Tuning electronic band topology of rare-earth monopnictides

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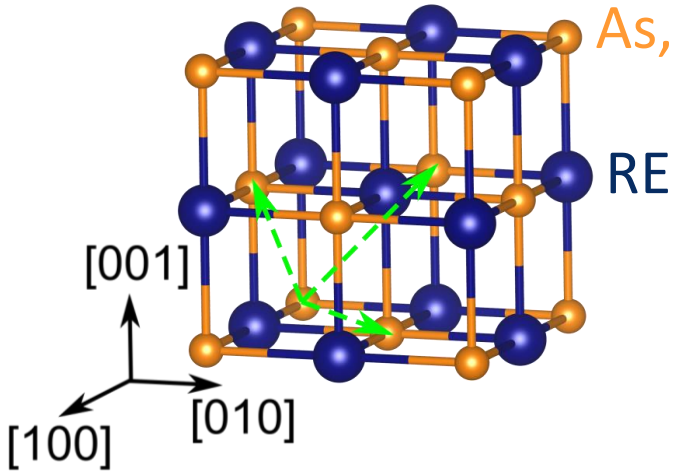
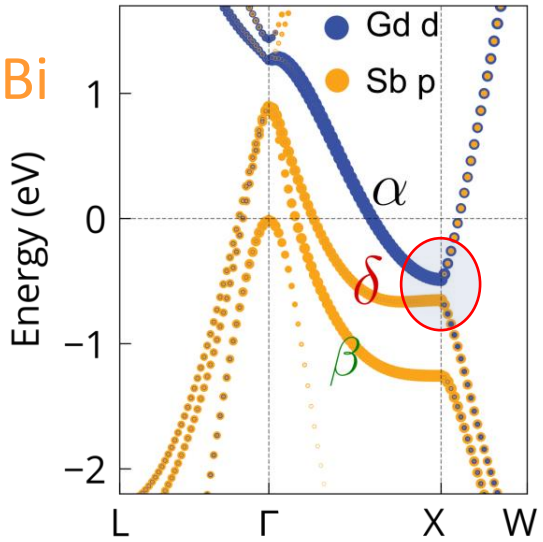
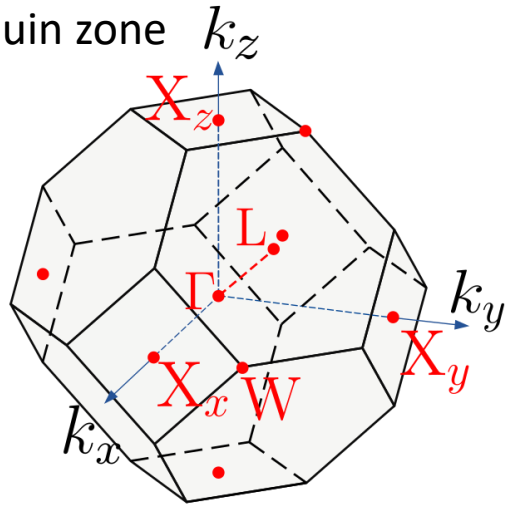
RE-V: a semimetallic with many interesting properties

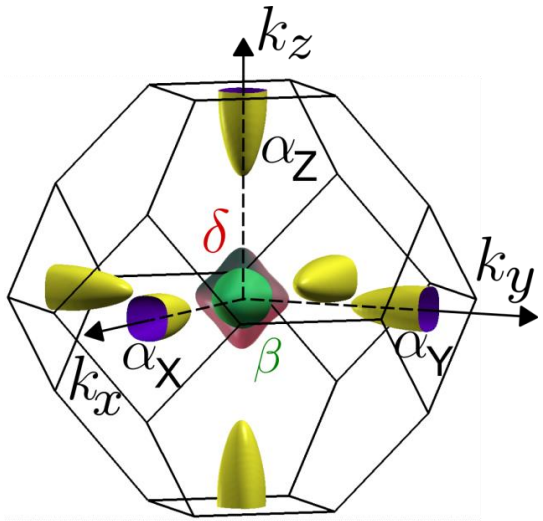
FCC crystal structure





Bulk Brillouin zone





- Compensated semimetalics used for spintronics, thermoelectric materials, low contact resistance materials, etc.
- Depending on the overlap between electron and hole at the X point: trivial semimetal or topological insulator

=> How to control topological property of a given RE-V?

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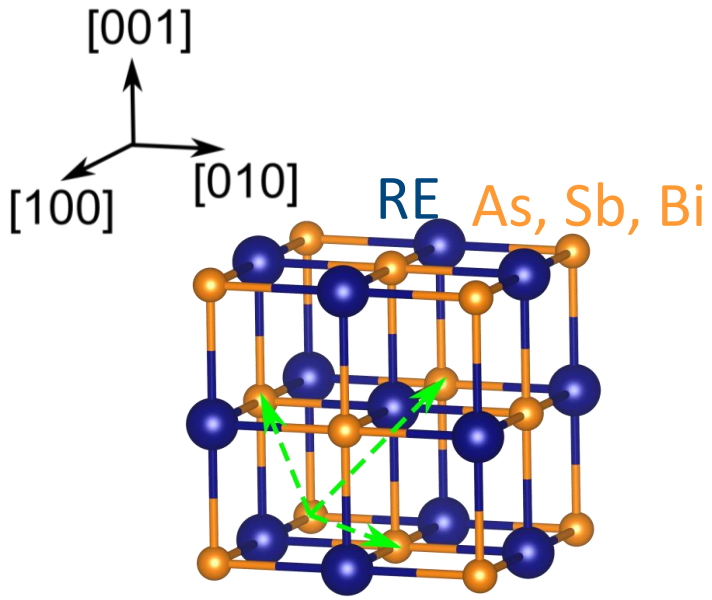
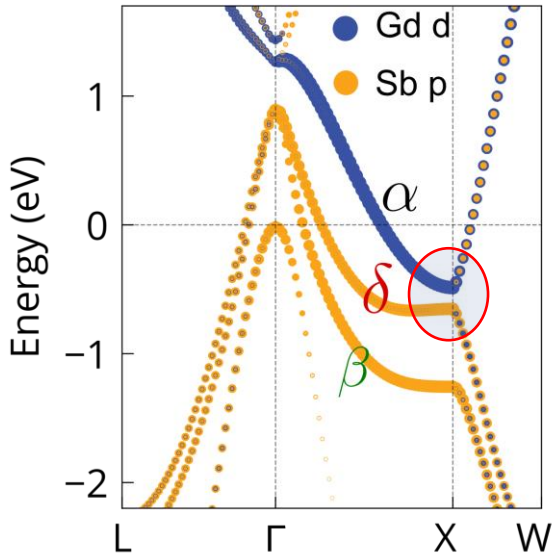
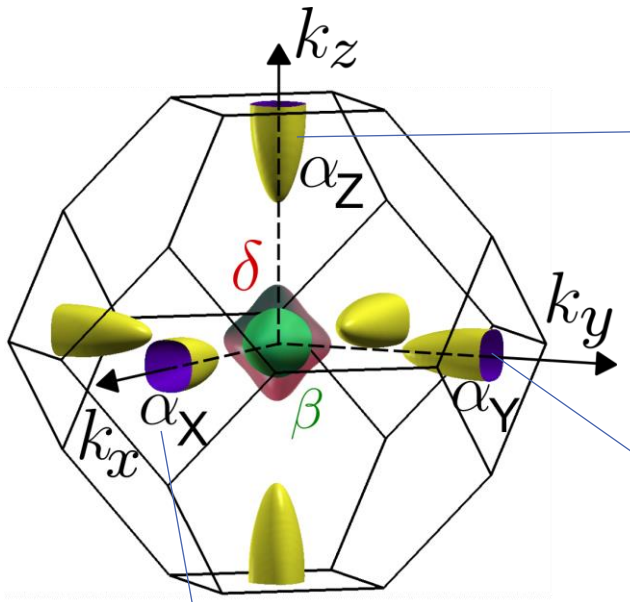
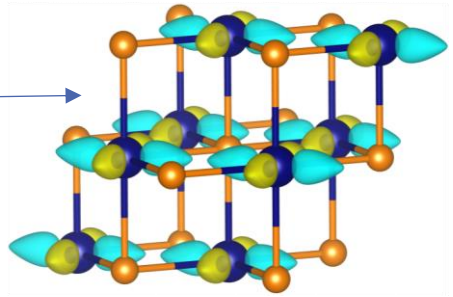
Ho *et al.*, *ACS Nano* 2023, 17, 21, 20991–20998
Natali *et al.*, *Progress in Materials Science* 2013, 58, 1316–1360

Directional characteristic of electron pockets

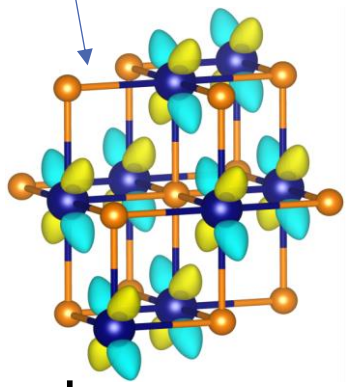




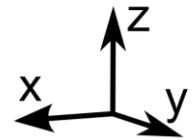


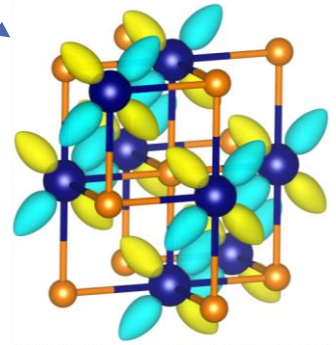


α_Z: d_{xy}



α_X: d_{yz}





α_Y: d_{xz}

- In-plane dispersion such as electron pockets $\alpha_{X,Y}$ derived from d orbital pointing out of plane
- Out-of-plane dispersion: electron pockets α_Z derived from d orbital lying in-plane

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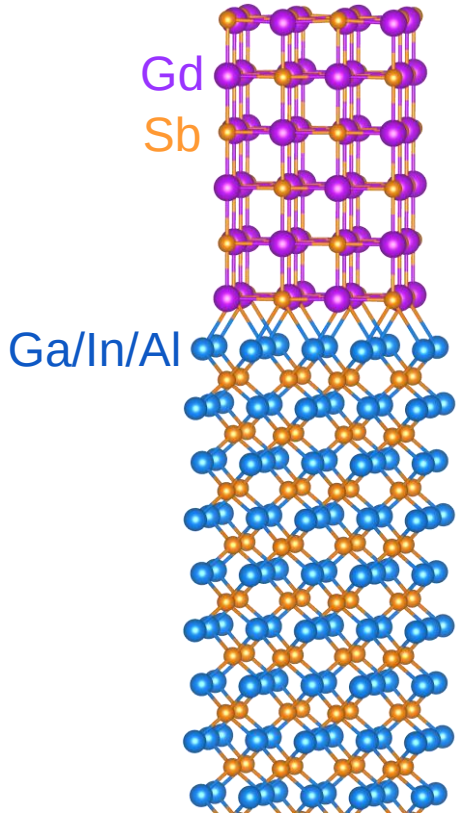
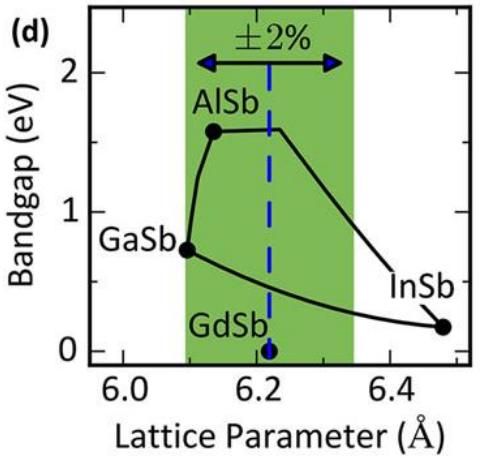
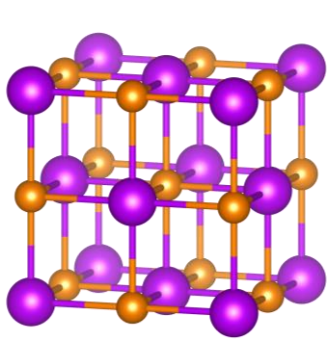
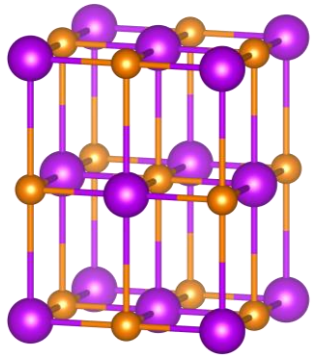
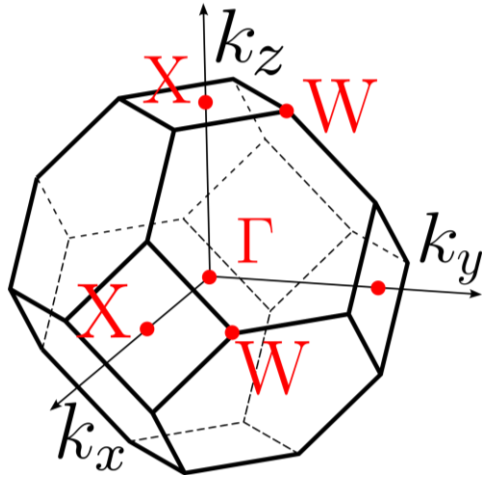
Electronic topology under strain

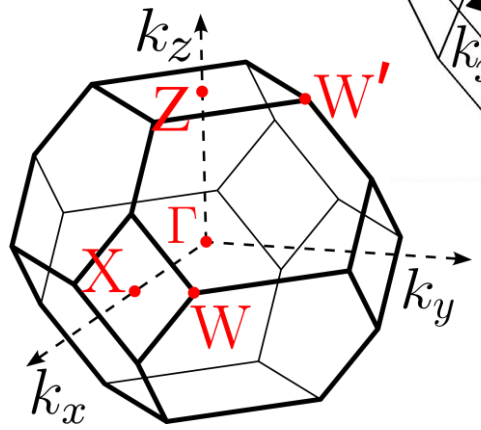


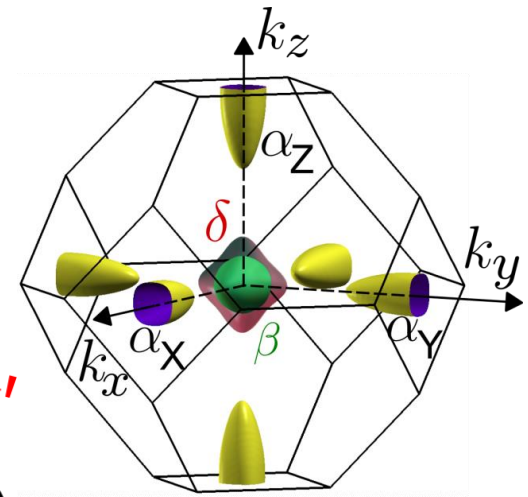












- Electron pockets with orbitals *lying perpendicular to film plane* will not be affected by in-plane strain
- Electron pocket at Z with in-plane dxy orbital will be more affected

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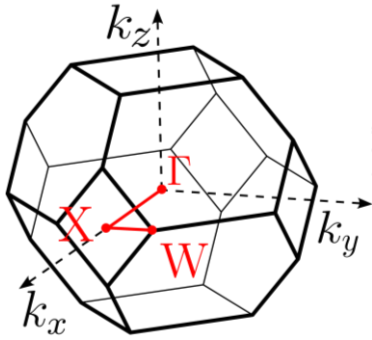
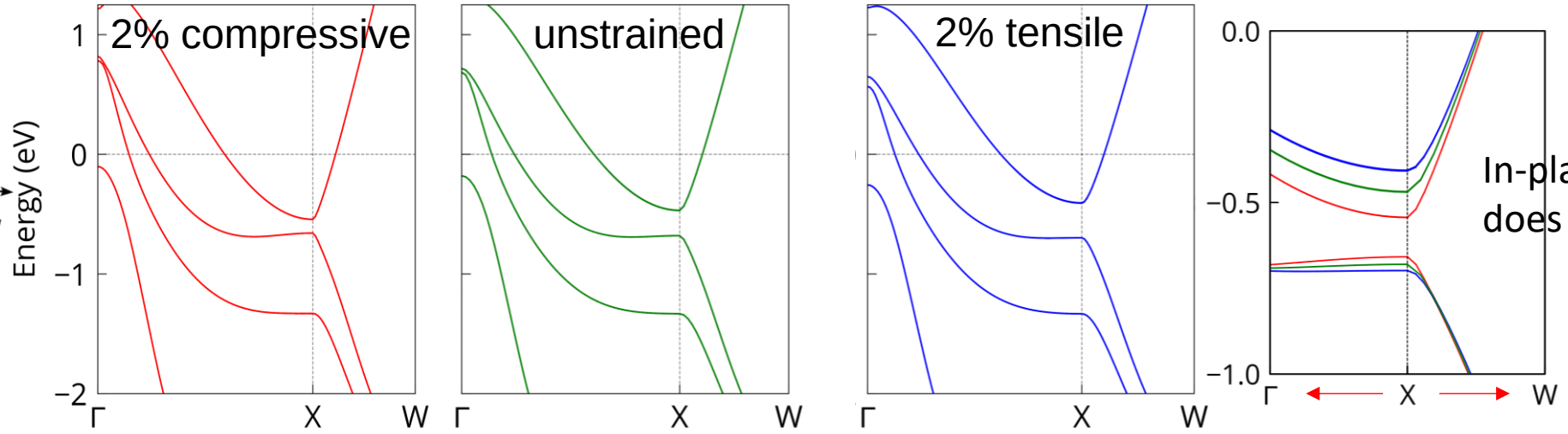
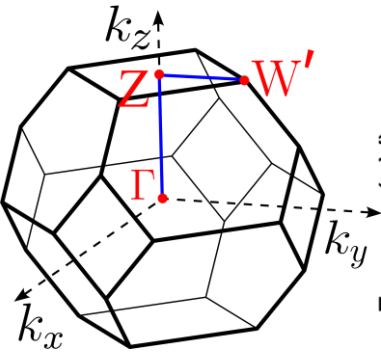
Effect of strain to band dispersion and band topology



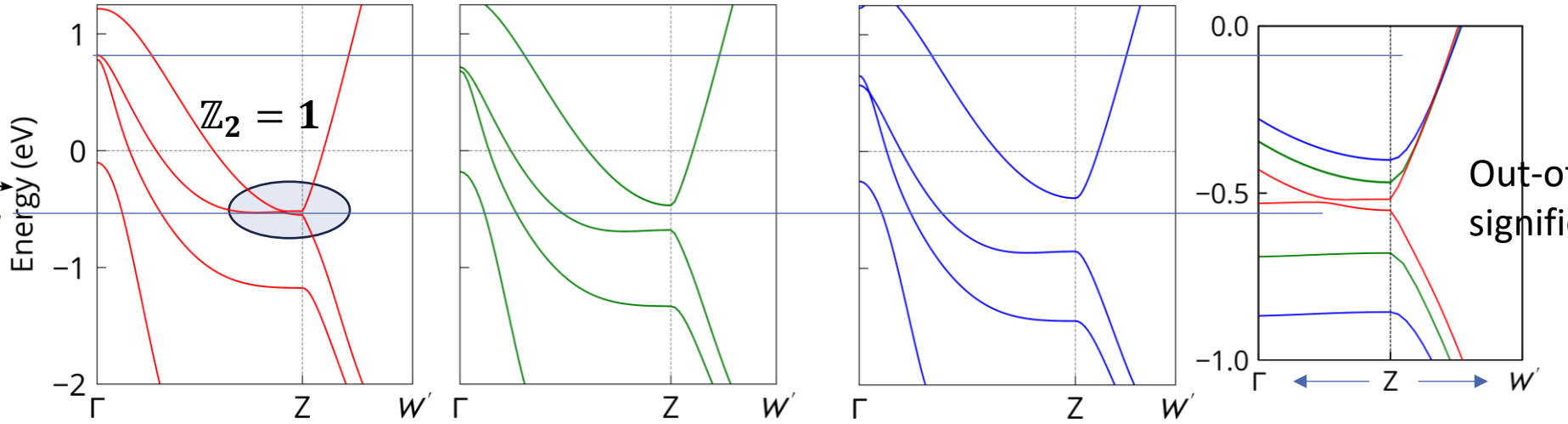
In-plane dispersion



In-plane dispersion does not change much



Out-of-plane dispersion



Out-of-plane dispersion significantly changed

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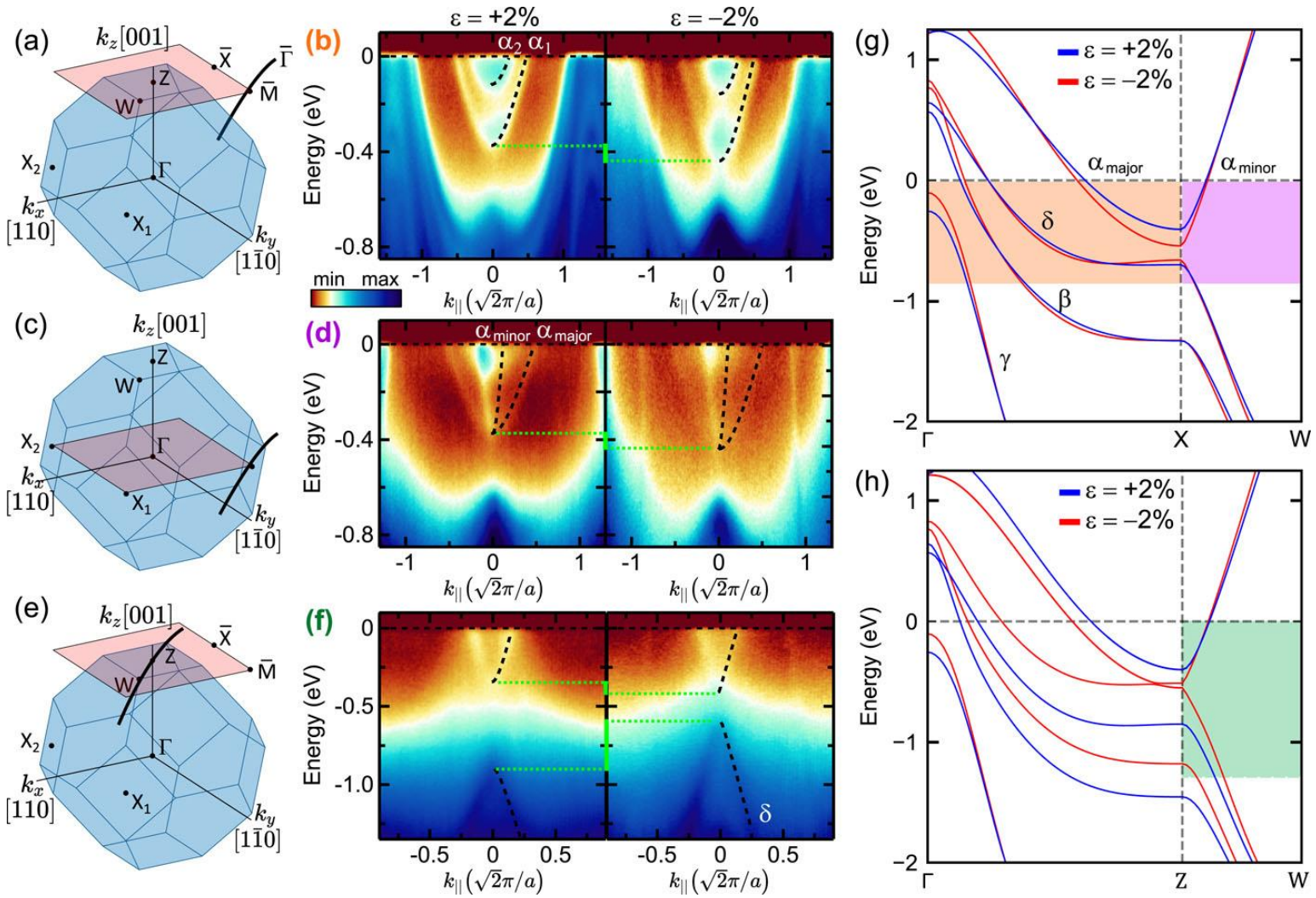

- In-plane electron pockets: lower energy for compressive strain than that of tensile one
- In-plane hole pocket: relatively unchanged

- Out-of-plane electron pockets: lower energy for compressive strain than that of tensile one
- Out-of-plane hole pocket: moving up quite significant, lowering the gap at Z

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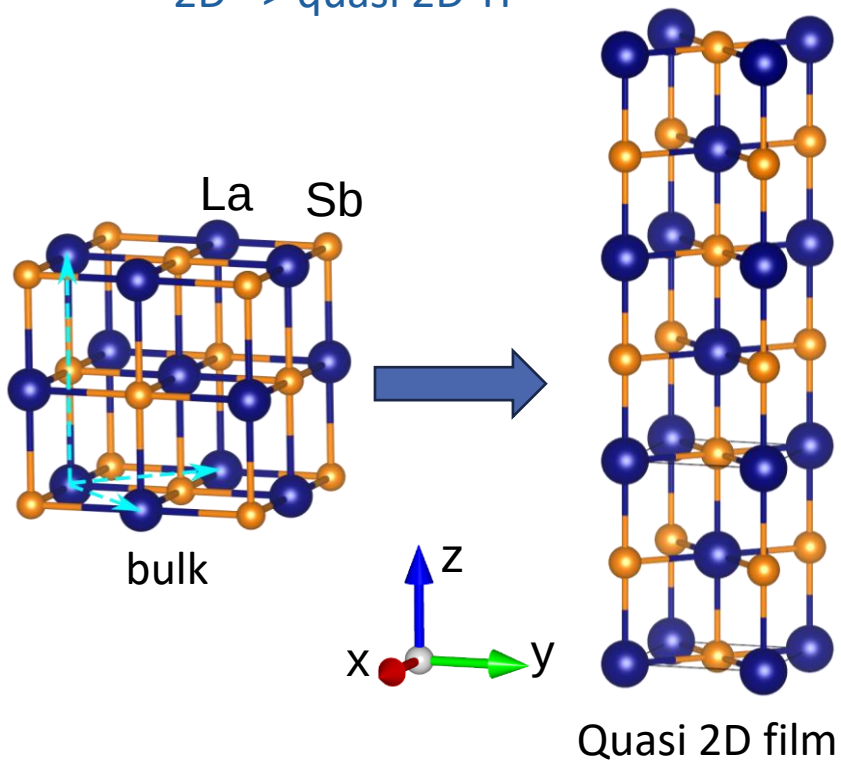
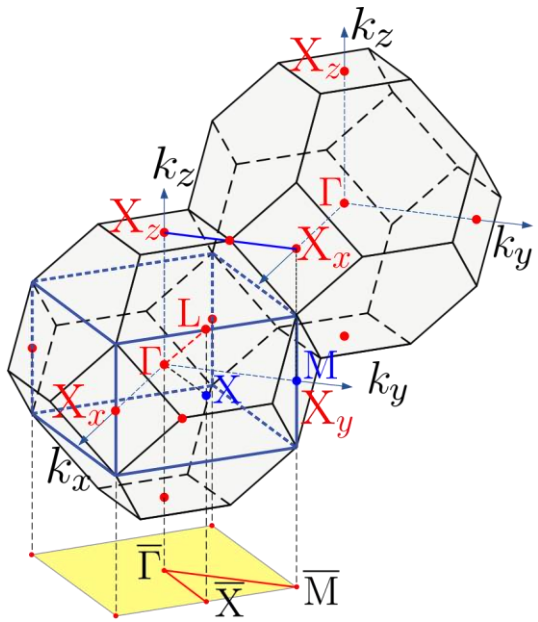
Electronic structure in ultra-thin film limit

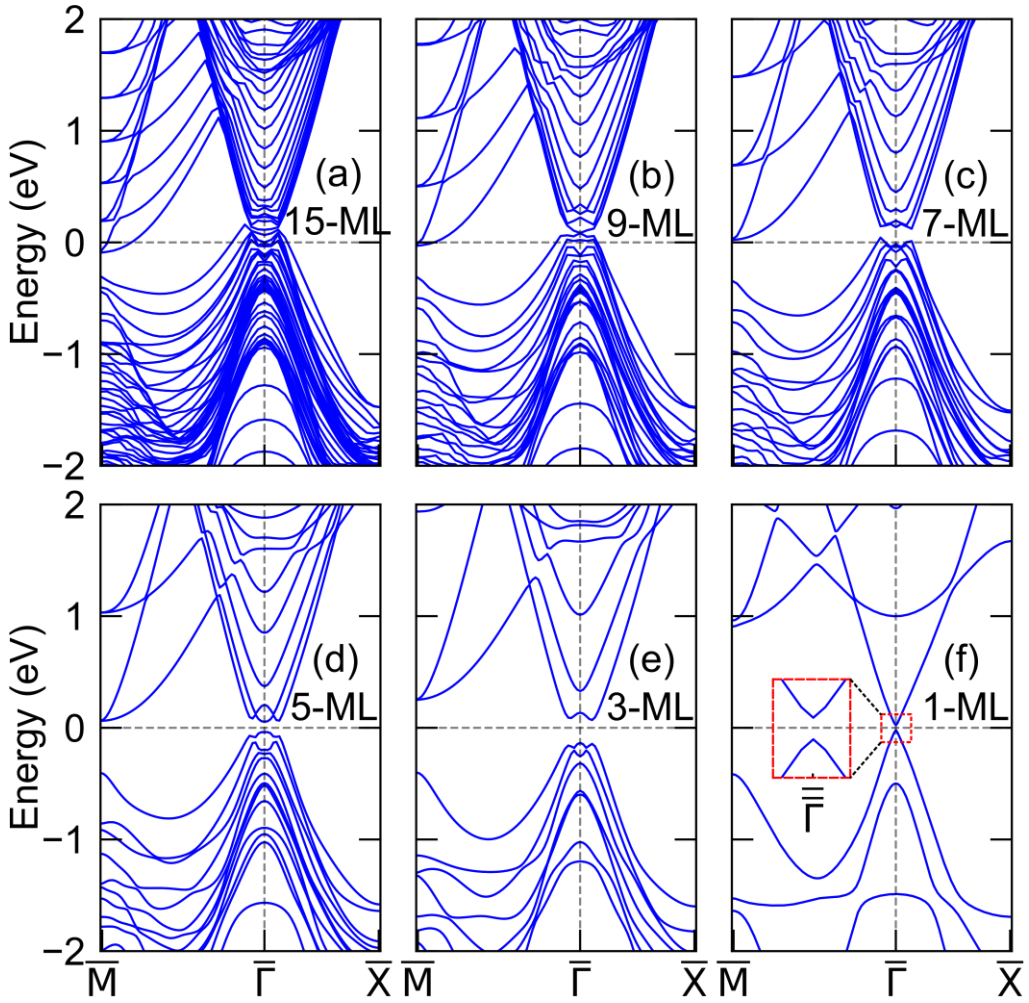
- *In-plane* electron pockets along x and y are strongly influenced by quantum confinement effect
- Electron pocket along z are much less affected

=> band inversion at BZ center

- Starting from 7ML, a gap is opened throughout the whole BZ of 2D => quasi 2D TI







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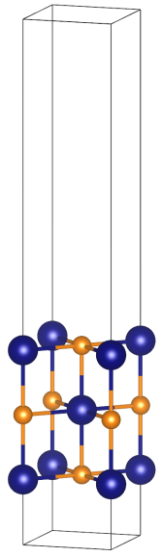
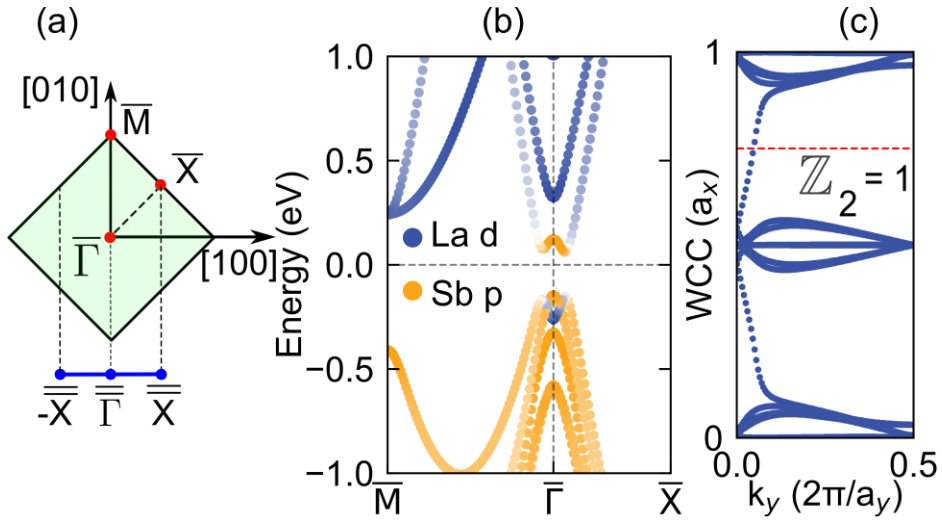
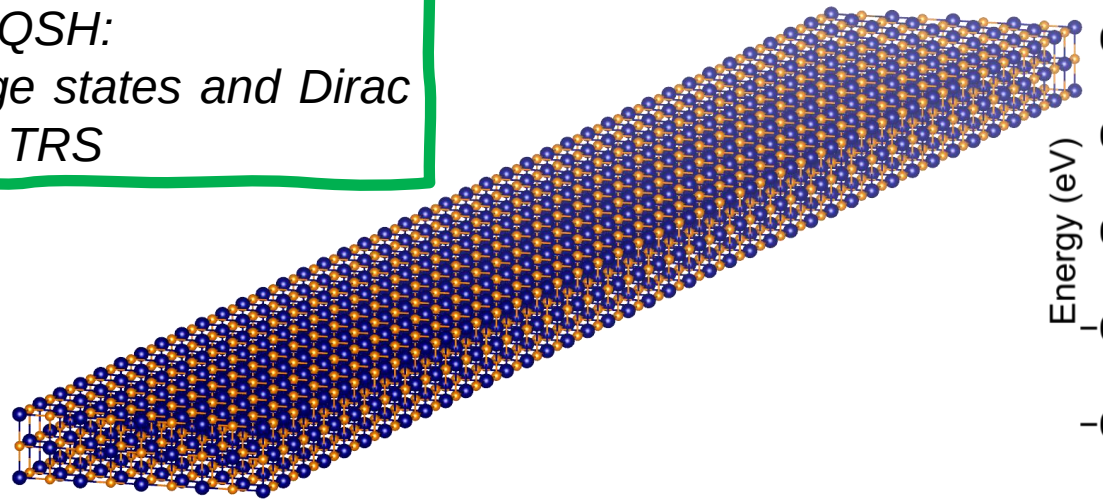
Signature of quantum spin Hall insulator in ultra-thin films

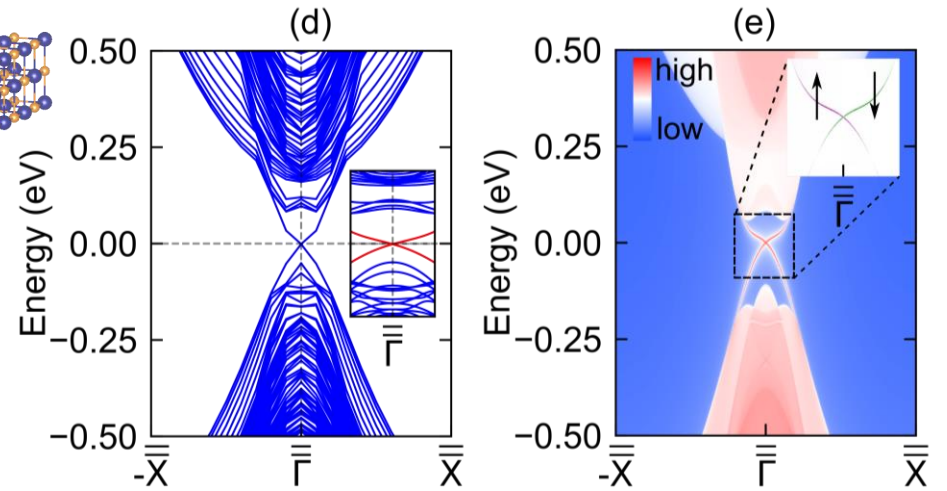
Characteristics of QSH:
- ✓ $\mathbb{Z}_2 = 1$
- ✓ *evolution of WCC*





Characteristics of QSH:
spin-polarized edge states and Dirac point protected by TRS





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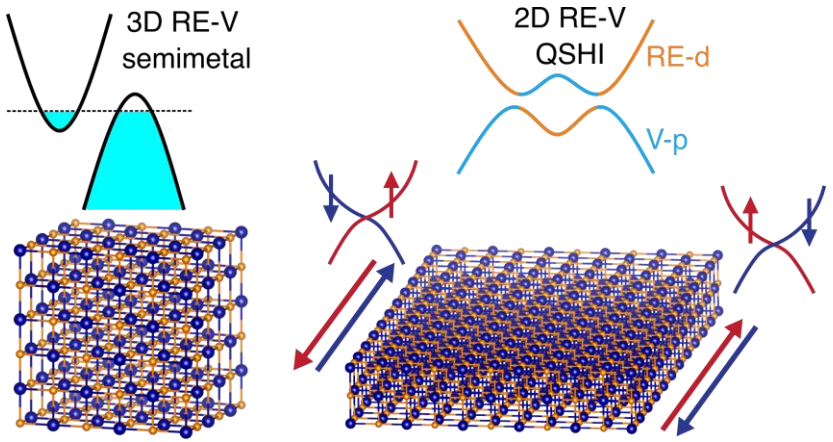
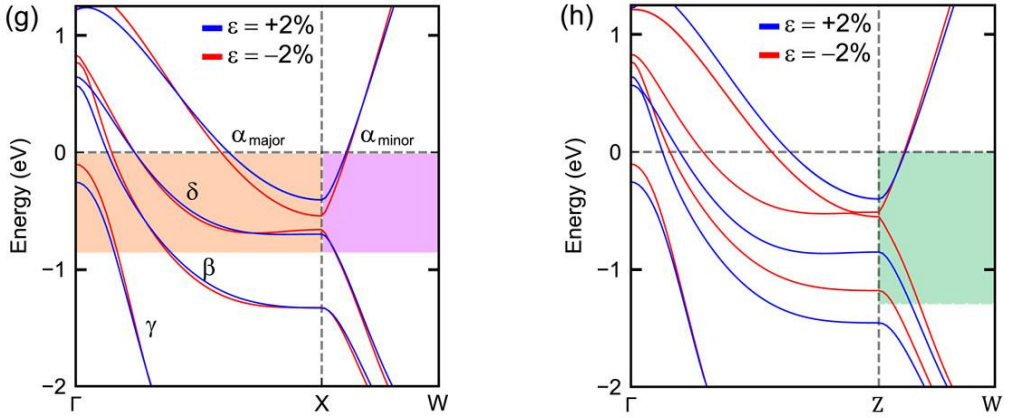
Conclusion





- ✓ 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 Γ and gap opening by SOC.
- ✓ This phenomenon could be observed for other RE-Vs

- ✓ Observation of phase transition for GdSb from a trivial semimetal to topological insulator phase characterized by $\mathbb{Z}_2 = 1$ due to expitaxial strain
- ✓ Origin of the topological phase is due to band inversion at the Z point tunable by expitaxial strain.
- ✓ Epitaxial strain is an effective way to tune electronic structure of RE-Vs

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