Transport properties of the lateral multilayer/monolayer PtSe₂ diode

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Research Article

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Abstract

A heterostructure of trilayer/monolayer platinum diselenide has been introduced and further studied. Applying the non-equilibrium green function tuned with density functional theory, it has been shown that such a junction forms a diode structure. The current voltage characteristic shows proper diode characteristics in nanoscale. Using the transmission spectrum and projected density of state, we have demonstrated that in forward bias, the conduction band and the valence band are aligned. Therefore, the possibility of tunneling enhances and this leads to the increase of current while in reverse bias such a possibility does not exist. We have also investigated the atoms of the junction and have identified the effective ones in the transmission.

1. Introduction

It is not a trivial matter to say that the current technology owes its structure to the diode. The Diode by controlling the flow of current in a specific direction is commonly used in everyday technology from rectifying currents to even separate photo-generated electron-hole pairs. Various structures of Diode have been devised so far, for instance, structures made of bonding two materials with the same bandgap to which homojunction refers, or structures of two different bandgap materials joined together, called heterojunctions.

Introducing two-dimensional materials in 2004, open up a new horizon in the Diode. So far, two major architectures for them have been introduced, structures that contain two materials connected on the same plane, known as the lateral junction, and two-body stacked face to face that is called vertical junctions. Since in the former one the junction is happening in one-dimensional interfaces and the latter one in two-dimensional overlap, they exhibit very different properties. Also, one of the exceptional properties of two-dimensional materials which is the dependence of the energy gap on the number of layers introduces new ideas for the construction of the Diode. Such property, in addition to the expressed architectures, can act as a structure called 2D homostructure lateral diode. Limited research has been done in this field and several materials have been introduced for this purpose.

Early studies show that platinum diselenide (PtSe₂) in its bulk form is a layer structure with an interlayer of almost 2.5Å° and has an indirect semi-metallic bandgap [1]. As expected, reducing the number of layers may lead to new properties and studies confirm for PtSe₂. For instance, the growth of thin-film Pt on substrates contain Se atoms may lead to forming a thin layer of PtSe₂ with new characteristics [2]. Primary studies on few-layer to monolayer structure of PtSe₂ show that these layer as member of transition metal dichalcogenide (TMD) family has potential for basic electronic devices due to tunable band-gap and high mobility and can be fabricated using simple mechanical exfoliation as their ancestors, MoS₂. Other techniques for the fabrication of pristine PtSe₂ were also introduced including but not limited to chemical vapor transport and the direct reaction of species under high pressure [3, 4]. Based on theoretical predictions, PtSe₂ has good potential for water splitting technology while it is stable in water and undergoes a semi-metallic to semiconductor transition without any external effects such as

pressure and only by reducing the number of layers [5, 6]. The potential of the PtSe₂ then experimentally is shown in FET devices. The bandgap of PtSe₂ can alter from metal to 1.17 by the number of layers due to exceptionally strong interlayer electronic hybridization of Pz orbital of Se atom which is in the range of near-IR and has good stability in the air [6]. Also, it is demonstrated experimentally that monolayer PtSe₂ can detect photons in mid-infrared by altering the number of layers [4]. Such a strong layer dependency can be engineered for possible semiconductor-to-semimetal evolution [7]. Besides, high drain current modulation is shown for the PtSe₂ FET-based devices which are promising for digital electronics [6].

While the low carrier mobility of TMDs at room temperature has limited practical applications, [8–10] recent theoretical studies have shown that PtSe₂, can afford higher carrier mobility [11–16]. The mobility of PtSe₂ is almost four times large than MoS₂ [6]. Soon another potential of this material was revealed and used as a gas sensor to detect NO₂ gas molecule at room temperature [17]. Strain also can tune the electronic properties of monolayer and bilayer PtSe₂ [18].

An interesting investigation studied the imperfection in the crystallography of monolayer PtSe₂ and shows that Se vacancies cannot introduce spin properties to this material [19]. Soon scientists make these materials mesoporous so they can work much better in various usage including sensing applications [20] while such properties are also theoretically investigated [21, 22]. The doped PtSe₂ push the boundaries of the pristine one and introduced theoretically remarkable properties including long-range ferromagnetic and half-metallic behavior [23].

The optoelectronic potential of this material is also explored both theoretically and experimentally which shows that removing undesirable effects of the substrate may happen using hBN and can lead to good photo-gain [24]. Combining PtSe₂ with other 2D materials can introduce even more remarkable properties. For instance, heterojunction based on graphene and PtSe₂ is simulated and shows that this form of junction can open bandgap in graphene and make PtSe₂ a good substrate for graphene [25]. PtS/ PtSe₂ heterostructure simulated as good candidate as photodetectors recently [26]. The more advanced usage of this material is introduced by forming hetero-structure between monolayer Ptse₂ and bulk and nanowire Silicon to use as a rectifier and self-driven photodetectors [27, 28]. The transport properties and effect of electrode contact have also been reported before [29].

Based on what has been stated and since PtSe₂ has shown strong thickness-depended band-gap and high mobility in previous studies, the ability of this material to construct the structure of lateral diode is investigated. Hence, the effect of the number of layers on bandgap is studied using density functional theory (DFT) and compared with previous reports, then the possible lateral junction is found and transport properties in the ballistic region is investigated using non-equilibrium green function coupled with density functional theory (DFT). Similar to other members of the TMD family, PtSe₂ in the chemical vapor deposition technique, produces multi-layered interconnection structures of their own and do not need post-processing for creating a lateral junction. This is one of our main reasons to consider this architecture in this research.

2. Method

Non-equilibrium Green function linked with DFT has proven itself as one of the most adequate techniques to predict the electrical and transport properties of devices in nanoscale. In this paper, such a technique has been used as implanted in Siesta and TranSiesta package [30].

The norm-conserving pseudopotential with exchange-correlation of the form Generalized Gradient Approximation (GGA) as defined in Perdew-Burke-Ernzerhof (PBE) and the basis set of double zeta polarized approximation is used in all sections of the calculation [31]. The mesh cut-off and kpoint sampling in optimization, electronic and transport properties are defined after proper converge test. We considered as 75Ha for mesh cutoff and $16 \times 16 \times 1$ kpoint sampling for the optimization and electronic properties and $4 \times 1 \times 150$ kpoint for non-equilibrium green function calculation. In addition, 8×1 kpoint sampling is considered for transport function. All the structures are relaxed until the force on each atom is less than $0.01 \text{ eV/\AA}$ and converged of the total energy is achieved when the value of two interactions are less than $10 - 5 \text{ eV}$. The $20 \text{ \AA}$ vacuum is taken to avoid the interactions among the nearest neighboring PtSe₂ layers.

3. Results And Discussion

The monolayer of PtSe₂ is formed in two different structures known as 1T, 2H. Also, the stacking of layers is in AA or AB structure for bilayer, and the same rules are applied for trilayers in theory [5] However, it has been shown that PtSe₂ in experimental form is almost 1T and in form of AA stacking [6]. Figure 1 shows the structure of the monolayer and trilayer of PtSe₂ in its final optimized stacking in addition to band structures. As can be seen, the 1T structure in AAA is considered for trilayer one and 1T for monolayer which is defined after comparing total energies of different configurations of PtSe₂ and it is in good agreement with the experiment [6]. The bandgap of the monolayer is almost 1.177 eV while the trilayer has almost 0.15 eV which is in good agreement with previous reports [4]. Such differences in the bandgap due to interlayer effects and the possibility of growing PtSe₂ multilayer-monolayer junction, just like other transition metal dichalcogenide family, in simple CVD growth inspire us to study this lateral junction.

The transport properties are modeled with a semi-infinite trilayer PtSe₂ and a semi-infinite monolayer one as contacts. To model these semi-infinite structures, three primitive unit cells in form of a supercell are considered as starting of an iterative algorithm. The channel is modeled with five unit-cells of monolayer and trilayer that form a junction. The model then optimized properly to define the lateral junction. Figure 2 shows the device.

The current-voltage characteristic of the junction illustrates in Fig. 3. As can be seen, a clear diode characteristic is observed from the junction. When voltage is applied on the trilayer contact, the current would be positive and rises around 1 V while under reverse bias no current would be transmitted. Such characteristics can be better understood by reviewing the transmission which shows in Fig. 4. As can be

seen, the transmission of the trilayer device is not zero for small values of Energies that lead to higher transmission in low applied voltages which is due to a small bandgap. On the other hand, the monolayer one shows small transmission in large energies due to its large bandgap.

The transmission at different energies varies depending on the kpoint perpendicular to the transmission direction. Figures 5a, 4b, and 4c illustrate this transmission for monolayer, trilayer, and the junction, respectively. As can be seen, the transmission is dominant around the Γ point. It should be noted that the transmission of the junction is depending on the scattering of the wave function due to junction and hence it is voltage-dependent. Figure 6 illustrates the transmission of the junction in various bias voltages. The dark lines show the bias window in which the transmission inside these lines is considered for the current. As can be seen, the transmission is altered due to applied bias voltages. Interestingly these changes are different in forwarding bias versus the reverse one which led to diode characteristic for the device. The clear difference can be seen by comparing the transmission in 1.25 V forward and reverse bias voltages. The k-point transmission shows that in 1.8V voltage bias at $E=-0.71$ the transmission is in the highest amount inside the bias window and would not happen at $\Gamma(0,0)$ point but $(0,0.25)$. To understand the reason for such dependency of transmission on the voltage bias, we have studied the projected device density of state (PDDOS) in different voltage bias is shown in Fig. 7.

Figure 7a illustrates the PDDOS for a zero-voltage biased device. The bandgap of both left and right can be seen and the lowest valence band of trilayer considered as the reference for fermi level. The interesting DOS can be seen at the junction, which is the leak of orbitals from the trilayer to the monolayer part of the device. As the forward bias is applied and shown in Fig. 7b, the PDDOS is bent till the conduction layer of the trilayer is in front of the valence band of the monolayer which improves the possibility of transmission through the barrier from tunneling effects. This effect is the main reason for the improvement of current in the forward bias. On the other hand, in the reverse bias, the valence part of the trilayer of the device is not seen the conductance of the monolayer due to the differences of the bandgap between them. In this case, the tunneling is highly unlikely and hence the current is not possible as seen in Fig. 7c. The supplementary animations show the forward and reverse bias PDDOS in different voltages and the tunneling possibility in forwarding bias would be visible. The animated PDDOS in supplementary materials shows such bending in different forward biases for more clarity.

To see which part needs more engineering in future investigations, the eigenstate of transmission in the 1.8V bias voltage at the $E=-0.71$ for the kpoint of $(0,0.25)$ is considered and shown in Fig. 8. As illustrated the main drop of the eigenstate happens near the junction. This shows that engineering the junction of the device can improve the working of this lateral trilayer/monolayer PtSe₂ diode as now is under investigation.

4. Conclusions

Due to the unique properties of nano-scale PtSe₂ and the dependency of its bandgap on the number of layers, a heterostructure based on the junction between trilayer and monolayer of them is proposed. The

transport properties of such junction are investigated using a non-equilibrium green function tuned with density functional theory. It is shown that the junction is the form of a diode. As the forward bias is applied the conduction band and valence band is aligned which increased the possibility of tunneling and leads to an increase in the current while in reverse bias such possibility does not exist. Also, the eigenstate of transmission shows that the atoms at the junction between trilayer to monolayer are the most effective atoms on the current-voltage characteristic.

Declarations

Funding: Not applicable.

Conflicts of interest/Competing interests: The authors declare no conflict of interest.

Availability of data: The data that support the findings of this study are available from the corresponding author, M. Berahman, upon reasonable request.

Code availability: the software used in this paper is available through the official website of Siesta package.

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Figures

(a)

(b)

Figure 1

The 1T unit cell and band structure of (a) monolayer and (b) trilayer PtSe₂

Figure 2

The device of the monolayer/ trilayer PtSe₂ heterojunction. The red balls show the Pt atoms while the orange balls are Se. The two yellow box shows the contacts.

Figure 3

The current-voltage characteristic of PtSe₂ junction

Figure 4

The transmission vs Energy of trilayer monolayer and the junction

Figure 5

Transmission vs Energy in different k point perpendicular to transmission direction for (a) monolayer (b) trilayer and (c) junction PtSe2

Figure 6

The transmission of junction PtSe₂ vs energy in different bias voltages

Figure 7

The projected device density of state of PtSe₂ junction for (a) equilibrium (b) forward bias (c) reverse bias

Figure 8

The eigenstate at the max transmission ($E=-0.71\text{eV}$) at kpoint of (0,0.25).