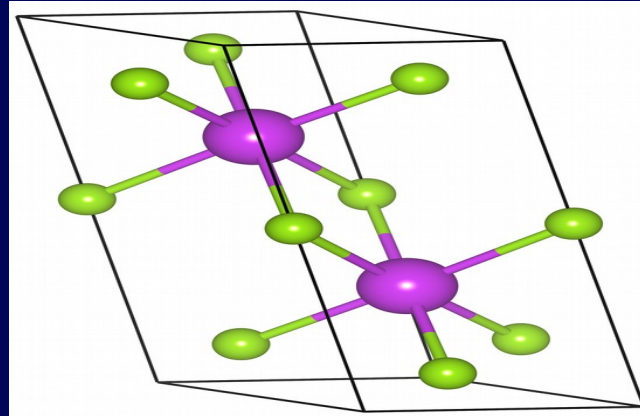


Origin of band inversion in topological bismuth selenide (Bi_2Se_3)

STEPHEN CHEGE MBUGUA



The Technical University of Kenya

NICIS

NATIONAL INTEGRATED
CYBERINFRASTRUCTURE SYSTEM

CHPC



What are topological insulators?

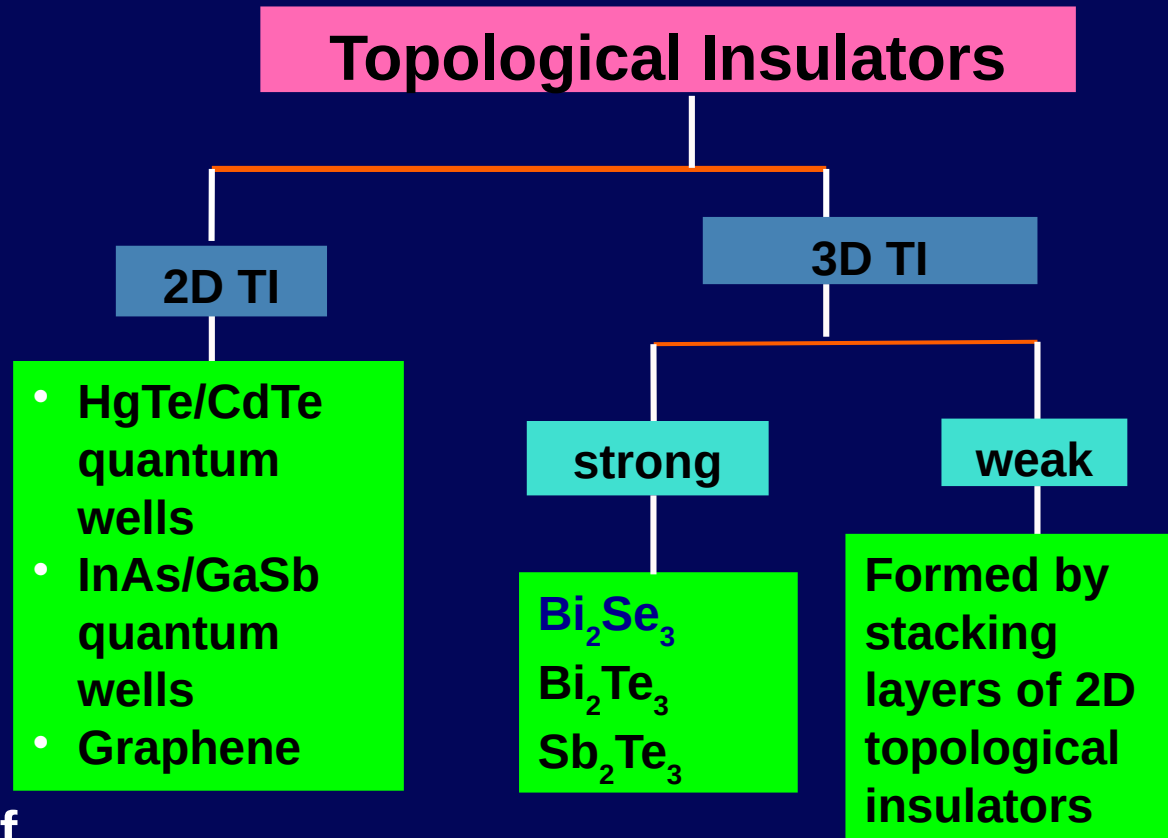
- Topological insulators in bulk have insulating properties but often exhibit conducting edge or surface states protected by time reversal symmetry.

Purpose of Research

- In this research we seek to investigate the origin of band inversion in topological Bi_2Se_3 .

Why topological Bi_2Se_3 ?

- It has applications in the fields of quantum computing, spintronics and thermoelectric topological devices.
- Moreover, knowledge about origin of band inversion in topological insulators will aid in engineering of materials in different phases in a non-volatile manner.

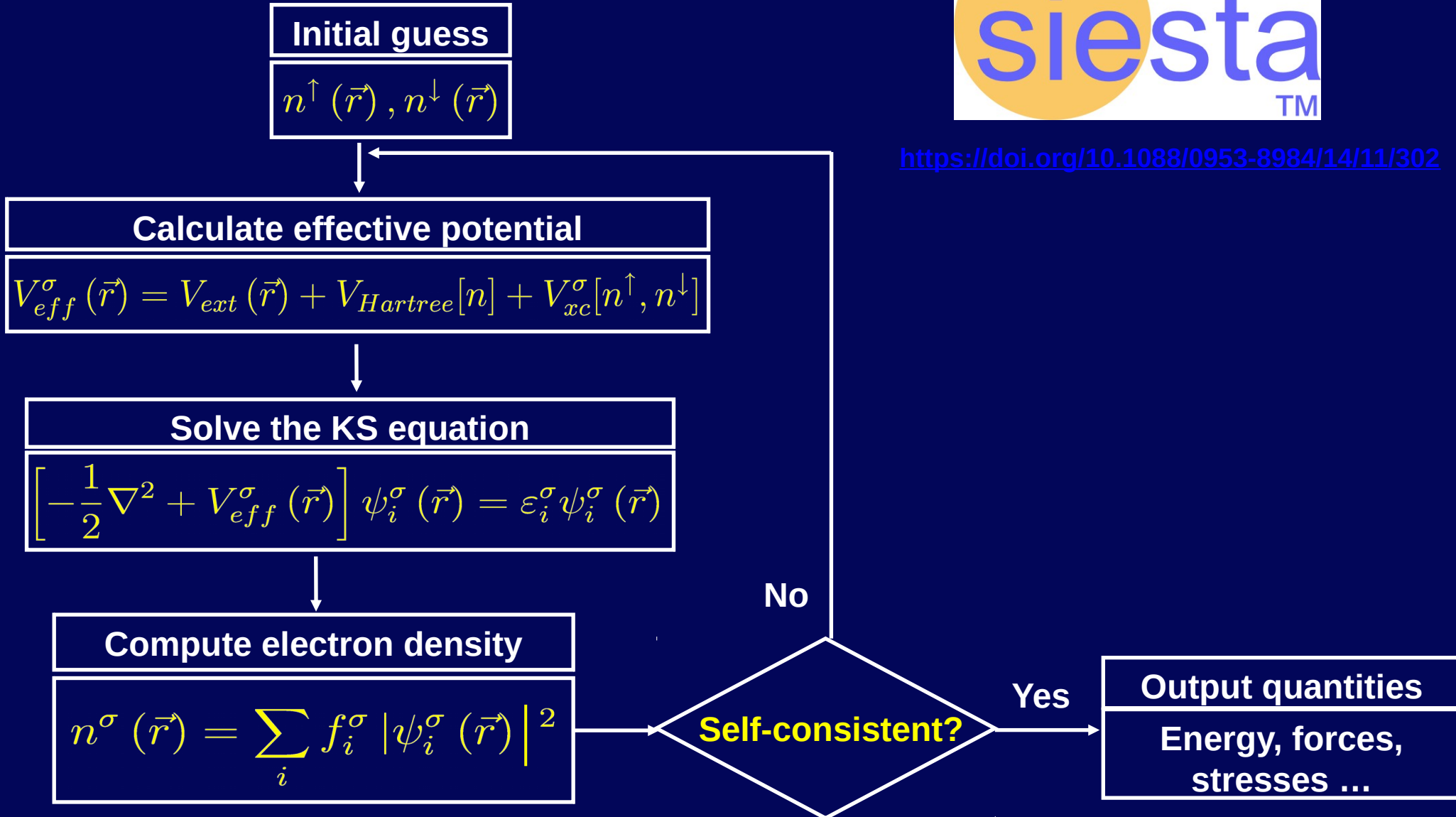


<https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.82.3045>

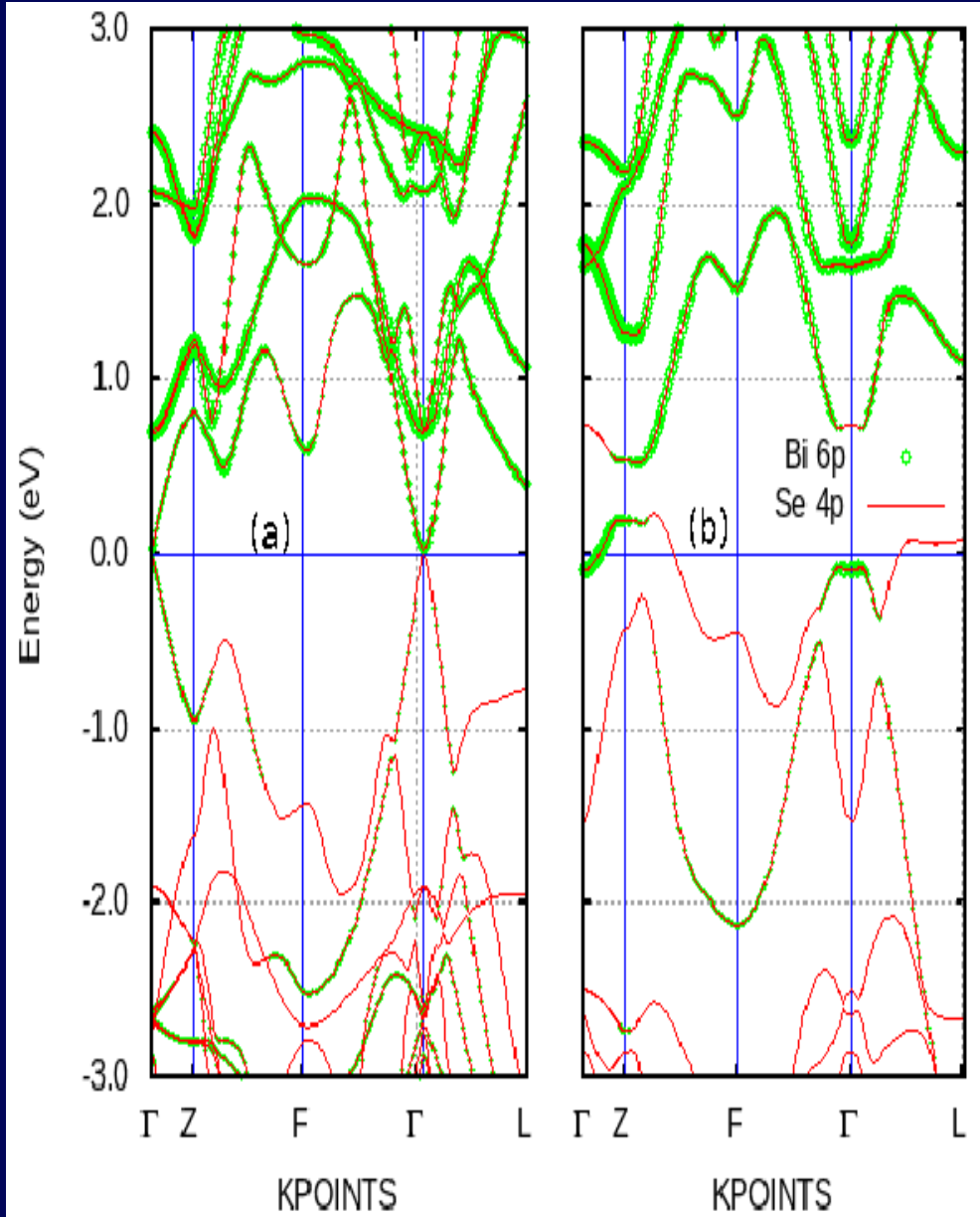
Method



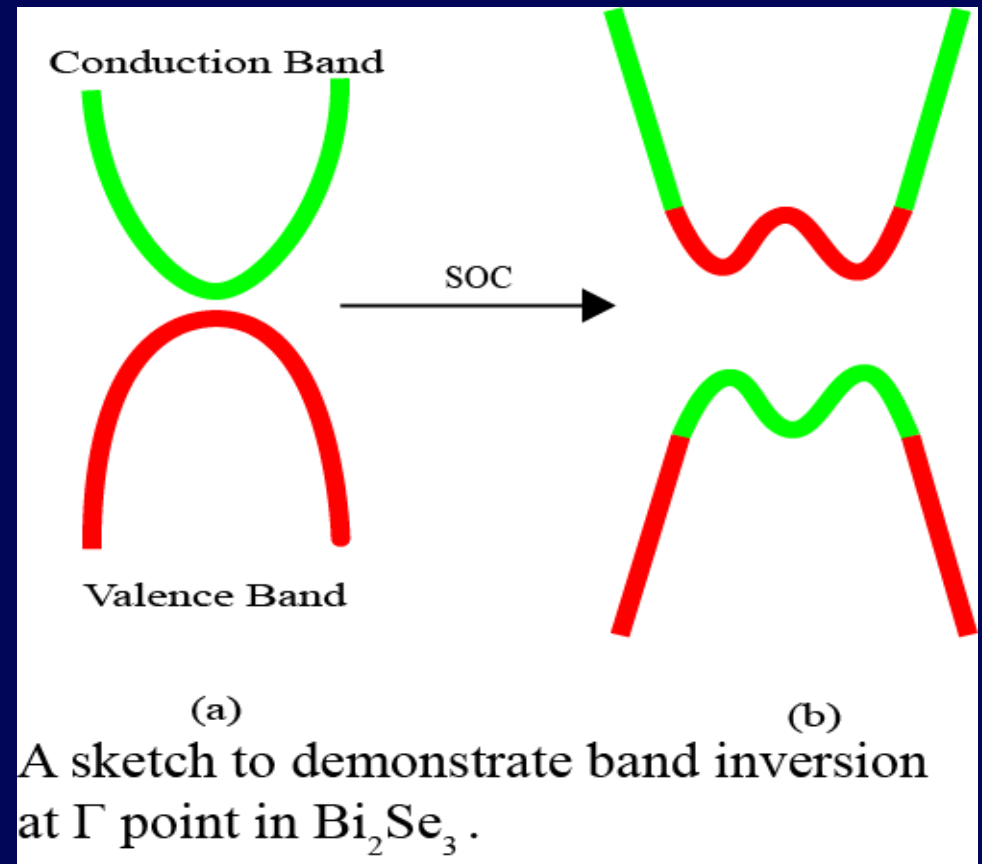
<https://doi.org/10.1088/0953-8984/14/11/302>



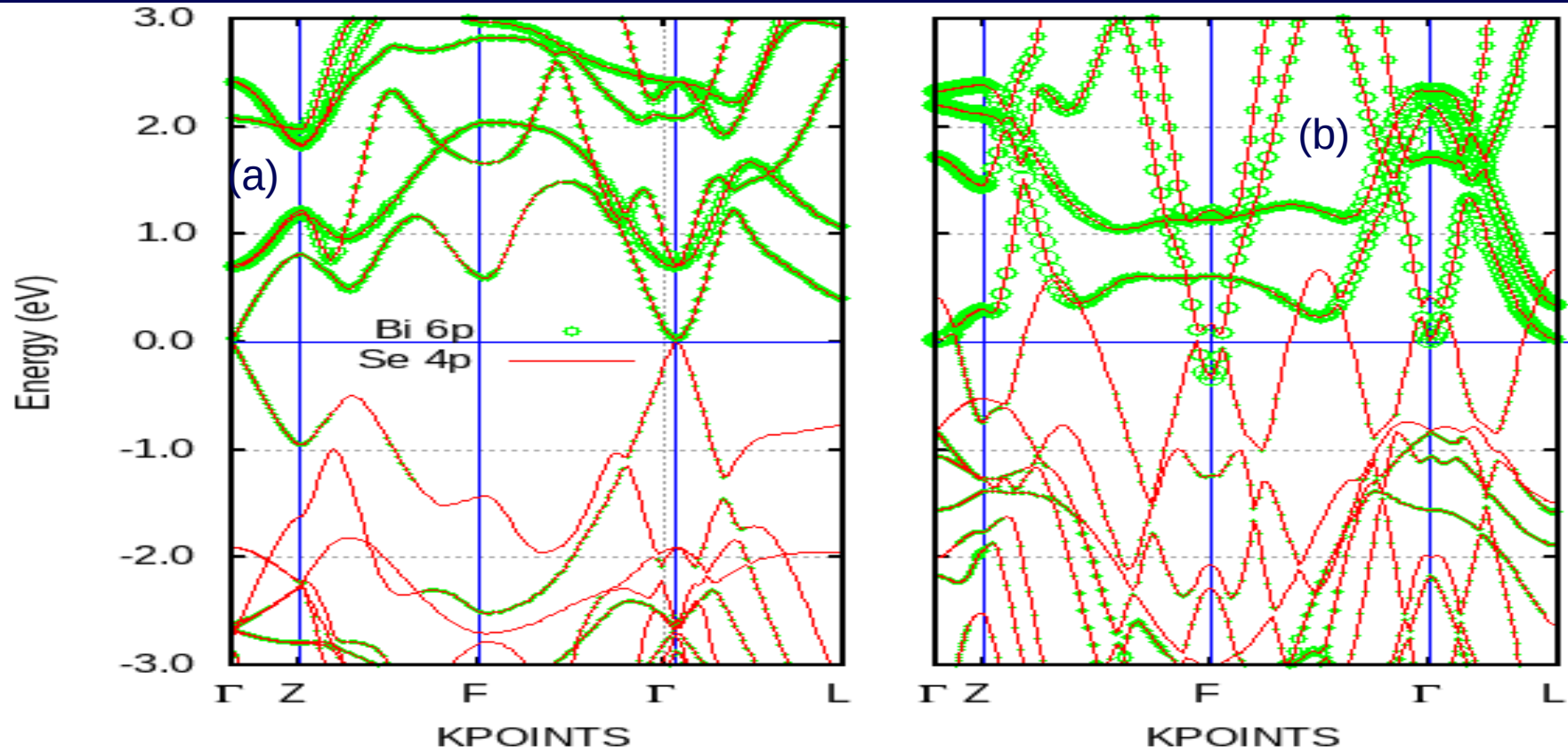
Results and discussion



- Fat bands of Bi_2Se_3 illustrating band inversion at Γ point. The Fermi level has been set to zero in both (a) and (b).
- (a) without SOC (b) with SOC



Results and discussion



Band inversion occurred at F and Γ points as illustrated in fig.(b) which is a scalar relativistic calculation. Thus band inversion is caused by;

- (i) scalar relativistic effects such as mass velocity and Darwin terms.
- (ii) lattice distortions in the crystal.

SOC is necessary for the opening of the gap but necessary to obtain inversion in our case.

Conclusion

From this research:

Fundamental band inversion in topological Bi_2Se_3 , which is a result of both scalar relativistic and fully relativistic effects was demonstrated.

Spin-orbit coupling is necessary in opening of the band structure for topological insulators but not the driving force for band inversion.

Scalar relativistic effects and lattice distortions are the origin of band inversion in topological Bi_2Se_3 .

For more info:

<https://aip.scitation.org/doi/full/10.1063/5.0022525>

THANK YOU :)