Tantalum phosphide: A topological weyl semimetal.

African Light Source Workshop(AfLS3)

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course outline

- Topological semimetals.
- Tantalum phosphide (TaP).
- Objective.
- Methodology
- Results and discussion.
- Conclusion.
- Acknowledgement.
- Selected references

Topological Semimetals

- In this class, the bulk of the material is semimetal and their valence and conduction bands touch at near Fermi level.
- The band crossing points are known as the weyl nodes.
- There are three types of topological semimetals; Dirac semimetal(DSM),Node line semimetal (NLSM) and Weyl semimetal(WSM).

Tantalum phosphide (TaP)

- TaP has been classified as a WSM with only a single type of Weyl fermions.
- We expect energy gap when SOC is turned on in the system.
- TaP exists in three phases: hexagonal phase, orthorhombic phase and tetragonal phase.
- In this work, we shall study tetragonal phase of TaP because its the only phase that has shown the topological properties.
- Gupta et al examined TaP under pressure (up to 25GPa) using Raman spectroscopy and synchrotron x-ray diffraction and their results revealed that TaP did not show phase transition up to 27GPa (Gupta et al., 2018)

Tantalum phosphide (TaP)

- They also noted from the crystal structure that TaP lack spatial inversion symmetry.
- However, they did not explain to what extend TaP remains a WSM .
- In this work, we shall calculate the band structure in TaP and how the spin-orbit interaction alters the single Weyl fermions.
- We shall engage the state of art ab initio methods based on the Density functional Theory (DFT), as implemented in SIESTA code (Soler et al, 2002)

objective

Our main goal will be to calculate the band structure in TaP and how the spin-orbit interaction alters the single Weyl fermions.

Methodology

- We carried out simulations of topological TaP using the density functional formalism as implemented in the Siesta method.
- Exchange and correlation were treated within the generalized gradient approximation.
- The band crossing points are known as the weyl nodes.
- Core electrons were replaced by ab initio norm-conserving (Hamann et al, 1979) and fully separable, Troullier-Martin pseudopotentials.
- A Fermi Dirac distribution with a temperature of 0.090 meV was used to smear the occupancy of the one-particle electronic eigenstates.
- In order to get converged system, we had a two step procedure:

Methodology cont'

- We first relaxed the atomic structure (with and without spin orbit) and the one particle density matrix with a sensible number of k-points (10x10x10 Monk horst-Pack) k-point mesh and secondly, freezing the relaxed structure and density matrix, we performed a non-self consistent band structure calculation with a much denser sampling of 60x60x60.
- In the real space integrations, a uniform grid with an equivalent plane-wave cutoff of 600Ry was used.
- In this calculation, all the atomic coordinates were relaxed until the forces were smaller than 0.01 eV/ A.

RESULTS AND DISCUSSION

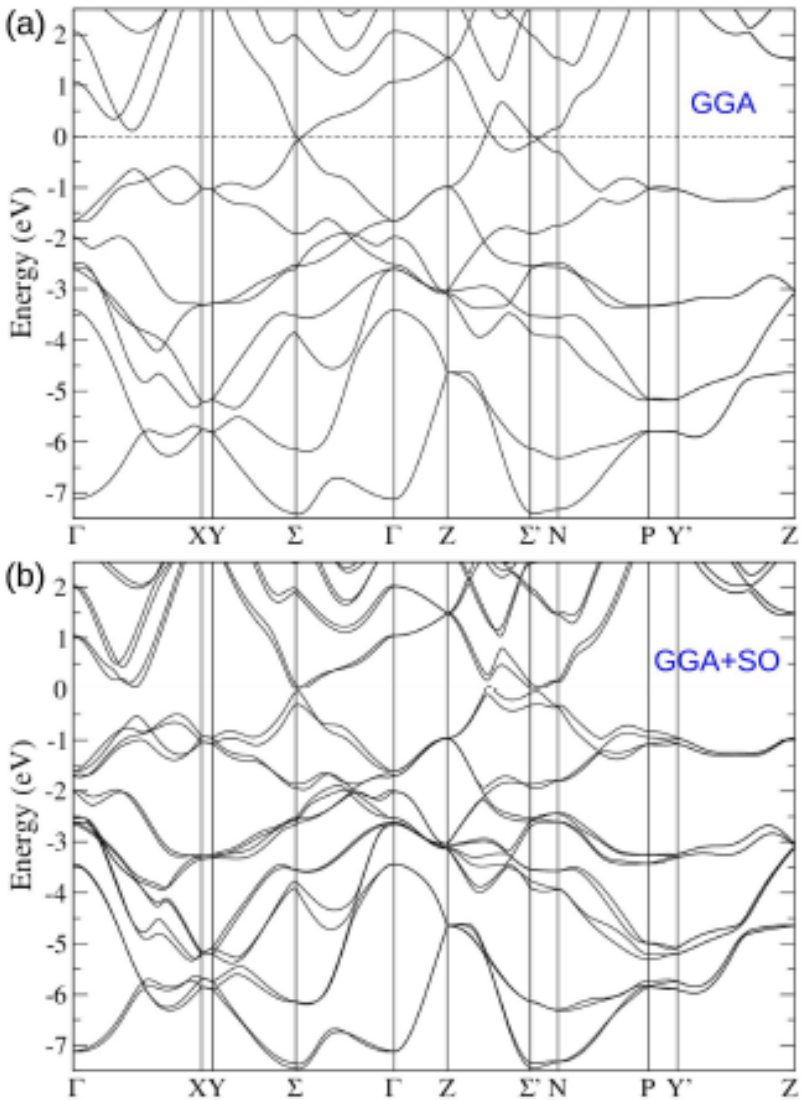

Figure: Band structure of TaP

RESULTS AND DISCUSSIONS

- In the figure above, we show the calculated band structure along some high-symmetry lines.
- It can be seen that the conduction and valence bands cross each other near the N points, giving rise to a semimetal ground state.
- In the absence of spin-orbit coupling (SOC), it can be seen that the overlap of the conduction and valence bands yields two ring-like crossings, or nodal lines.
- The lowest conduction band and the highest valence bands which are basically derived from d states, yields a small energetical overlap which leads to formation of semimetals.

RESULTS AND DISCUSSIONS

- when SOC is turned on, it lifts the double degeneracy of a band except at the Kramer's points, which shows the break of inversion symmetry but the respect of TR symmetry.
- Three regions exhibiting a small or vanishing gap and band crossings can be observed along direction near weyl one node along the N lines coming closer to trivial points.
- Our results are consistent with other DFT studies

structural properties

Table: Indicating calculated lattice parameters, Bulk modulus, volume per atom and minimum energy of tetragonal primitive cell TaP using PBESOL exchange correlation in comparison to other studies.

XC	Ref	a_o(Å)	c(Å)	$B_o(GPa)$	Vol/atom (Å
PBESOL	This work	3.31	11.15	130.42	15.2
Theory	(chang et al., 2016)	3.34	11.43	-	15.9
EXPT	(Lee et al., 2015)	3.32	11.36	-	15.5
EXPT	(Besara et al., 2016)	3.32	11.34	-	15.6

RESULTS AND DISCUSSIONS:structural properties

- We begin to determine the geometry structural parameter of TaP WSM. TaP belong to the space group of I41md (c11 4v, no.109) primitive cell and the first Brillouin zone (BZ) along the high symmetry lines.
- We observed that our results are in agreement with previous reported DFT results and the experimental value with an error of -0.003
- The calculated lattice parameters, bulk modulus and volume per atom are reported in the table1 with some other available data though little have been done on this material.

Conlusion

- We have performed first principles calculation on tetragonal topological TaP. The goal of our work was to calculate the band structure in TaP and how the spin orbit interaction alters the single Weyl fermions.
- Our results have shown that the bands crossing at low symmetrical points in BZ with three regions exhibiting a small or vanishing gap and band crossings along direction near weyl one node along the N lines coming closer to trivial points.
- The band gap was observed to open up when SOC was turned on.

Conlusion

- This shows that SOC has an effect of opening up of energy gap for a topological Weyl semimetal of TaP.
- We also calculated the lattice parameters, volume per unit atom and bulk modulus for TaP. Our results is consistent with both the available DFT and experimental data.
- However, there was no experimental data for the bulk modulus for TaP and therefore we have provided a platform for future experimental studies.

Acknowledgement

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THE END
THANK YOU
GOD BLESS YOU