Graphene like ZnO 2D structure from semiconductor to conductor behaviour by doping F

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Abstract. 2D ZnO honeycomb structure was recently fabricated. This new semiconductor material with band gap about 1.67 ev is great for applications which needs this gap and such dimension. This material has a great electronic structure, which was investigated in this article by details for the first time by this view. Due to this especial electronic structure here we found that this material could be change its behaviour from semiconductor to metal material with different Fermi surfaces which could be used for different applications by doping F elements on the surface. The first section in your paper

1. Introduction

In recent years many 2D structures were fabricated such as graphene [1], transition metal dichalcogenides (TMDs)[2], hexagonal boron nitride (hBN) [3] etc. with thicknesses ranging from a single to a few atomic layers which, open new area of research in physics. These materials have great electronic structures that is different from their bulk structures [4]. In modern electronic devices area, low dimension material is going to use for miniaturization of electronic devices. 2D crystals are great of interest to understand in fundamental physics at reduced dimension because of their unique and functional properties. These 2D materials exhibit charming and great physical properties, from conductor to semiconductor range of materials, which could be used in the wide range of applications in nano scale electronic and photoelectronic devices [5-9].

In this situation, founding new 2D Structure that could be stable in the nature would be great of interest; actually, if it could be tunable from semiconductor to conductor material. One of the structures that fabricated in recent years is 2D ZnO graphene like honeycomb structure [10, 11].

Bulk zinc oxides structures are widely used in different studies in environmental and energy-related applications such as solar cell devices [12], sensors[13], photo catalysis[14] etc.. However, the new structure (2D ZnO with honeycomb structure) has more interested structure because of less band gap and his unique electronic structure, which is investigate in this article with more details. Because of the open surface area that is due to monolayer structure and its double chemical bond between Zn and O elements this structure could have tunable electronic structure.

2. Calculation methods

First-principles calculations within density functional theory (DFT) is used for achieving to our results by using Wien2k and FHI-aims packages. Generalized gradient approximation GGA functional use as
exchange-correlation potential. All structures have been treated within supercell geometry using the periodic boundary conditions. The interaction between ZnO monolayers in adjacent supercells examine as a function of their spacing. Since we used the spacing of 100 Å which these monolayers have not interaction with each other in the calculations. In the self-consistent potential and total-energy calculations, the Brillouin zone is sampled by 12*12*1 special k points for 2D honeycomb ZnO and also for doping with F element. All structure was relaxed and the structure stability was checked out.

3. Result and discussion

At first the electronic structure of single ZnO layer was investigated. As could be seen in the DOS results (see picture 1) the band gap is 1.67 ev which is have great agreement with Topsakal et all results [10]. On the other hand as could be seen we have 2 different type of hybridization in this material:

1- In the XY plane the hybridization is included of S, Px and Py orbitals of Oxygen ; S, Px,Py,dX²Y² and dXY orbitals of Zinc and also dZ² orbital of Zinc because as you know this orbital have Electronic Cloud in XY plane. This hybridization create σ chemical bond.

2- Due to Z direction the hybridization is include of Pz orbital of Oxygen and Pz, dXZ, dYZ and dZ² orbitals of Zinc. This hybridization create Π chemical bond. Which the second type band is located in the middle of the first band duo to the energy and locate in out of XY plane in the Z direction duo to the space.

The Zn-O bond length in this structure was obtained 1.90 Å.

Figure 1. This pictures shows the band structure and pDOS of ZnO honeycomb structure in 2 way of in plane and out of plane direction.

Therefore, because of this electronic structure by doping hole in the second type orbitals (the orbitals which are located out of XY plane) metallic characteristic behavior could be induced to this material by broken Π bond and could construct dangling bond. In this situation, we doping F elements to the surface of ZnO sheet by different concentration (One, two and three F elements for each three ZnO hexagon). The results show all of the structures could be metallic (see figure 2). These three structures have different Fermi surfaces, which could be used for different applications (see figure 2 around fermi level).
4. Conclusion:

Therefore, 2D ZnO honeycomb structure was fabricated. This material has a great electronic structure which was investigated in this article by details. This material has semiconductor electronic character with 1.67 eV band gap and chemical double bond between Zn and O elements. Due to this especial electronic structure we found that this material could be change its electronic characteristic from semiconductor to metal with F elements doping by break the π bonds.

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