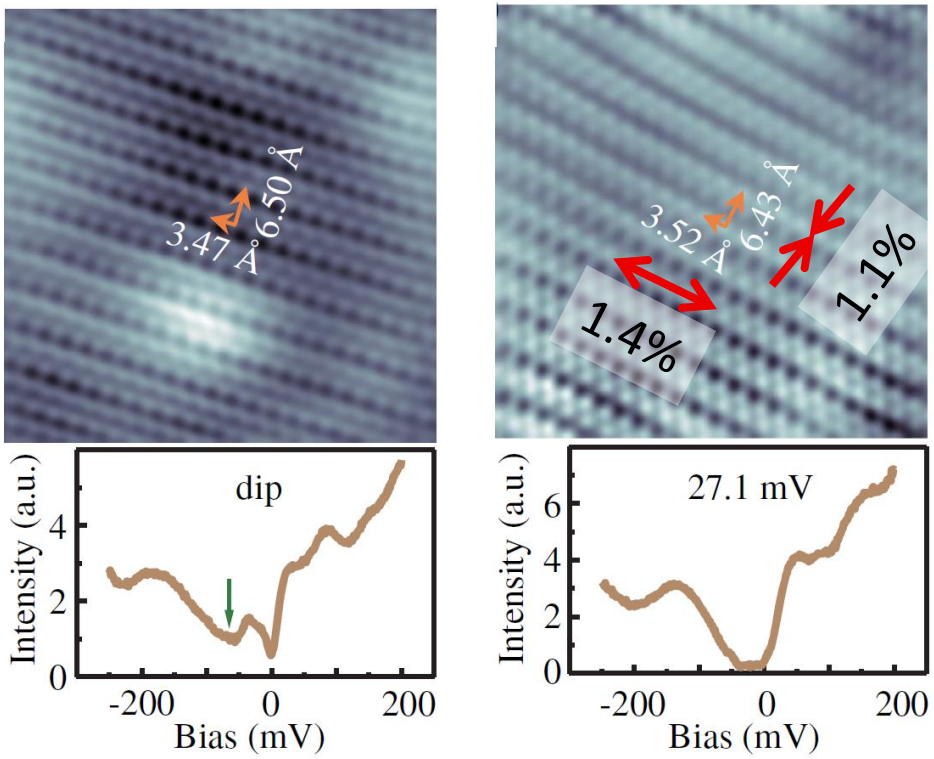


- Periodical QSH states at the junctions



- strain with lattice mismatch increases the bandgap ~10 meV (DFT calculations)

Strain-engineered Experiments



C. Zhao et al., Phys. Rev. Lett. 125, 046801 (2020)

Monolayer WTe_2

- Increased bandgap
  ~20 meV
- Superconducting gap
  ~1 meV

The increased bandgap is essential for Majorana qubit manipulations.

Summary

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Quantum spin Hall states of WTe_2

- Electronic properties of the steps in bilayer Td-WTe_2
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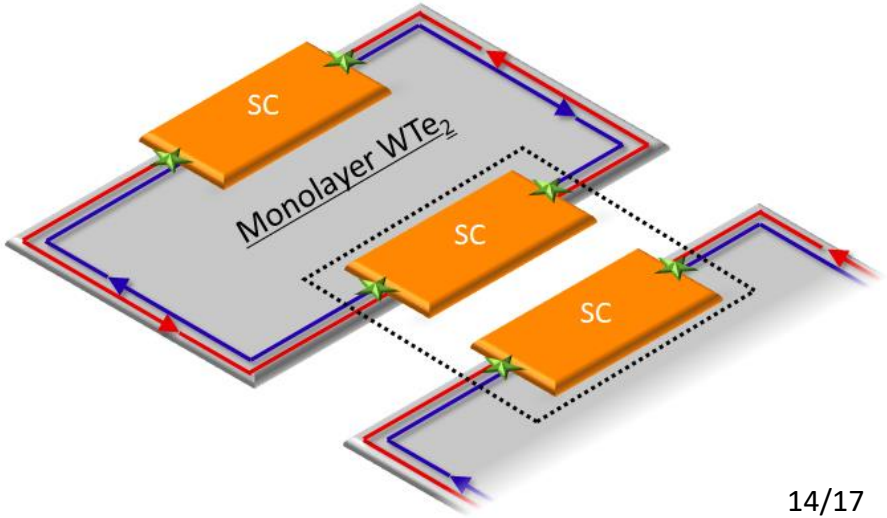

Platform for integrating Majorana qubits

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Thank you