



# Confinement-induced topological phase transition in thin film LaSb

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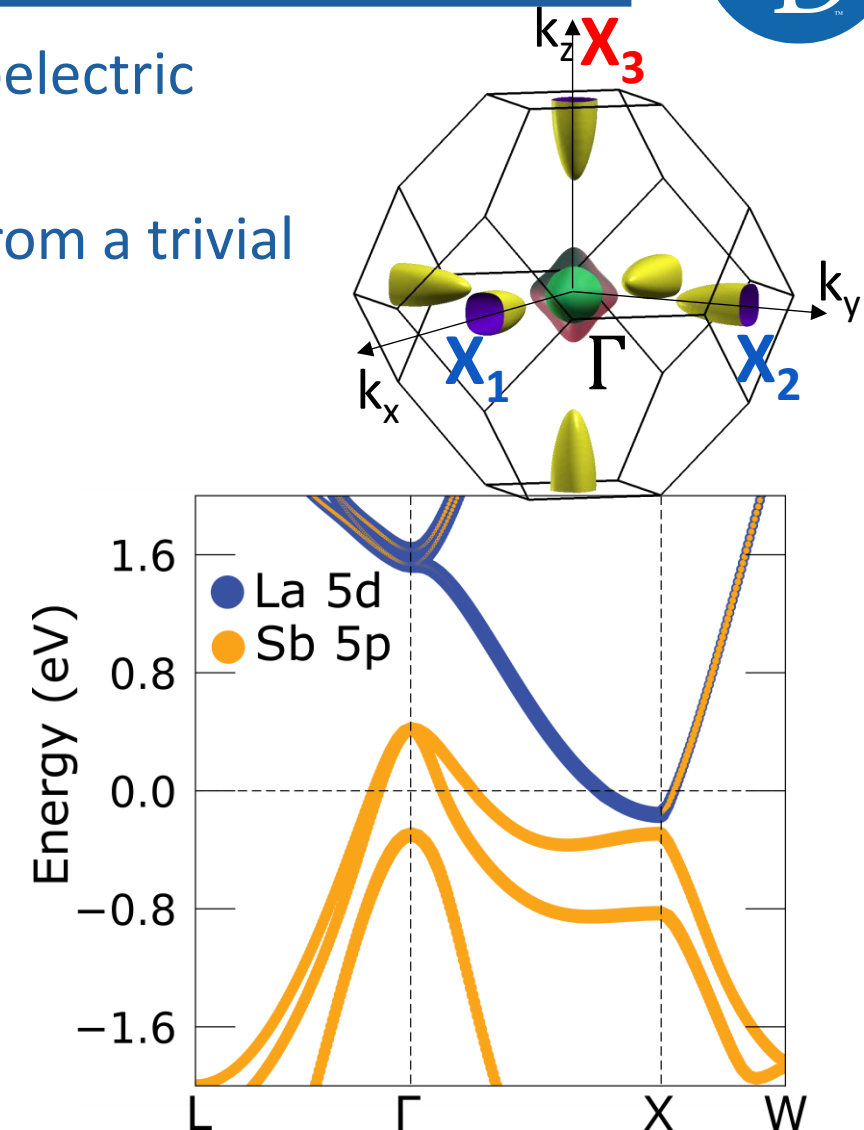
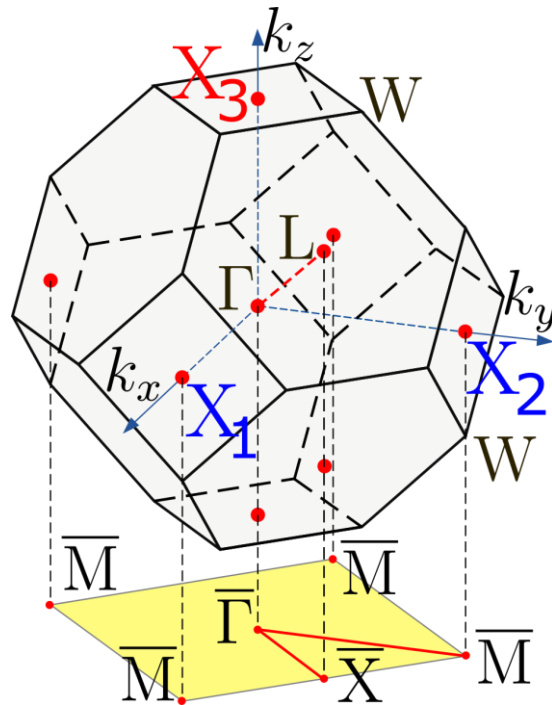
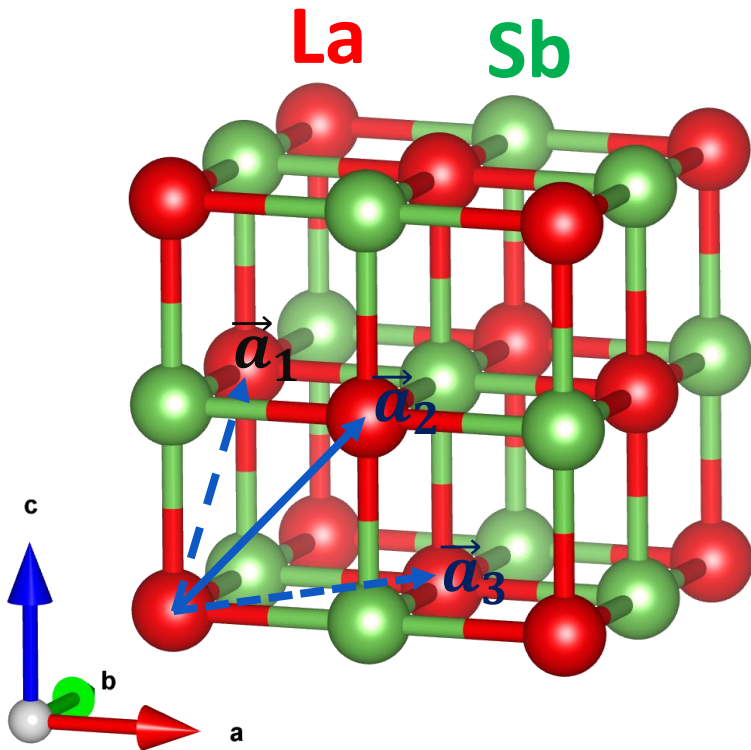
February 8, 2025



# Introduction to Rare-earth monopnictides RE-Vs



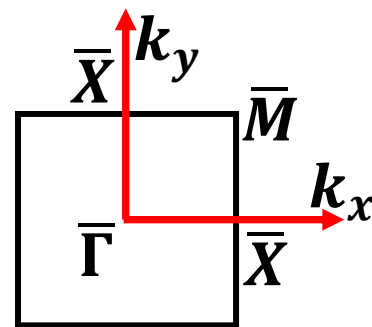
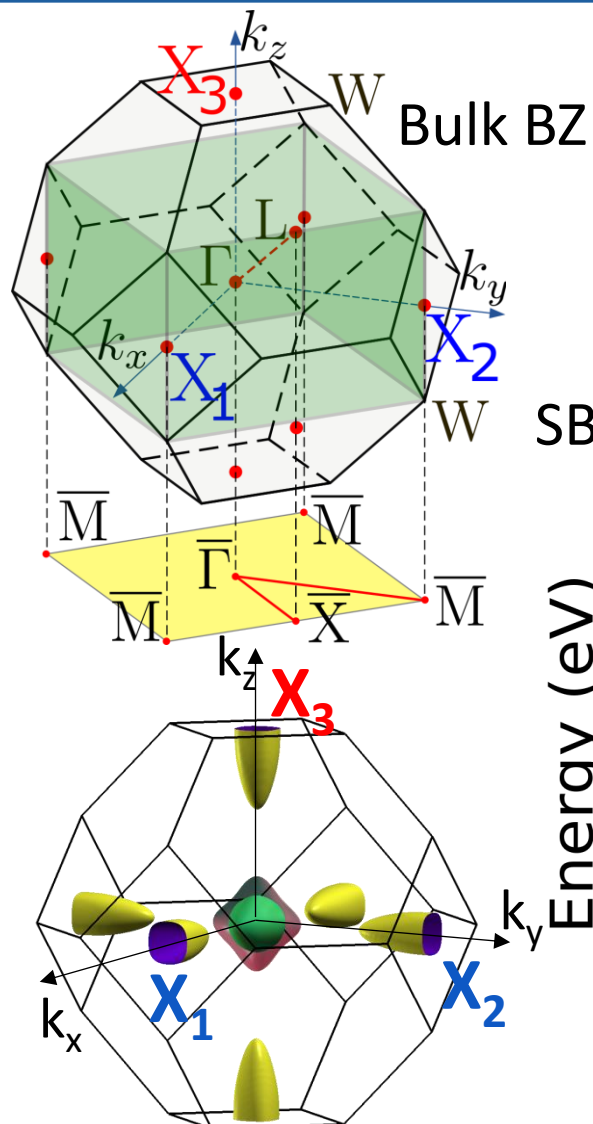
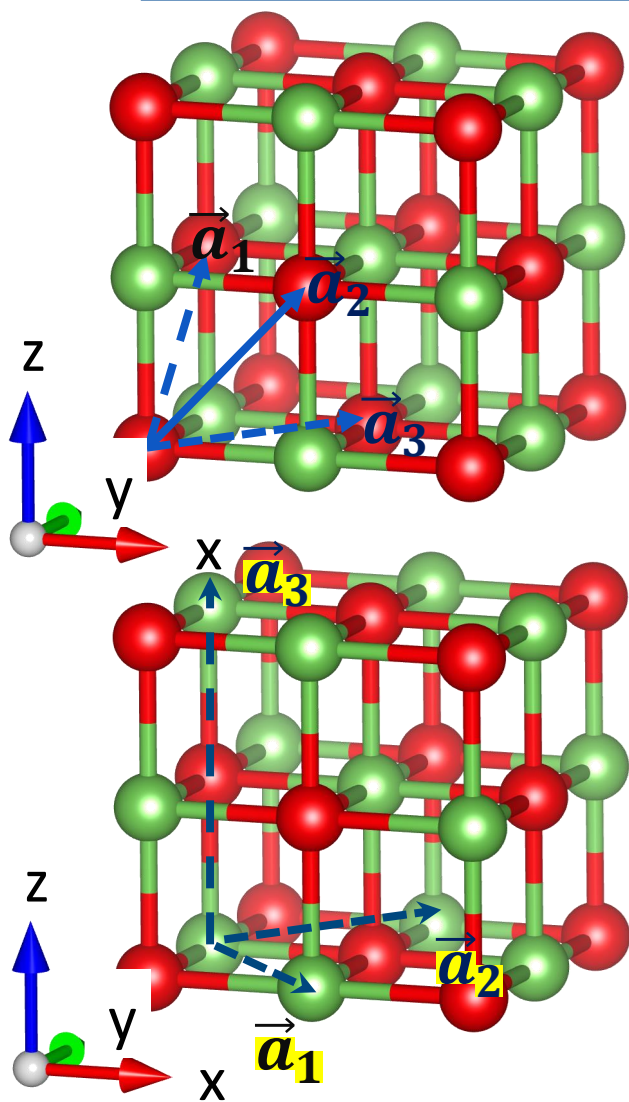
- Compensated semimetals used for spintronics, thermoelectric materials, low contact resistance materials, etc.
- LaSb is an XMR material and on the verge of transition from a trivial semimetal to a topological semimetal



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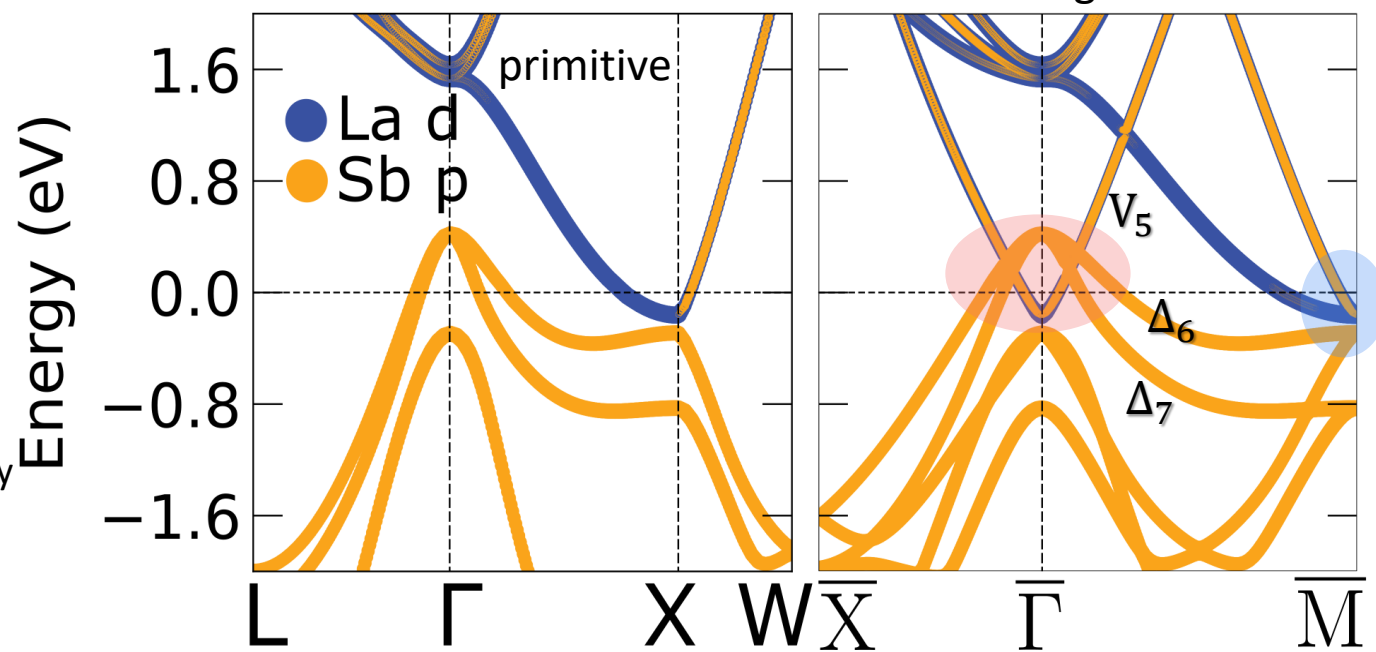
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# Electronic structure of bulk LaSb

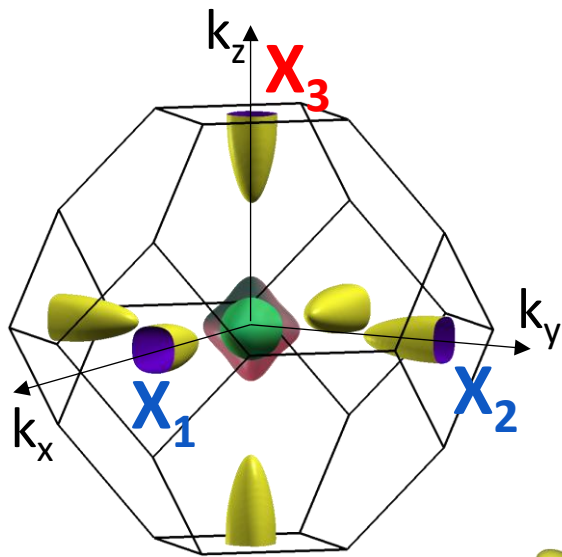
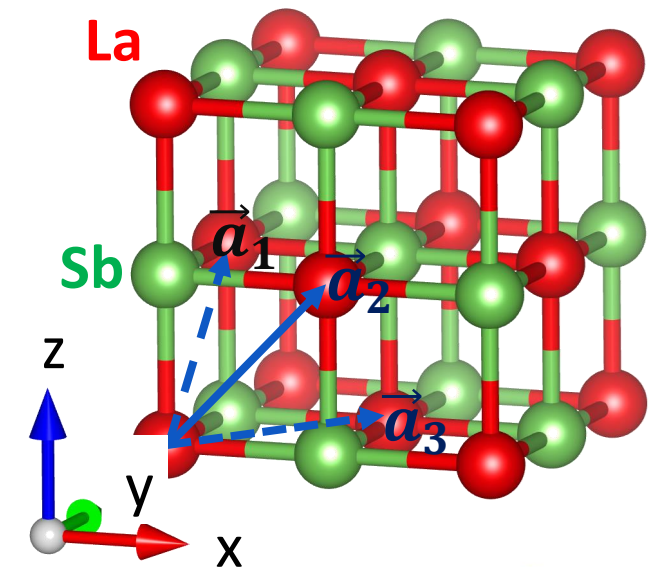


✓  $X_1$  and  $X_2$  projected to  $\bar{M}$   
 ✓  $X_3$  and  $\Gamma$  project to  $\bar{\Gamma}$

SBZ/thin film along [001] BZ

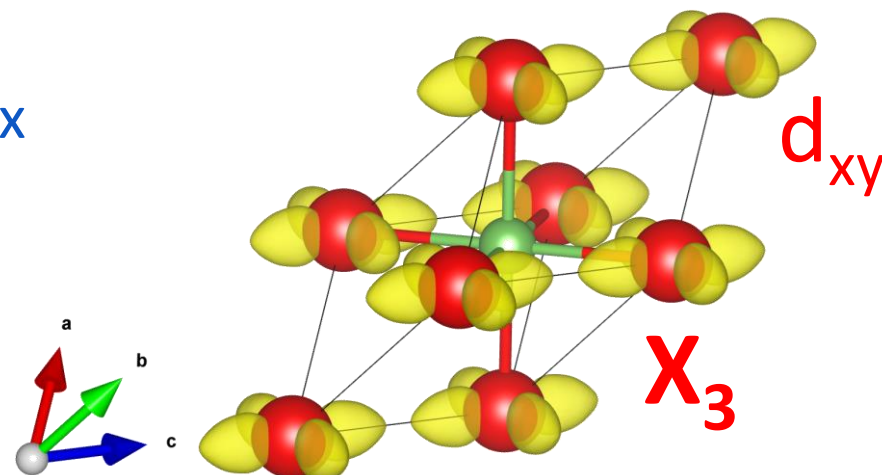
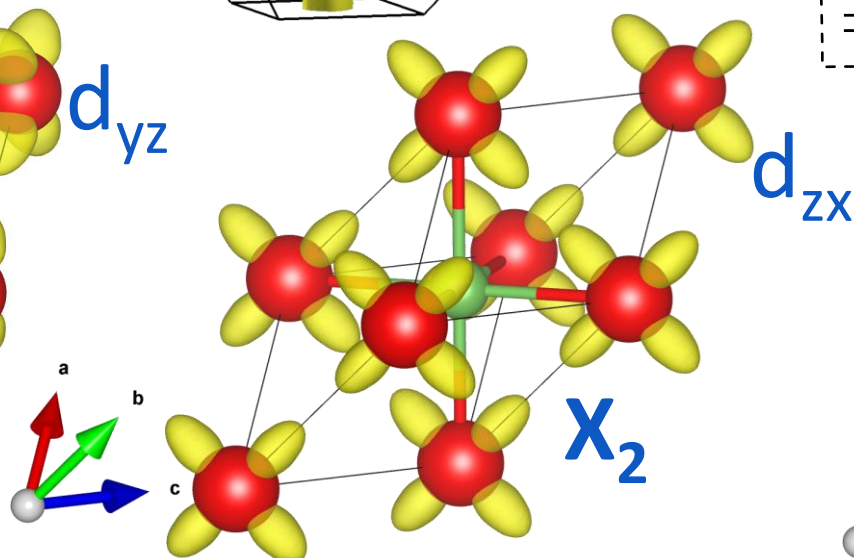
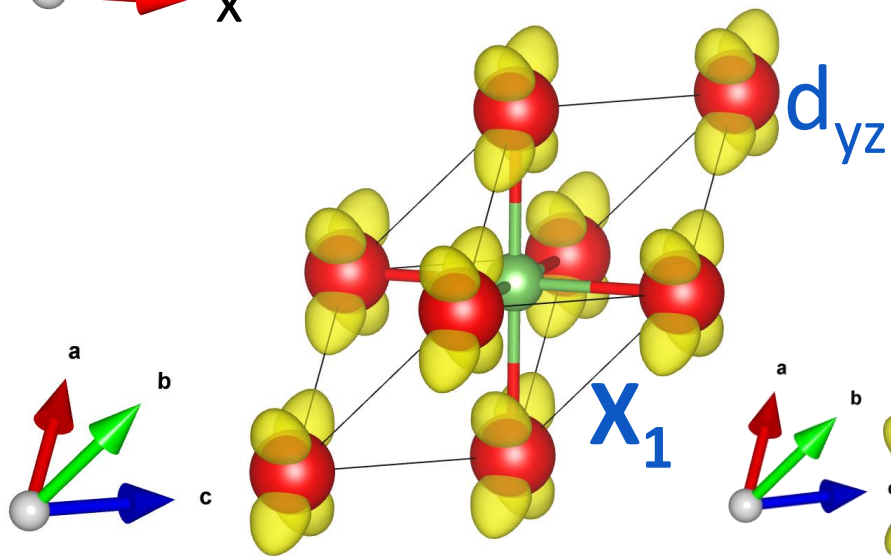


# Orbital composition of e-pocket at $X_i$



Prediction

- ✓  $X_1$  and  $X_2$  composed of *out-of-plane* La-La  $d_{yz}$  and  $d_{zx}$  interactions, respectively
  - ⇒ Strongly affected by size quantization
- ✓  $X_3$  composed of *in-plane* La-La  $d_{xy}$  interaction
  - ⇒ less suffering from confinement

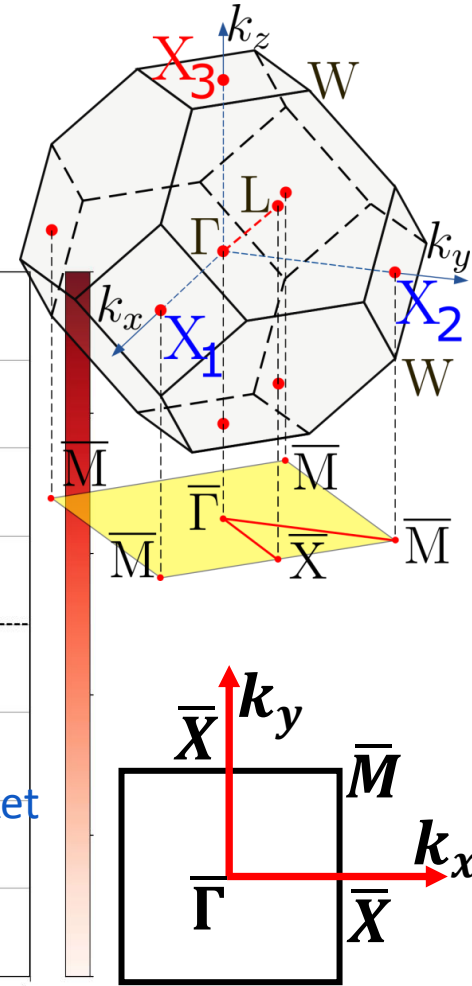
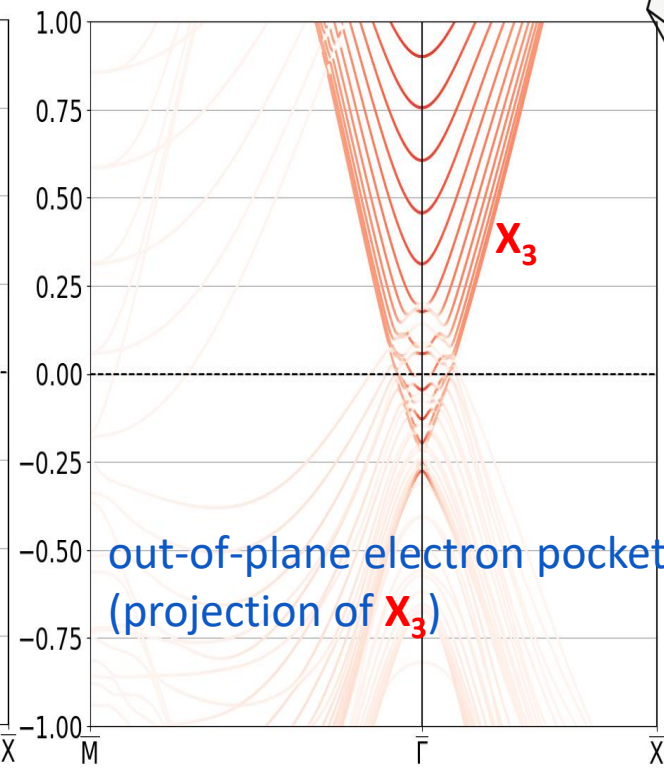
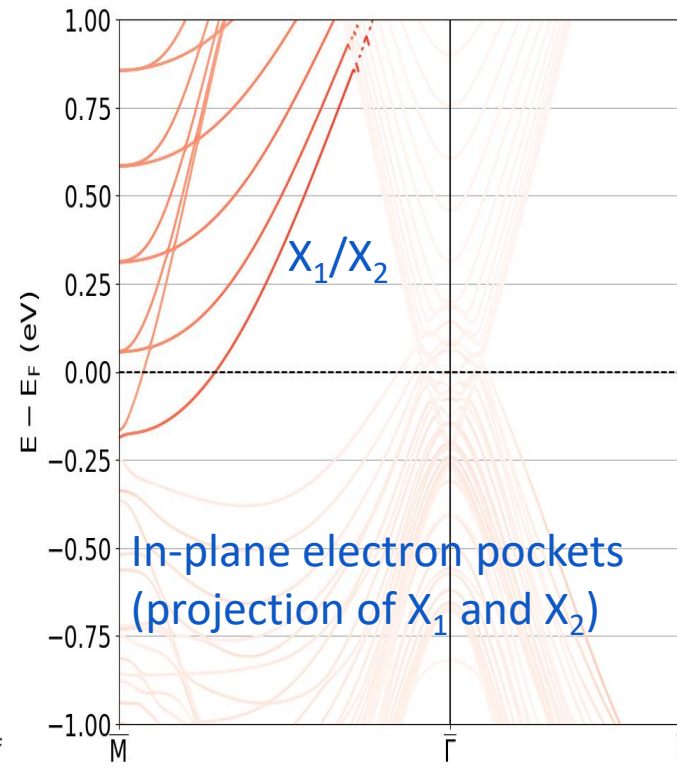
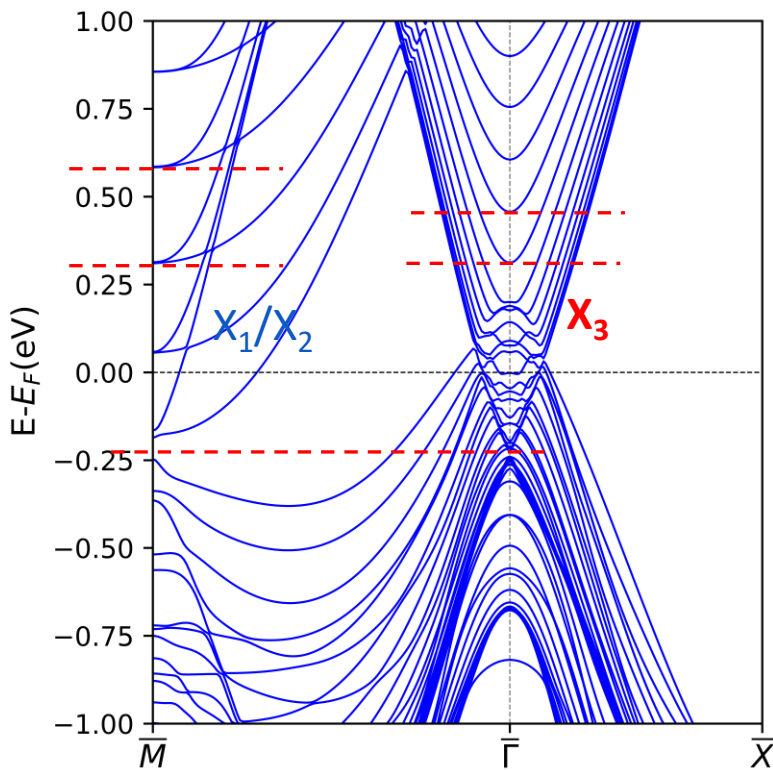


# Electronic structure of 15ML freestanding film LaSb

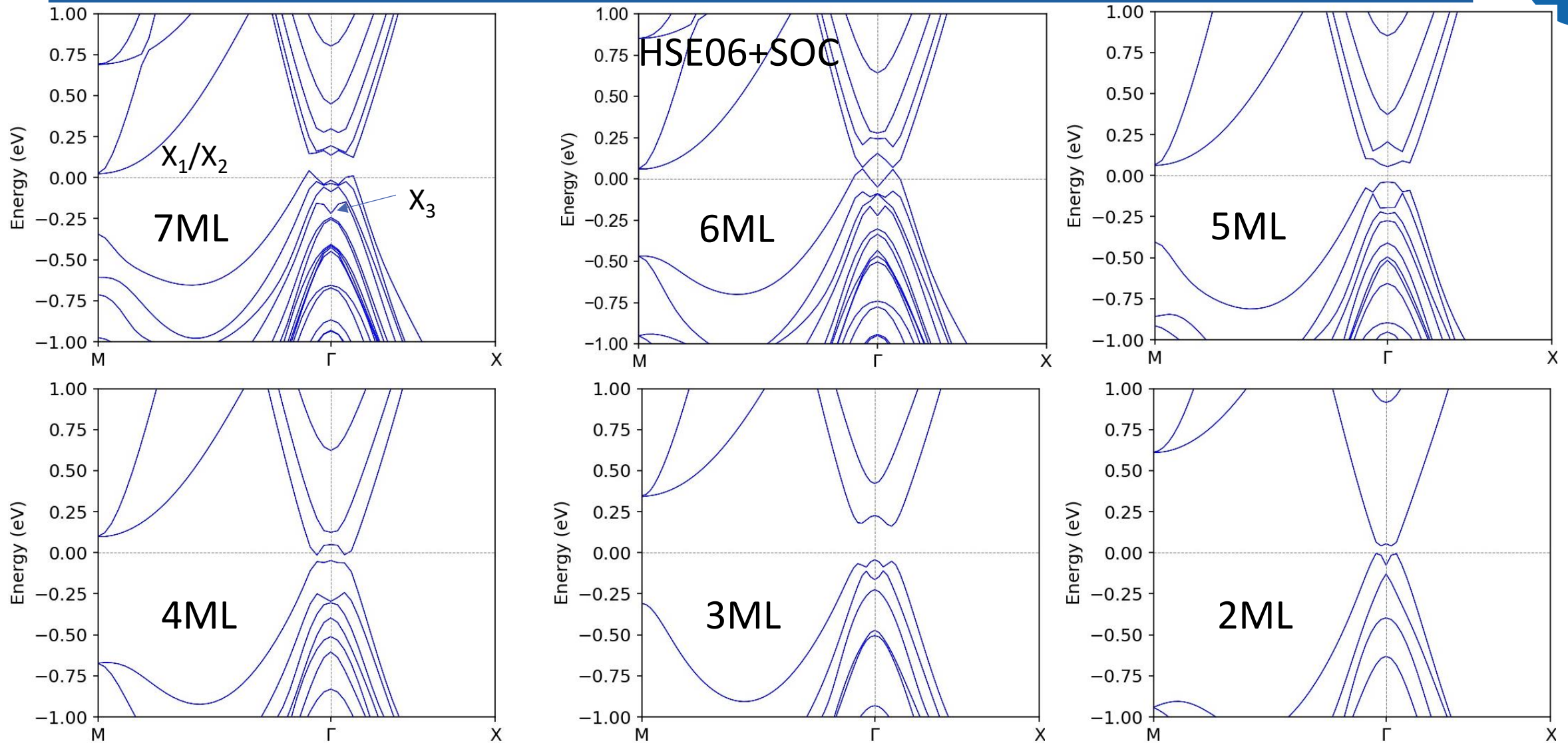


## GGA+U+SOC

- Too many metallic state => the thin film remains metallic
- Difference in the extent of electron pockets movement is not significant
- Substantial quantization effect for in-plane electron pockets
- Interesting interaction around  $\bar{\Gamma}$



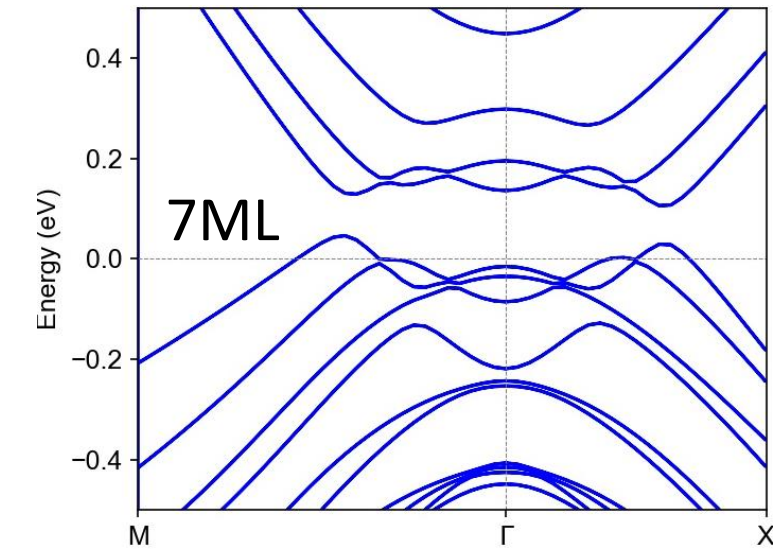
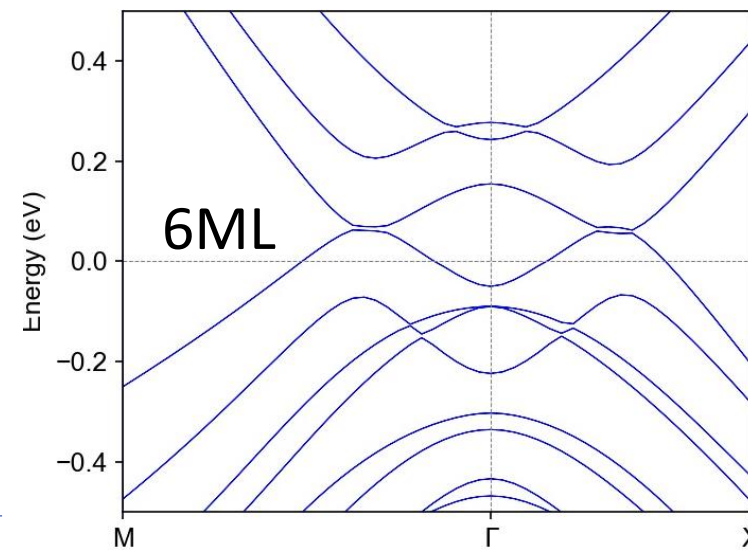
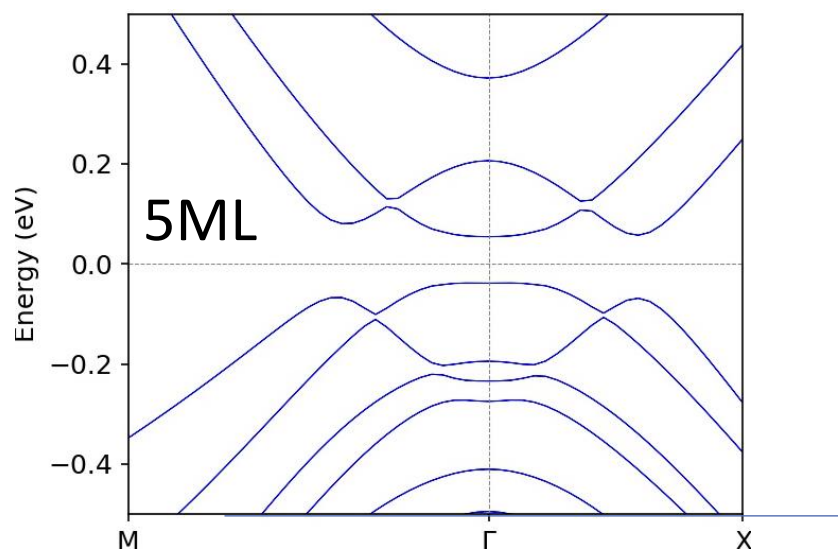
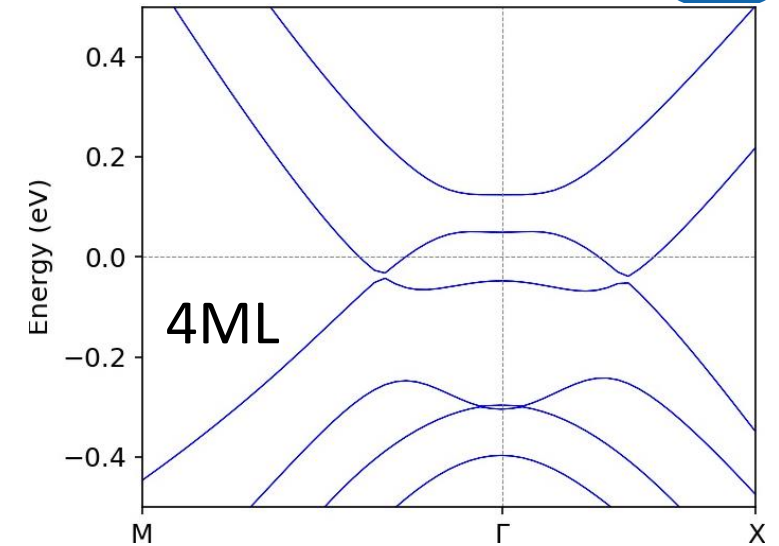
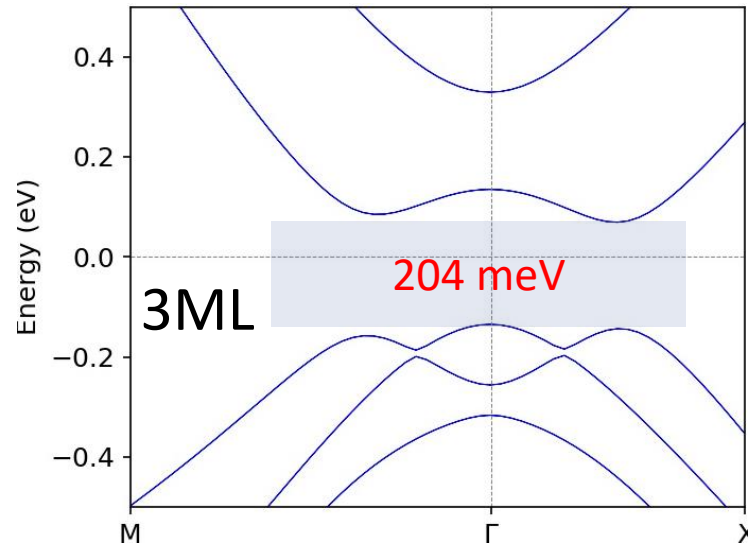
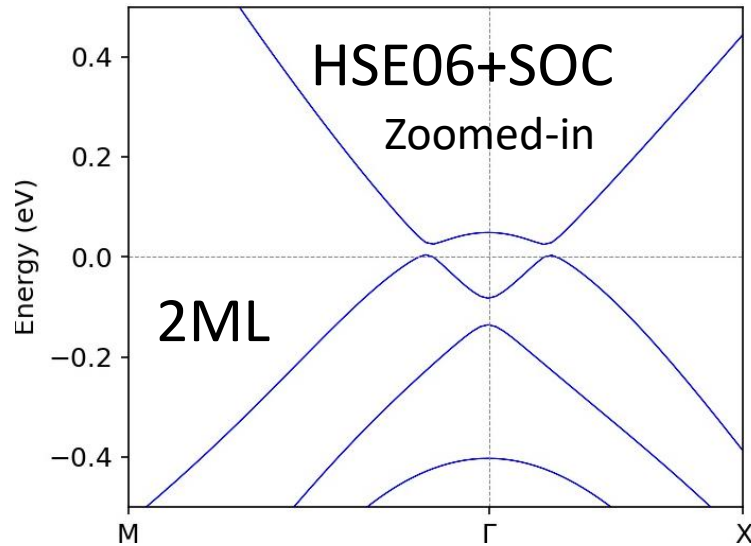
# Electronic structure of thinner LaSb films



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# Electronic structure of thinner LaSb films: a closer look

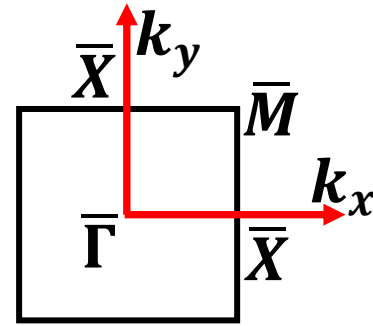


# Electronic structure of 3ML LaSb

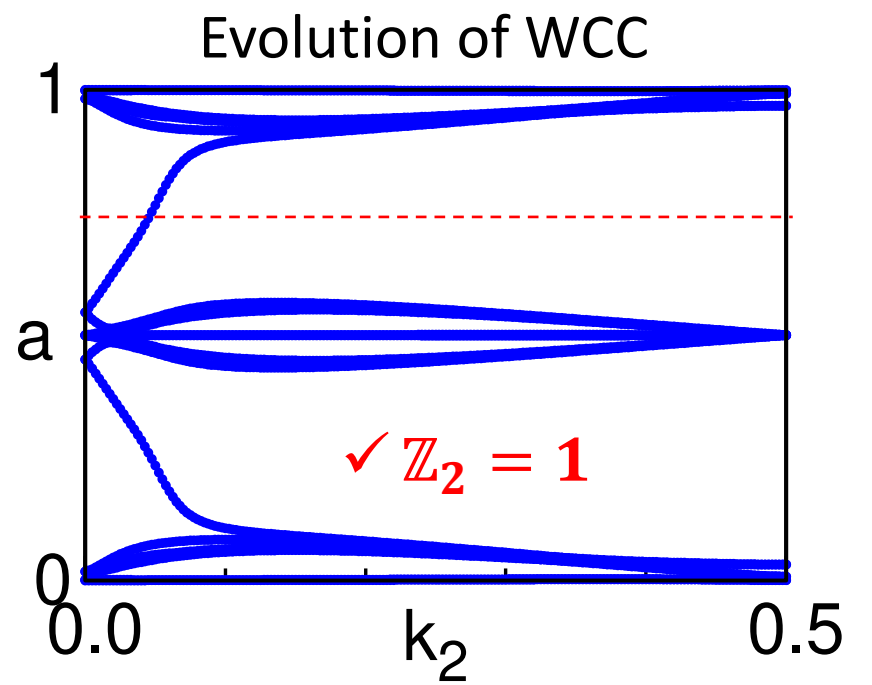
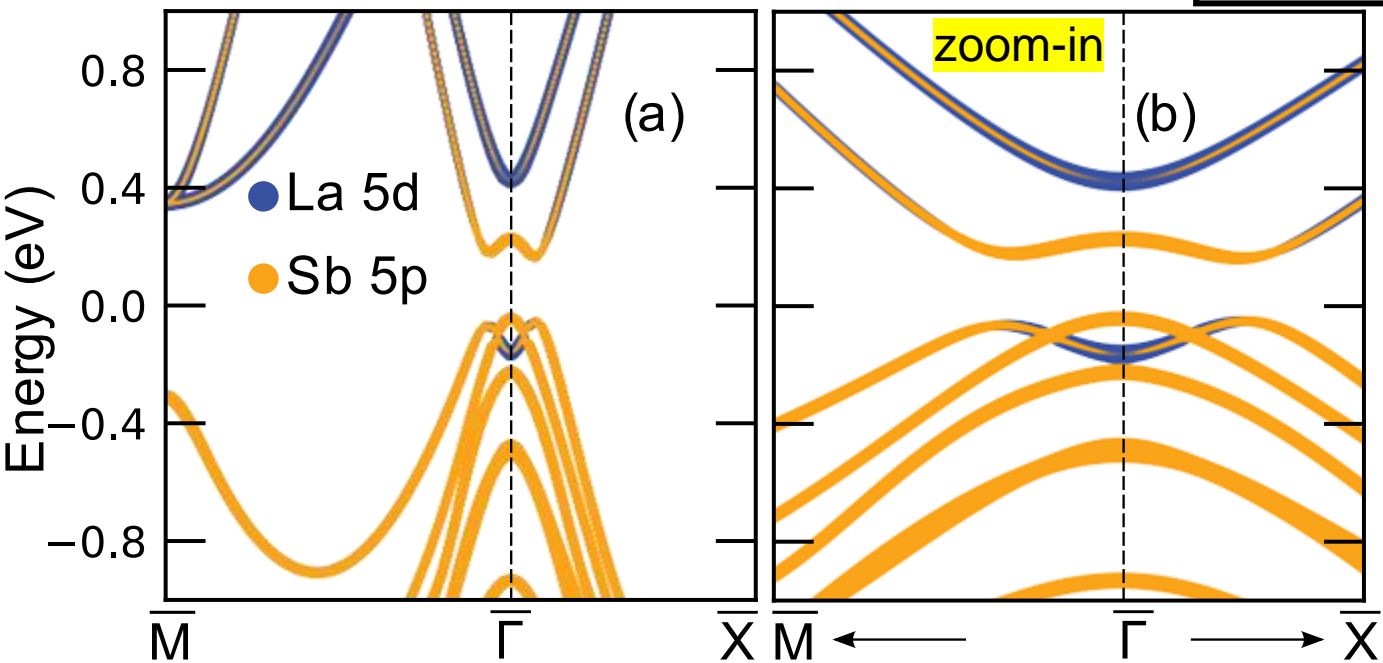


HSE06+SOC calculation

- ✓ Non-magnetic system
  - ✓ Inverted and sizable gap
- => Possible Quantum Spin Hall insulator



*Characteristics of QSH:  
 $\mathbb{Z}_2$ , evolution of WCC?  
spin-polarized edge states and  
Dirac point protected by TRS?*

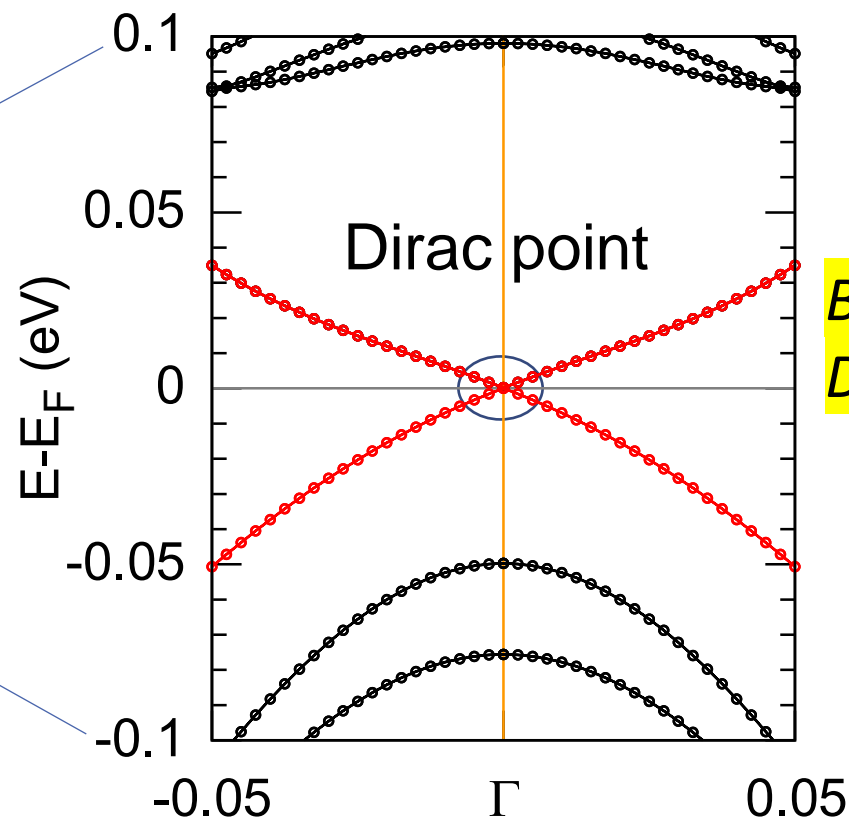
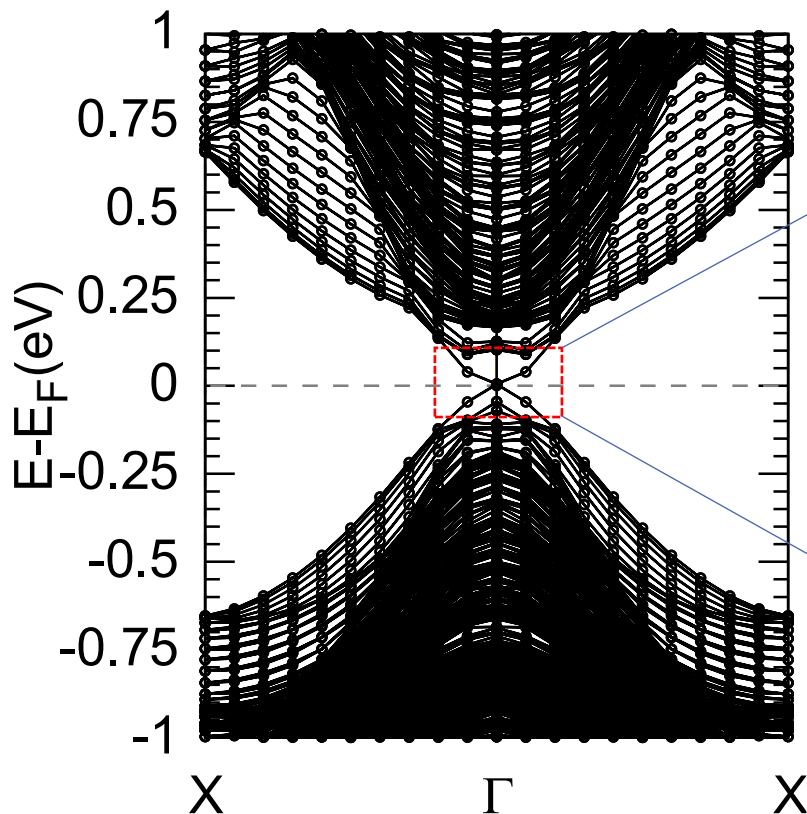
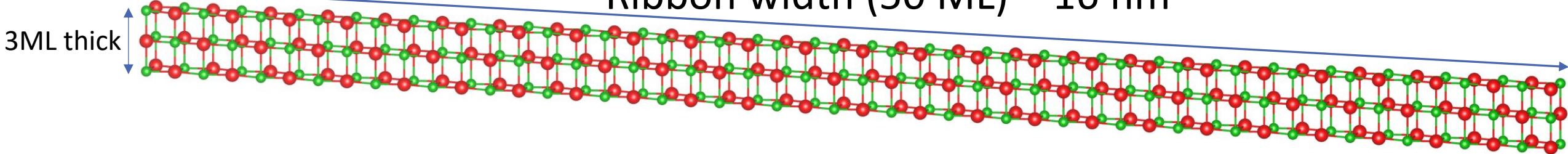




# Observation of edge states and Dirac point



Ribbon width (50 ML)  $\sim$  16 nm

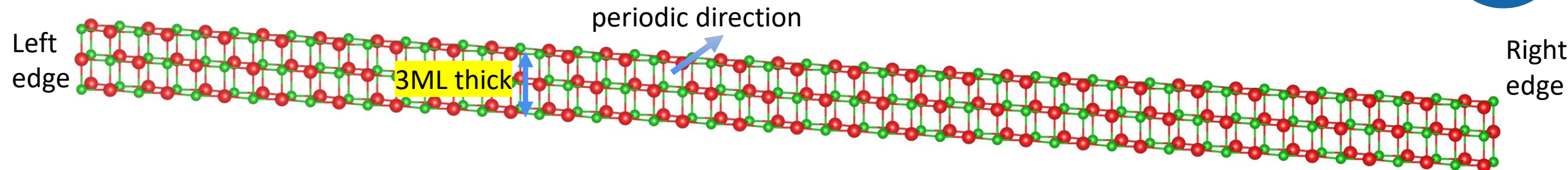


*Band crossing featuring  
Dirac point observed!*

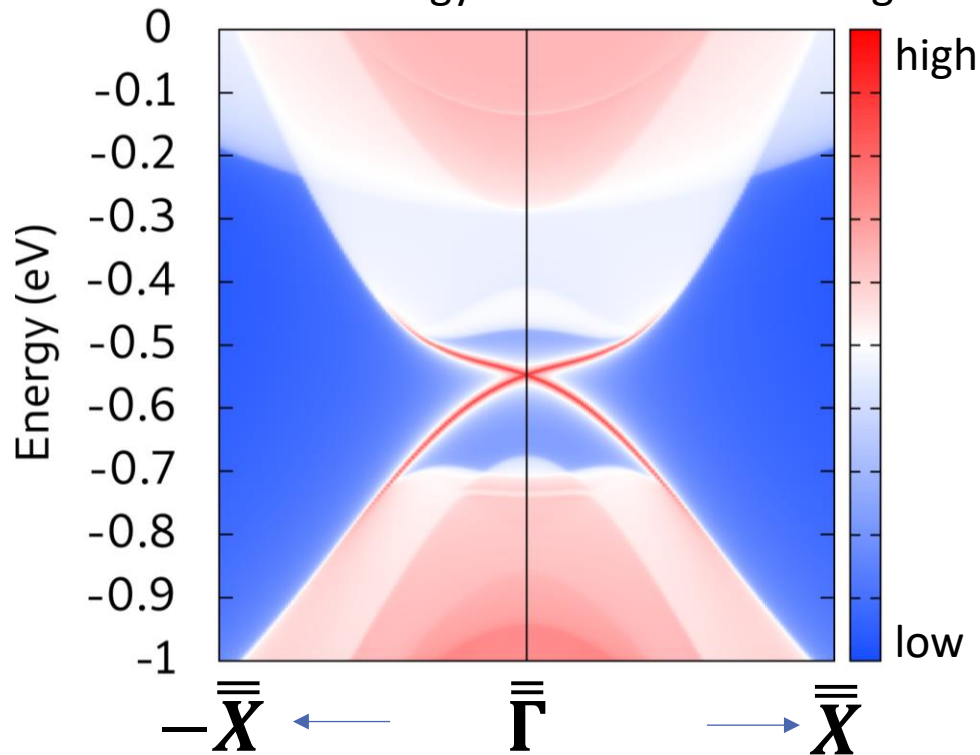
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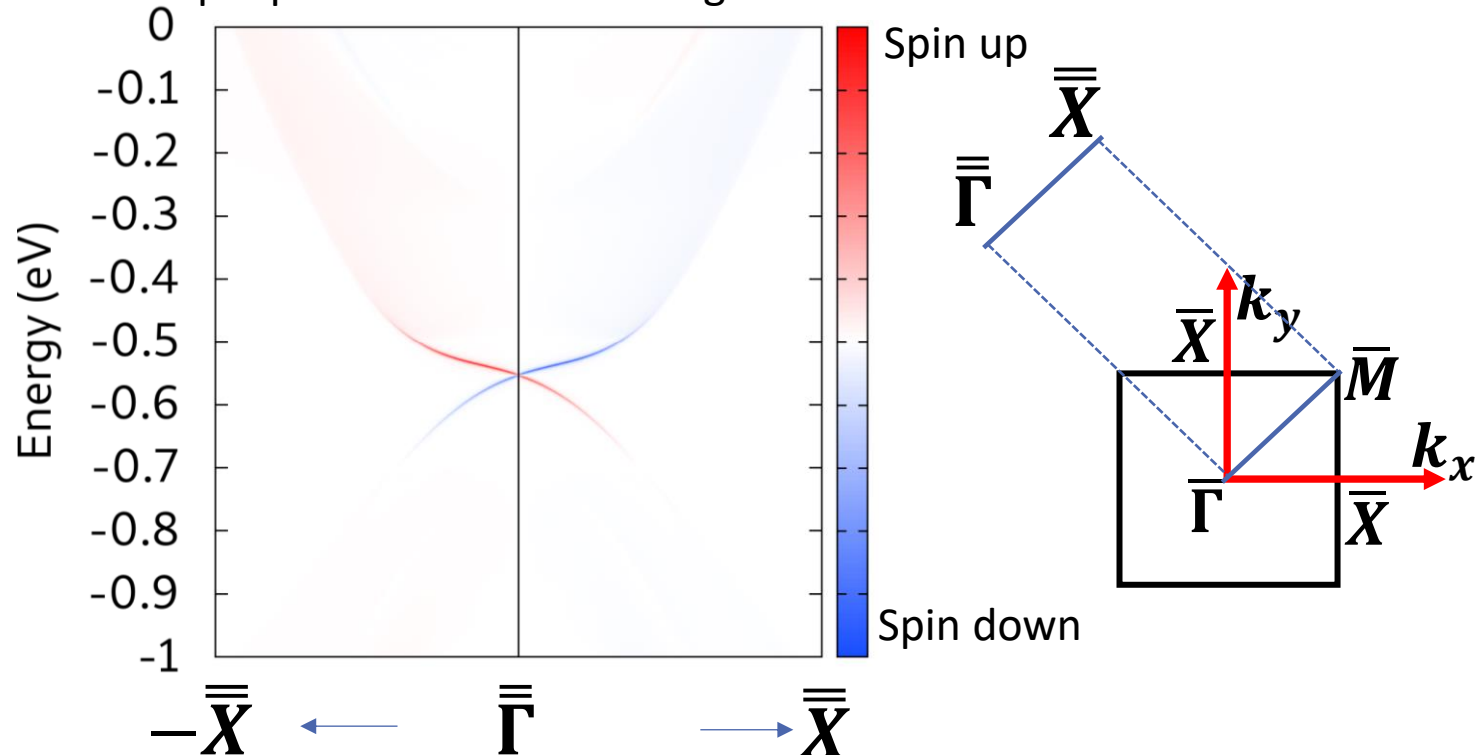
# Spin polarization of edge states in momentum space



momentum and energy resolved DOS for edge states



Spin polarization for the edge states



- ✓ Observation of phase transition for LaSb from a trivial semimetal in the bulk to a sizeable gap QSH insulator in the ultrathin film limit characterized by  $\mathbb{Z}_2 = 1$ , TRS-protected Dirac point, and spin-polarized edge states
- ✓ The origin of the QSH phase is due to inverted band feature between La-d and Sb-p at  $\Gamma$  and gap opening by SOC.
- ✓ This phenomenon could be observed for other RE-Vs

# Acknowledgements

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- NSF MRSEC project for funding
- XSEDE for computational resources
- Dr. Janotti at UD and Dr. Bryant at NIST research groups

