Bulk Band Structure of Bi_2Te_2Se

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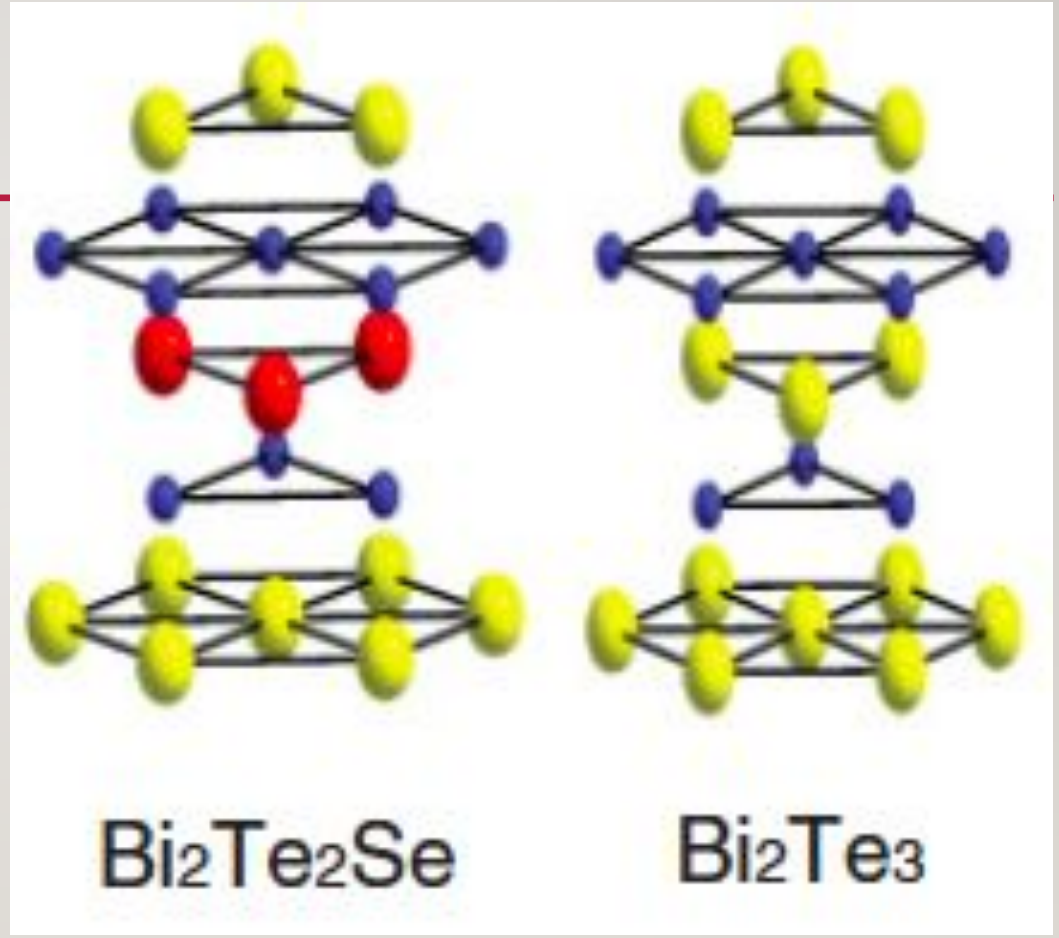
STRUCTURE & COMPOSITION

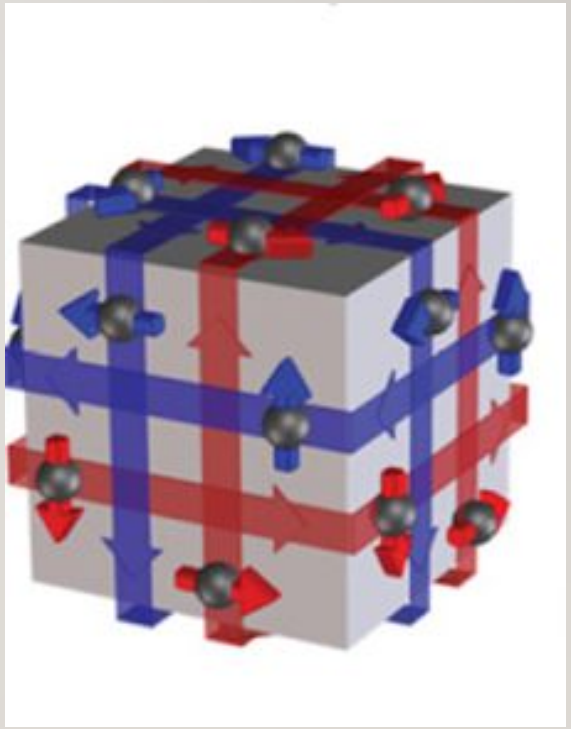
- **Tetradymites, Chemical formula of M_2X_3 where M is a group V metal and X is a group VI anion; also rhombohedral**
- **Formed by stacks of quintuple layers connected by van der Waals bonds**
- **Induced electrical interactions that are intermolecular**



S. Jia et al., PRB **84**, 235206

WHY INTERESTED IN BI_2TE_2SE?

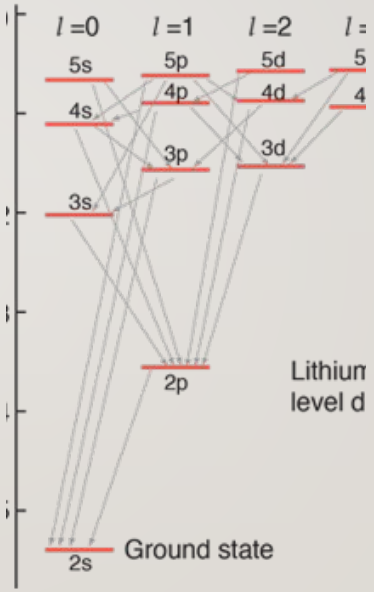
- **Bi_2Te_2Se is a topological insulator(TI)**
- **Materials that are insulating at the bulk and conducting at the surface**
- **TI's have applications in computer memory such as non-volatile random access memory (NVRAM) due to spin-momentum locking**
- **Difficulty observing transport properties of surface states**

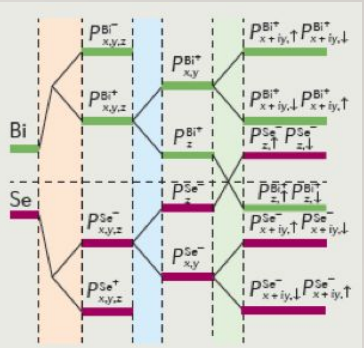


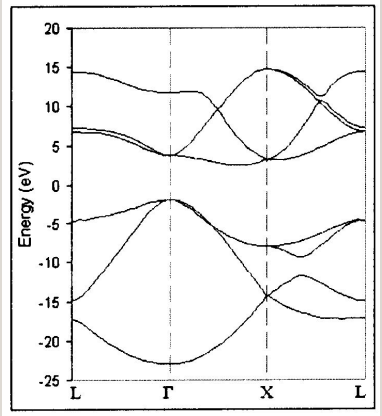
http://research.physics.berkeley.edu/lanzara/research/ti.html

WHAT IS BAND STRUCTURE?

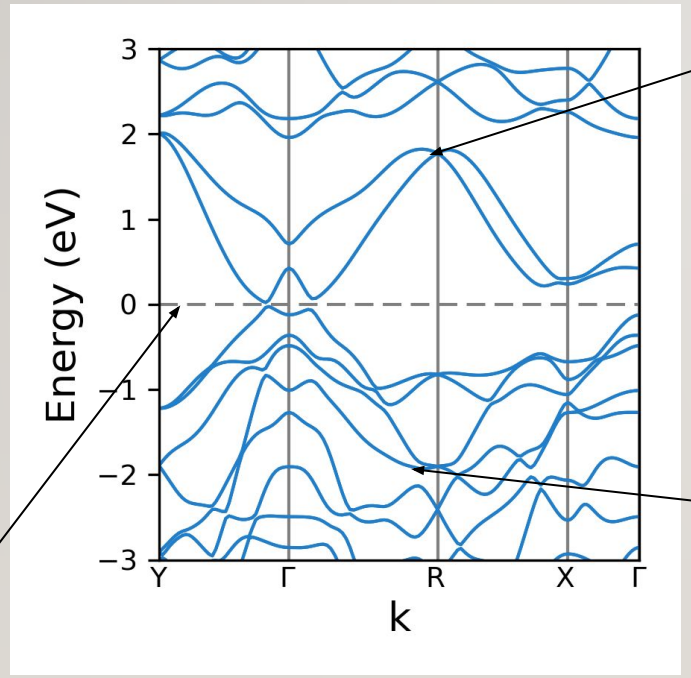
- **Representation of the energies of crystalline orbits in crystalline materials**
- **Atoms have discrete energy levels that are degenerate**
- **Degeneracy is lifted through processes such as crystal-field splitting and spin-orbit coupling(SOC)**
- **Can predict certain physical properties**







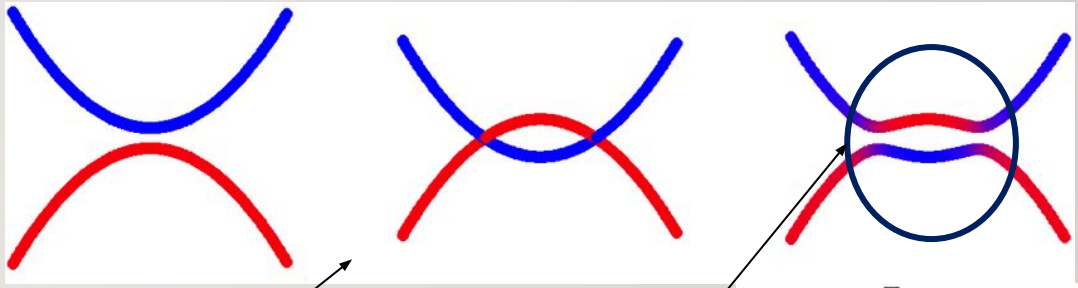
GENERAL BAND STRUCTURE



Conduction Bands

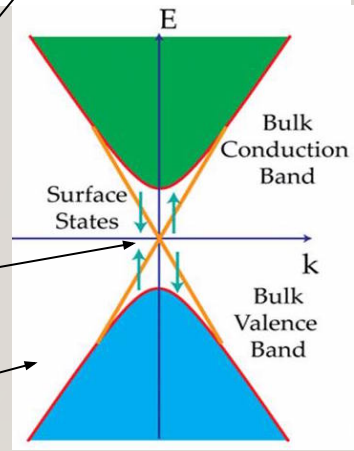
Valence Bands

Fermi Energy



Band Inversion

Camelback Feature



Dirac Point

TI Surface Band Structure

https://hungpham2017.github.io/mcu/plotting1D.html

H. Wang et al, Adv. Phys. **64**, 18732

OBSERVATION OF SURFACE TRANSPORT PROPERTIES

- **Requires Surface Bandstructure Dirac point to be at the Fermi energy level and electrically insulating bulk**
- **Bi_2Se_3 Dirac point is at the fermi level yet is intrinsically a n-type semiconductor, making it difficult to obtain an insulating bulk**
- **Bi_2Te_2Se is determined to be more chemically stable**

Bulk Bi_2Se_3

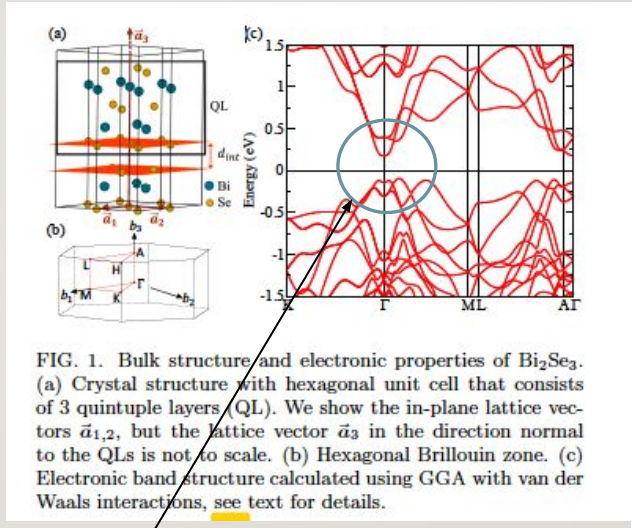


FIG. 1. Bulk structure and electronic properties of Bi_2Se_3. (a) Crystal structure with hexagonal unit cell that consists of 3 quintuple layers (QL). We show the in-plane lattice vectors $\vec{a}_{1,2}$, but the lattice vector $\vec{a}_3$ in the direction normal to the QLs is not to scale. (b) Hexagonal Brillouin zone. (c) Electronic band structure calculated using GGA with van der Waals interactions, see text for details.

Dirac Feature

Surface Bi_2Se_3

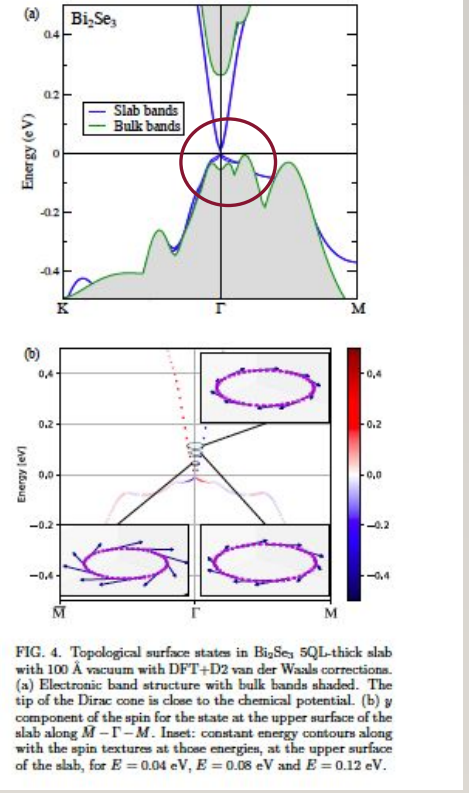
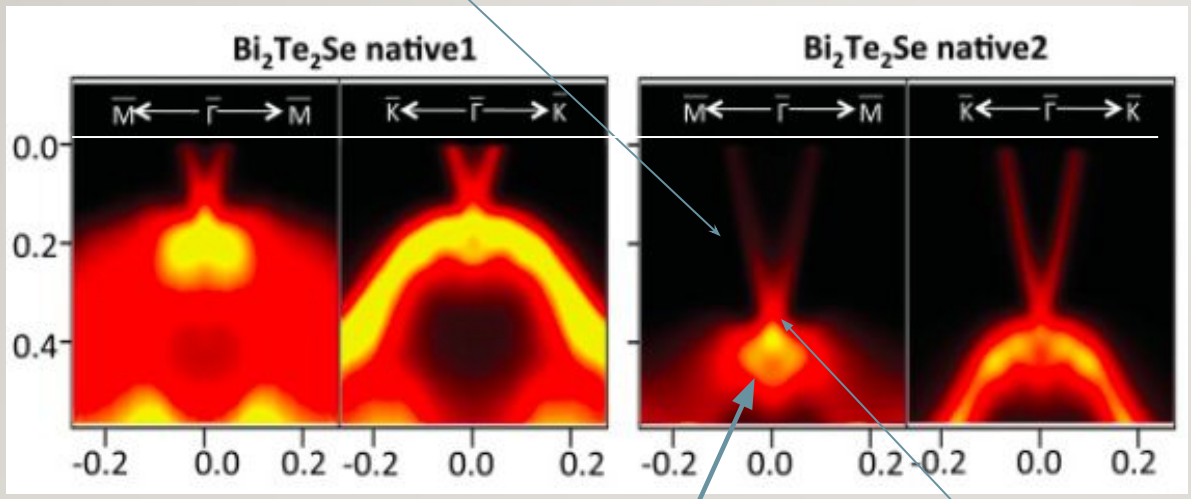


FIG. 4. Topological surface states in Bi_2Se_3 5QL-thick slab with 100 Å vacuum with DFT+D2 van der Waals corrections. (a) Electronic band structure with bulk bands shaded. The tip of the Dirac cone is close to the chemical potential. (b) y component of the spin for the state at the upper surface of the slab along $\bar{M}-\bar{\Gamma}-\bar{M}$. Inset: constant energy contours along with the spin textures at those energies, at the upper surface of the slab, for $E = 0.04$ eV, $E = 0.08$ eV and $E = 0.12$ eV.

Shirali K, Shelton WA, Vekhter I.
arXiv preprint arXiv:1905.01269. 2019.

PAST EXPERIMENTAL DATA



- **Angle-Resolved Photoemission Spectroscopy(ARPES)**
- **Location of Dirac Point varies from experiment to experiment**

M. Neupane et al, PRB **85**, 235406

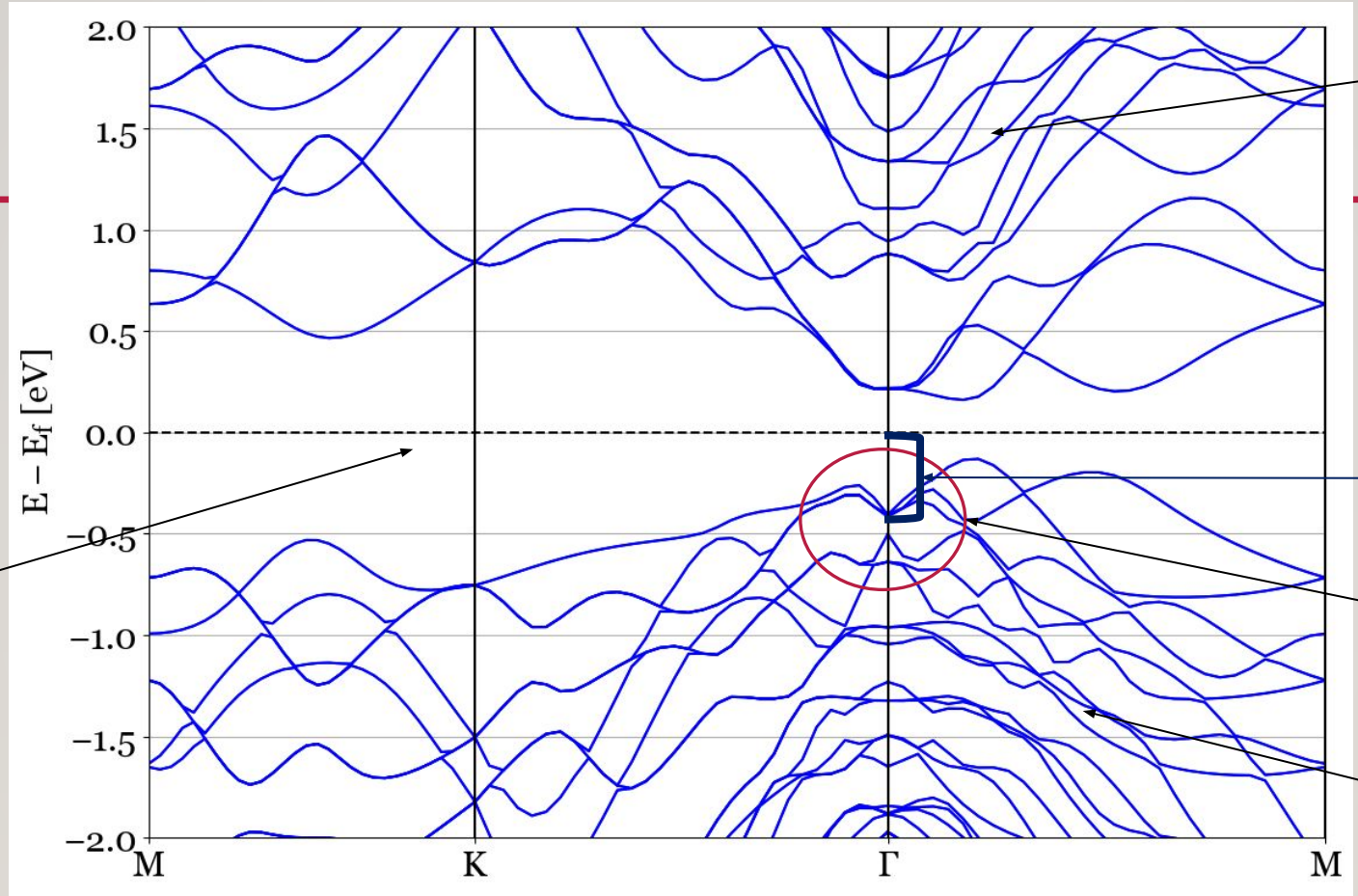
METHOD

- **Vienna Ab initio Simulation Package(VASP)**
- **Density Functional Theory(DFT)**
  - **Ground state energy can be expressed as functional of density**
  - **Iterative**
  - **Convergence of density functional and ground state energy**
- **Ionic Relaxation: Optimizes atom positions and lattice parameters**
- **Plane Wave Pseudopotential Method**
  - **Solution as linear combination of plane wave basis or Fourier series**
  - **Core electrons represented as effective potential, not included in plane wave basis**

VAN DER WAALS CORRECTIONS

- **DFT does not take into account van der Waals interactions; lattice parameters are overestimated as a result**
- **Two calculations were done: one without the corrections and one with the corrections(DFT-D2 method of Grimme)**

	Without Corrections	With Corrections
c	30.61Å	30.08Å
a	4.384Å	4.278Å
Avg. % Difference c	2.306%	0.535%
Avg. % Difference a	1.916%	-0.512%
Fermi Energy	5.095 eV	6.026 eV
Ground State Energy	-62.87 eV	-68.73 eV
Energy Gap	0.232 eV	0.285 eV



Conduction Bands

Fermi Energy Level

$\Delta E \sim 0.4\ eV$

Dirac Feature

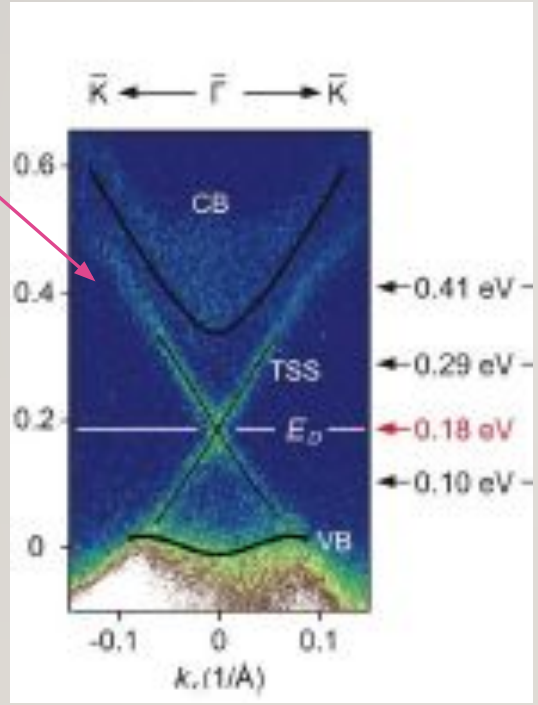
Valence Bands

CONCLUSION

- **Bulk band structure calculations were carried out for Bi_2Te_2Se**
- **Accuracy of bulk band structure calculations can be supported by agreement of the optimized lattice parameters with the experimental lattice parameters**
- **Bi_2Te_2Se might not be an adequate material to observe transport properties of surface states since the Dirac feature is far from the Fermi energy level**
- **Accurate bulk band structure can give a strong foundation to valid surface band structure calculations**

FUTURE DIRECTION

ARPES Measurement Of Sb_2Te_3



S. Zhu et al, Sci. Rpt **5**, 13213

- **Calculate surface band structure using similar parameters from the bulk calculations**
- **BSTS Compounds: $(Bi_{1-x}Sb_{x)2}(Te_{1-y}Se_y)_3$**
- **Some combinations of x and y are determined to be chemically stable**
- **Possibility of higher location of Dirac point; based on Sb_2Te_3**

ACKNOWLEDGEMENTS

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Thank You for Your Attention!