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Energetics and Electronic Properties of Pt Wires of Different Topologies on Monolayer $MoSe_2$

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Abstract. The energetics and electronic properties of different topology of Pt wires including linear, zigzag and ladder structures on $MoSe_2$ monolayer have been investigated in the framework of density functional theory (DFT). The predicted order of stability of Pt wire on $MoSe_2$ monolayer is found to be: linear > ladder > zigzag. Pt wires induce states near the Fermi level of $MoSe_2$ that results into metallic characteristics of Pt-wire/$MoSe_2$ assembled system. Valence band charge density signifies most of the contribution from Pt atoms near the Fermi energy of assembled wire/$MoSe_2$ system. These findings are expected to be important for the fabrication of devices based on $MoSe_2$ layers for flexible nanoelectronics.

Keywords: DFT, Electronic Structure, Density of States
PACS: 31.15.v-71.20.-b 73.22.-f 77.22.ch

INTRODUCTION

Transition metal dichalcogenides (TMDs) possess layered structures [1] with strong intra-layer bonding and weak inter-layer van der Waals interactions that allows the successful exfoliation of single layer. TMDs monolayers with graphene-like hexagonal symmetry are direct band-gap semiconductors with band-gap value ranges from 1-2 eV [2].

The fabrication of next generation electronic devices generally requires the combination of conducting and insulating materials for higher performance and greater flexibility [3-4]. Noble metal wires anchored on MoS_2 monolayer are found to enhance the conductivity of monolayer [5] which is expected to have importance for the catalytic activity of monolayer MoS_2. In recent investigations, Pt contacts on $MoSe_2$ monolayer enhances the conductivity of layered MoSe2 by several order of magnitude that is found to be crucial for the development of flexible electronic devices and transparent conducting materials using ultrathin dichalcogenide layer materials [6].

In this paper, we study the energetics and electronic properties of different topologies of Pt wires with linear, zigzag and ladder configurations on $MoSe_2$ monolayer. Note that the linear, zigzag, and ladder Pt wires show distinct features in their free standing form [7].

COMPUTATIONAL DETAILS

All calculations were performed within the framework of density functional theory (DFT) by means of ab-initio pseudopotential and numerical atomic orbitals (NAOs) based SIESTA method [7] within generalized gradient approximation (GGA) using PBE functional. We have used relativistic Troullier Martin pseudopotentials, double zeta polarization (DZP) basis sets with confinement energy of 30 meV and real space cutoff 300 Ry for calculations. A vacuum layer of 20 Å is used to eliminate the interaction between the $MoSe_2$-Pt system images in the perpendicular direction. A (15x15x1)

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Monkhorst-Pack of k-points were used for electronic structure calculations.

RESULTS AND DISCUSIONS

Structural Properties

The GGA-PBE calculated lattice constant of monolayer $MoSe_2$ is 3.36 Å. Mo-Se bond length and bond angle between Se-Mo-Se is 2.49 and 82°, respectively which are in good agreement with the previous theoretical study [2]. The structure for different topologies i.e. linear, ladder and zigzag, for Pt wires is shown in Figure 1. The optimized lattice constant for these topologies are 2.5 Å, 2.4 Å and 2.5 Å, respectively are in good agreement with the previous theoretical study [7].

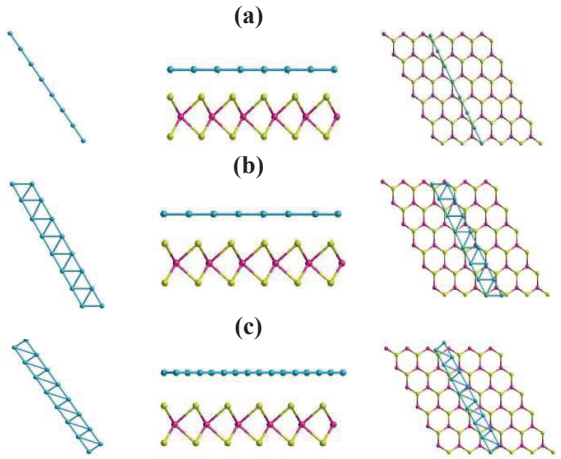

FIGURE 1. (a) Linear (b) Ladder (c) zigzag topologies of Pt wires with side and top view on $MoSe_2$ monolayer. Blue, Purple and Yellow balls correspond to Pt, Moand Se atoms, respectively

Due to lattice mismatch between the monolayer and wires, strain at the interface needs to be minimized by the suitable choice of supercell simulating the composite system. Our choice of supercell for wire (1x8) and monolayer (6x6) leads to lattice mismatch less than 0.03% for all topologies.

The binding configuration for considered topologies wires is as top site of monolayer i.e. the Pt atom of wire are directly on the top of Se atom of monolayer, which was on the case with Pt/MoS_2 system [5]. The equilibrium separation between wire and monolayer ($R_{wire\text{-}monolayer}$) is calculated as 2.5, 3.2 and 2.7 Å, respectively for linear, ladder and zigzag topologies (Table 1 and Figure 2).

Binding energy vs. $R_{wire\text{-}monolayer}$ curve (Figure 2) reveals linear topology of Pt to be energetically most

Table 1. The calculated optimized distance between wire and monolayer (Rwire-monolayer), and the binding energy (Eb) of the wire/monolayer system.

System	$R_{wire\text{-}monolayer}$(Å)	E_b(eV /atom)
$MoSe_2$-linear	2.5	- 0.62
$MoSe_2$-ladder	3.2	- 0.15
$MoSe_2$-zigzag	2.7	- 0.30

favorable on $MoSe_2$ monolayer with the binding energy of - 0.62 eV (Table 1). The binding energy of the monolayer-wire system is defined as $E_b = E_{wire\text{-}MoSe2} - E_{MoSe2} - E_{wire}$. A negative value of E_b indicates the stability of the assembled system. The predicted order of stability of different topologies on monolayer is linear > zigzag > ladder (Table 1) which correlates with the equilibrium separation between wire and monolayer. It is found that linear topology of Pt show gain of ~ 0.7e fractional charge from monolayer, while other two topologies have negligible charge transfer.

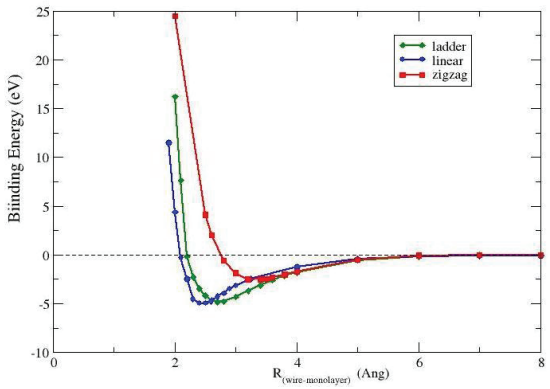

FIGURE 2. Binding Energy vs wire-monolayer separation ($R_{wire\text{-}monolayer}$) curve for the assembled system.

Electronic Properties

Monolayer $MoSe_2$ is known to be a direct band-gap semiconductor with calculated band gap value of 1.39 eV at DFT-PBE level of theroy.The interaction of Pt wire with semiconducting $MoSe_2$ monolayer significantly modifies its electronic properties. On analyzing the states around Fermi level of asembled wire/monolayer system, we found mettalic density of

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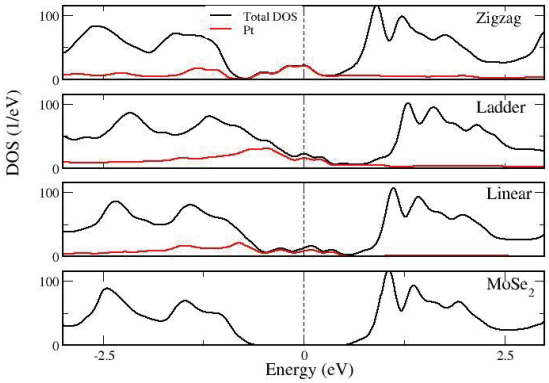

FIGURE 3. Density of States for Pristine and assembled system of $MoSe_2$.

states which are mainly contributrd by the Pt wires (Figure 3).

To examine the states near Fermi level, the valence band charge density of 0.5 eV below Fermi level is calculated. It is found that the states near Fermi level are due to Pt-atoms of metallic wire (Figure 4). In case of $MoSe_2$–ladder and $MoSe_2$-linear topology systems, the small contribution from Mo and Se atoms can also be seen while $MoSe_2$-zigzag topology assembled system has contributions mainly from the Pt atoms only.

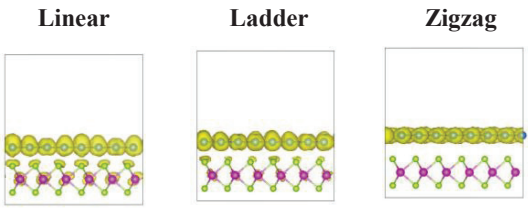

FIGURE 4. A side view of the valance band charge density of assembled systems with isosurface value 0.003 e/ $Å^3$

CONCLUSIONS

In conclusion, structural stability and electronic properties of various topology of Pt wires on $MoSe_2$ are investigated. Pt-wire of linear topology interacts strongly with $MoSe_2$ monolayer. All the considered topologies significantly change the electronic properties of monolayer from semiconductor to metal which is important for the applications of flexible electronic devices and the catalysis based on layered $MoSe_2$.

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