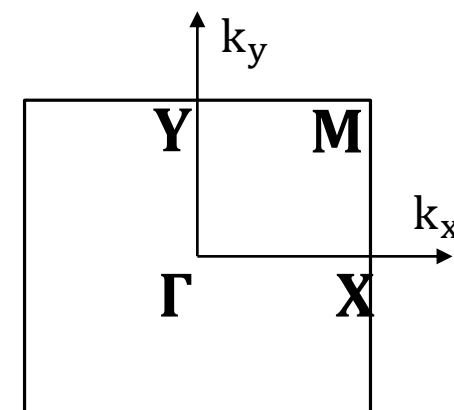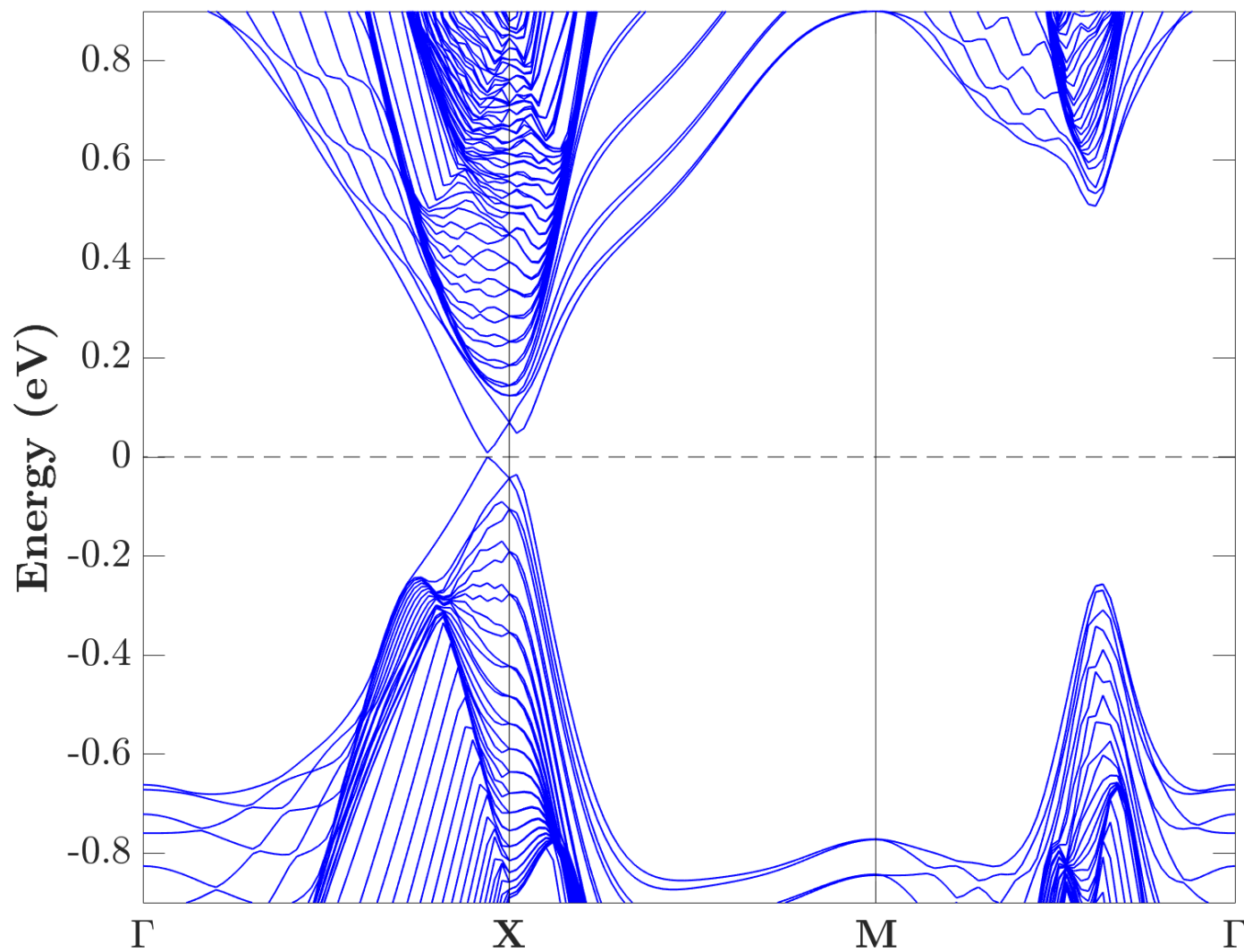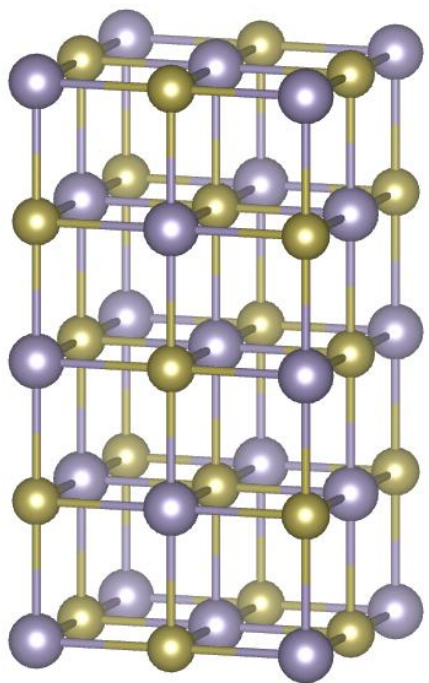# "Cutting Edge" Technology

洪逸群(YI-CHUN HUNG)[1,2]

1. DEPARTMENT OF PHYSICS, NATIONAL TAIWAN UNIVERSITY, TAIPEI, TAIWAN

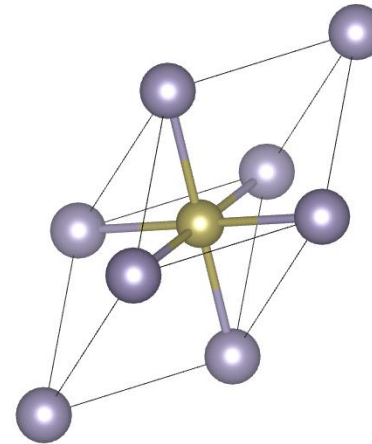2. INSTITUTE OF PHYSICS, ACADEMIA SINICA, TAIPEI, TAIWAN

NTU, Taipei, April 29, 2022.

SnTe[001] 40L

"Cut" a TB-slab ?
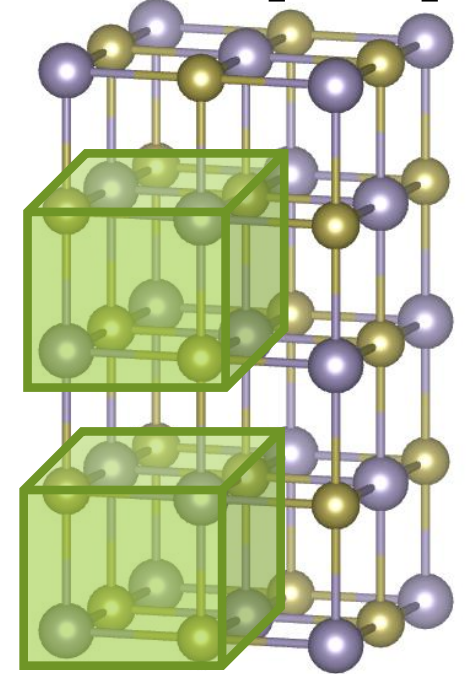
Construct a supercell

SnTe bulk

SnTe[001]

↓
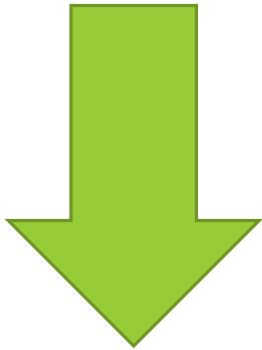
"Turn off" its inter-supercell hopping terms

How to construct a TB-supercell ?
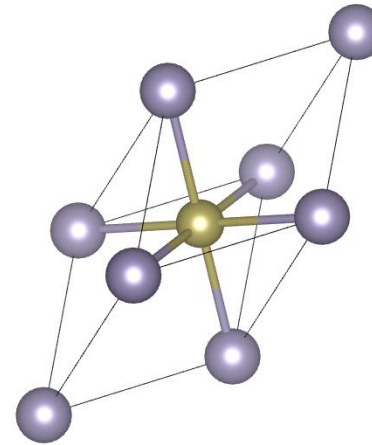
Find **positions of atoms** and **unit cell of slab**
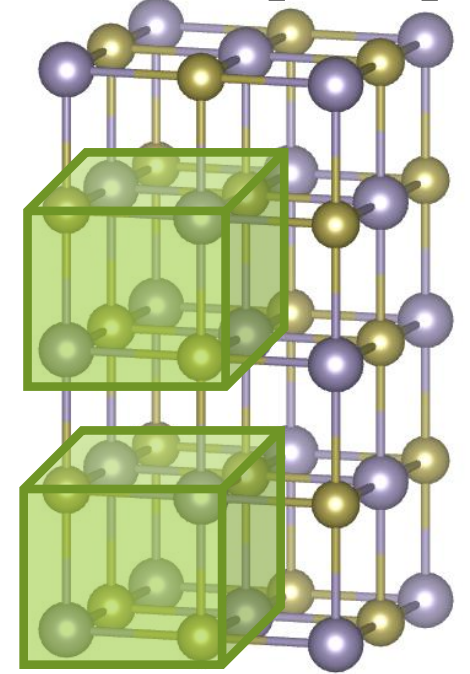
⬇

Select the hopping terms from bulk information

⬇

"Attach" the atoms through these hopping terms

SnTe bulk

SnTe[001]

Slab with different termination?
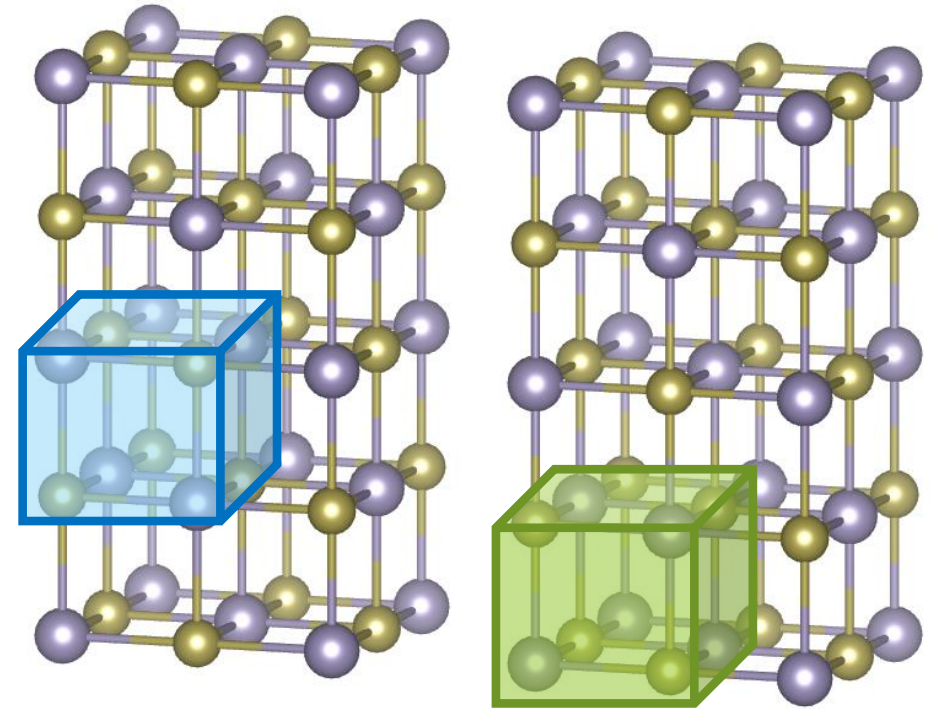
Change unit cell

Shift atoms' fractional coordinates

⬇

Transform TB-Model into **Wannier rep.**

⬇

Transform TB-Model back into **Bloch rep.**
using new coordinates

Slab with different termination?

Construct a Slab with **an extra layer**

Select the atoms
above the desired termination

"Turn off" the hopping terms involving these atoms

The hard way: attaching extra ATOMS ...