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Hole-doping and Contact Induced Spin-polarization in Weyl Semimetal TaAs

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Abstract. TaAs is an ideal Weyl semi-metal consisting of conducting surface states composed of massless Weyl fermions. We have investigated the effects of Nb doping in bulk TaAs. For TaAs/Au and TaAs/Ag interfaces, we have observed huge hole doping to the TaAs system. In addition, the introduced carriers impart a large spin polarization within otherwise non-spin-polarized TaAs.

INTRODUCTION

Materials possessing finite band gap between the valence and conduction bands are classified as insulators and those having overlapping bands are termed as metals. However, depending upon the difference of topology of band structure, insulators can again be classified into further varieties. Topological insulator is a special class of insulator, where gapless surface states are generated inside the bulk energy gap. The gapless nature of these surface states is protected by topology.¹ These surface states (TSS) are also observed on the surface of Weyl semimetals (WSM). Hermann Weyl (1929) discovered the existence of massless fermions in Dirac equation, which are known as Weyl fermions.² Recently, experimental results of WSM stimulate many exciting novel phenomena like superconductivity and strong spin-polarization.

Weyl semimetals have an electronic band structure with singly-degenerate bands dispersing linearly in three-dimensional (3D) momentum space through a node termed as Weyl point. The energy bands in a specific momentum space region obey Dirac or Weyl equation, which is distinctly different from traditional parabolic energy band dispersion.¹, ³

Although Weyl semimetal does not show topological ordering, they still have topologically protected states promising for various applications. Recently Huang et. al proposed the first weyl semimetal TaAs which is stoichiometric, inversion breaking and single-crystal material.³ Both the Weyl fermions and the Fermi arcs have been experimentally realized in TaAs by photoemission experiments.⁴

Although a lot of theoretical studies have been done to establish TaAs as a weyl semimetal, most of them are focused on finding the key aspect of electronic structure. The effect of doping and contacts in TaAs are still not investigated thoroughly. In this study, we perform first principles theoretical calculation on Nb doped bulk TaAs. We have also investigated the effect of gold and silver interfaces with pristine and Nb-doped TaAs.

COMPUTATIONAL DETAILS

First-principles spin-polarized density functional calculations are performed using Projector augmented wave (PAW) potentials for bulk TaAs supercell and interface of TaAs with Au and Ag in a rectangular box. Nb atoms of different percentages are doped in the above two systems.
The exchange-correlation interactions are treated by the generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) exchange functionals using Vienna Ab-initio Simulation package (VASP). The cutoff energy for the plane-wave expansion is set as 500 eV. A 3×3×1 supercell is used for bulk calculations and an interface of TaAs is created with Au and Ag, keeping the interfacial strain as ~1.3%. k-meshes of size 7×5×3 and 5×5×3 are used for interfaces and bulk complete geometry optimization and electronic structure calculations respectively. van der Waal’s interactions are incorporated in this calculation by using DFT-D2 method of Grimme, as implemented in VASP. The bulk TaAs and the Au/Ag-contacted TaAs are fully relaxed until the absolute value of force acting on each atom is less than 0.01 eV/Å.

RESULTS AND DISCUSSIONS

Bulk supercell of crystalline host semimetal is a 144 atom Ta72As72. Interface of TaAs/Au/Ag is constructed from Ta24As24 layer with 20-atoms double layered metals (Au/Ag), placed in a cubic box of size 5×15×27 Å3. For study of doping, Nb is substituted at the Ta-site at both supercell and interfaces. Using the ab initio methods described above, we have carried out an extensive analysis of electronic structure, doping nature and charge transfer process of for doped and pristine TaAs in bulk and interfaces.

We have investigated two different concentrations of Nb-doping in TaAs supercell. Size of Nb (~2.1Å) is slightly lower than Ta atom (~ 2.2Å), which indeed generates size-induced relaxations within the underlying pristine system. The impact of doping of Nb atom in the bulk TaAs supercell is depicted in the atom projected density of states (APDOS) shown in Figure 1. Figure 1a, b, c and d shows the APDOS of pure TaAs bulk structure and 2.77%, 5% in-plane (IP) and 5% out of plane (OP) Nb doped systems respectively.

![Fig. 1: Atom projected (APDOS) and of the systems a) TaAs supercell, b) 1.4% Nb doped TaAs, c) 2.77% (IP) Nb doped TaAs and d) 2.77% (OP) Nb doped TaAs.](image)

The valence configuration of Ta and Nb are 5d6s2 and 4d5s1 respectively, whereas As possesses 3d04p3 configuration. Because of larger range of 5d over 4d, the covalent charge sharing is more prominent for Ta than Nb. It will be evident from the lack of hybridization of Nb-4d states than Ta-5d with As-4p. Therefore, Nb doped systems show a gradual shift of Fermi-energy (E_F) towards valence band, indicating introduction of p-type carriers or holes within the system. For TaAs, the main contribution near E_F comes from Ta-5d and As-4p. Valence band top and conduction band bottom of the system are separated by a valley shaped density of states at the Fermi energy, which is a characteristic feature of semimetal. At E_F, there is a crossing between valence band and conduction band forming electron pocket and hole pocket respectively. With gradual increase of Nb-doping, we found the semi-metallic behavior is transforming to a normal metallic behavior with finite DOS at E_F.
Recent observation of tip-induced superconductivity in TaAs motivates us to explore the electronic properties of the system with metallic interfaces. In addition, contacts play very crucial role in nanoscale electronic device fabrication. We have investigated two types of interfaces with TaAs systems, a) TaAs/Ag and b) TaAs/Au and its corresponding doped systems. The APDOS of TaAs/Ag and TaAs/Au with the corresponding doped systems are presented in the Figure 2 and 3 respectively.

Fig. 2: Atom projected (APDOS) density of states of silver contacted systems a) TaAs supercell, b) 5.5% (IP) Nb doped TaAs, c) 5.5% (OP) Nb doped TaAs and d) 10% Nb doped TaAs.

Fig. 3: Atom projected (APDOS) density of states of gold contacted systems, a) TaAs supercell, b) 5.5% (IP) Nb doped TaAs, c) 5.5% (OP) Nb doped TaAs and d) 10% Nb doped TaAs.
In both of these interfacial systems, we have observed that the DOS is spin polarized in presence of metallic contacts. Bulk TaAs does not have any magnetic moment, whereas TaAs/Ag and TaAs/Au systems are having a moment of \( \sim 3.4 \mu_B \) and 3.1 \( \mu_B \) respectively. This spin polarization is mostly achieved by the charge-carriers introduced at the interface from the metallic contacts. This spin polarization of the system will be evident from the spin-density plots presented in Figure 4, where with the same iso-surface scale, TaAs displays no-spin polarization. Extent of spin-polarization is more for Au than Ag.

For the interfacial systems, we have observed a huge amount of \( p \) type doping, implying that Ag/Au layer dopes hole within the TaAs layer. This extent of hole-doping is even increasing in presence of Nb-doping. This hole-doping can be a possible cause for the recent observation of tip-induced spin-polarization and superconductivity in TaAs system. Further studies on related systems are ongoing.

**CONCLUSION**

This work demonstrates the impact of Nb-doping for the well-known Weyl semi-metal TaAs in bulk. In addition, we have observed interface induced hole-doping for TaAs/Ag and TaAs/Au interfaces. Nb-doping introduced additional \( p \)-type doping for the interfacial system. This study can provide an explanation to the tip-induced superconductivity and spin-polarization in Weyl semimetallic systems.

**REFERENCE**