The Study for Two-dimensional PtX2 (X=S Se Te) Which Have Geometrical Structures Fully Composed of Pentagons.

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The Study for Two-dimensional PtX$_2$ (X=S Se Te) Which Have Geometrical Structures Fully Composed of Pentagons.

Ping Wu
School of Physics and Technology, University of Jinan, Jinan 250022, China

Abstract. In this paper, we mainly use the first-principles method based on density functional theory to study the structure and electronic properties of three new two-dimensional materials consisting of five-membered rings, PtS$_2$, PtSe$_2$ and PtTe$_2$. Based on the structure of the pentagon tile of Cairo, the substitution of Pt, S and Pt, Se and Pt, Te between the atoms in the unequal position of the minimum repeating unit will result in different structures, and then different structures will be obtained. The obtained structure is optimized, and the phonon spectrum is calculated. Finally, the three phonon spectrum stable structures of penta-PtS$_2$, penta-PtSe$_2$ and penta-PtTe$_2$ are obtained. Then we proved the stability of these three structures from the aspects of dynamics and thermodynamics. Then their electronic properties were studied. From the calculated energy band diagram, we found that these three structures are indirect band gap semiconductors.

1. Introduction
We all know that carbon is one of the most widely studied elements in the periodic table. Carbon has many allotropes composed of C5, C6, and C7 rings [1-4]. However, graphene composed of six carbon rings has structural defects in stone-wales [5]. In the last two years, Wang et al. discovered a new type of allotrope of two-dimensional carbon elements, which has a deformed Dirac cone in its structure, this structure is composed of a regular arrangement of 5-6-7 carbon rings [6]. In recent years, researchers have discovered a new type of carbon material that consists entirely of five-membered rings. The new material can be stripped from the T$_{12}$ phase structure of carbon. More five-membered rings material was reported later, for example, penta-B$_2$C, and penta-SiC$_2$ and so on. And these Penta structures all have good properties. For example, penta-B$_2$C has a band gap that can be adjusted, while penta-SiC$_2$ has a unique electronic state distribution.

In this paper, we take the five-element ring structure as the basis, and assume whether the five-element ring structure exists in PtX$_2$(X=S Se Te) material. We first obtain the five-element ring structure through the method of atomic substitution, and then carry out structural optimization, phonon spectrum calculation, etc., to analyze their stability. And then finally for stable structures we calculate their electron properties.

2. Calculation method
In this article, we use the VASP software package, which is based on first principles. And the cutoff energy of the plane wave base set is 400 eV. The generalized gradient approximation theory (GGA-PBE) [8] is used to describe the exchange correlation energy between electrons, and the method of adding plane wave (PAW) [7] is used to describe the interaction between electrons and ions in the calculated system. In the calculation of this paper, the vacuum layer we defined is 15Å, and the k-mesh mesh of 15× 15× 1 is taken. The molecular dynamics time step was 1 fs and the simulation
duration was 6 ps. Our initial simulation temperature was 300 K. Bader analysis [9-10] was used to analyze the charge transfer in the system. Phonon spectrum is calculated using Phonopy babe [11], and in the calculation of phonon spectrum, we define the convergence standard of force as 0.1 meV/Å.

3. Calculation results and discussion

3.1. Geometric structure and stability of the three materials

The pentagon structure of Cairo is shown in figure 1, and a × b is used to represent its protocell in figure 1. A, B, C, D and E represent the unequal positions of Pt, S, Pt, Se and Pt and Te atoms respectively.

![Figure 1. The schematic diagram of Cairo pentagon](image1)

By making atomic substitutions in different places, we have optimized the \textit{penta}-Pt\textsubscript{n}X\textsubscript{m} structure and calculated the corresponding phonon spectrum.

![Figure 2. (a), (b) and (c) are respectively the structural diagrams of penta-PtS\textsubscript{2}, penta-PtSe\textsubscript{2} and penta-PtTe\textsubscript{2}](image2)

As can be seen from figure 2, the \textit{penta} structure formed by these three materials has slight folds to release the spatial stress, which is not completely the same as the Cairo pentagonal tile. Then we use Bader software to charge analysis; the formation energy \( E_\text{f} \) of these three structures is calculated by using formula (1). Positive (negative) for \( E_\text{f} \) is an exothermic (endothermic) reaction.

\[
E_\text{f} = E_{\text{Pt}X_2} + 2E_X - E_{\text{PtX}_2}
\]

![Figure 3. Table 1. Lattice constant formation energy and charge distribution of the three materials](image3)

| Structure | Lattice/Å | \( E_\text{f}/\text{eV} \) | Charge/e | \( E_\text{Pt}X_2 \) |
|-----------|-----------|---------------------------|----------|------------------|
| Pt\textsubscript{2}S\textsubscript{4} | 5.59      | 1.03                      | 9.8      | 12.2             |
| Pt\textsubscript{2}Se\textsubscript{4} | 5.99      | 0.68                      | 10.12    | 11.88            |
| Pt\textsubscript{2}Te\textsubscript{4} | 6.44      | 0.86                      | 10.5     | 11.5             |

What we found out by calculation, the kinetics of the \textit{penta}-PtX\textsubscript{2} configuration is stable, because there is no imaginary frequency in the phonon spectrum, then we calculate the molecular dynamics of
penta-ptX₂ structures with stable phonon spectrum to analyse their thermal stability. We’re expanding the 5 × 5 supercell to reduce the error. The initial simulation temperature of molecular dynamics is 300 K. and the temperature rises at an interval of 50 K. After that, we analyze the final structure of the simulation. As shown in Figure 3, penta-PtS₂, penta-PtSe₂ and penta-PtTe₂ are stable at 1100K, 1000K and 650K, respectively.

In FIG. 4, we analyze the mechanical stability of the three material structures. We made the calculation by using the protocell. From figure 4, we can clearly see that for the two materials penta-PtS₂ and penta-PtSe₂, they can withstand the biaxial stress of 13%, and penta-PtTe₂ can withstand the biaxial stress of 14%, showing a good static stability.

Figure 3. (a) figure on the left side of penta-PtS₂ phonon spectra, and the right to at 1100 k temperature curve of simulation time and the total potential energy (b) the figure on the left side of penta-PtSe₂ phonon spectra, and the right to at 1000 k temperature curve of simulation time and the total potential energy (c) figure on the left side of penta-PtTe₂ phonon spectra, and the right to at 650 k temperature curve of simulation time and the total potential energy. The illustration in the three diagrams is the structure diagram after simulation.

FIG. 4. (a), (b) and (c) are biaxial stress curves of penta-PtS₂, penta-PtSe₂ and penta-PtTe₂ respectively
In addition, in order to further test their stability, we use the finite deformation method to calculate the corresponding Young's modulus and Poisson's ratio. The results are listed in Table 2.

**Table 2. Young's modulus and Poisson's ratio of the three materials**

| Structure  | Elasticity/N/m | ν  |
|------------|----------------|----|
| Pt₅S₄      | 89.85          | 0.26 |
| Pt₅Se₄     | 43.19          | 0.28 |
| Pt₅Te₄     | 49.73          | 0.31 |

These data demonstrate the mechanical stability of the three materials.

3.2. Study on the electronic properties of the three materials

We proved the stability of penta-PtS₂, penta-PtSe₂ and penta-PtTe₂ with different methods above. We then studied the electronic properties of these three structures, as shown in Figure 5. As can be seen from the band diagram, all three materials are indirect bandgap semiconductors with large band gaps, which have good applications in semiconductor devices.

**FIG. 5.** (a), (b) and (c) are energy band diagrams of penta-PtS₂, penta-PtSe₂ and penta-PtTe₂, respectively.

**FIG. 6.** (a), (d), (b) and (e) respectively represent phonon spectra and band diagrams of penta-PtS₂ and penta-PtSe₂ under 13% biaxial stress, and (c) and (f) represent phonon spectra and band diagrams of penta-PtTe₂ under 14% biaxial stress.

It is well known that stress is very effective in adjusting the electronic properties of two-dimensional materials, which can be proved in many materials studied [12-13]. For the three two-dimensional materials penta-PtS₂, penta-PtSe₂ and penta-PtTe₂, we applied stress to them and calculated the corresponding phonon spectrum and electronic properties, as shown in FIG. 6. It can be
seen from figure 6 that when $\text{penta-PtTe}_2$ is applied with a biaxial stress of 14%, its electronic properties show metallic properties.

4. Conclusion
In this paper, we obtained three two-dimensional materials, $\text{penta-PtS}_2$, $\text{penta-PtSe}_2$ and $\text{penta-PtTe}_2$, and calculated their properties by using the first principle. The obtained data proved their stability from different aspects and analysed them. For example, in the calculation of phonon spectra, we can see that phonon spectra are stable, and no virtual frequency indicates that their dynamics are stable; Later, in the simulation calculation of molecular dynamics, we obtained that the melting temperatures of the three materials were 1100 K, 1000 K and 650 K respectively, indicating that the thermodynamics was stable. The calculation of formation energy shows that they are exothermic and easy to form. After applying the stress, $\text{penta-PtS}_2$, $\text{penta-PtSe}_2$ and $\text{penta-PtTe}_2$ were found to be able to withstand the stress of 13%, 13% and 14% of the biaxial stress. In addition, the calculation of electronic properties shows that these three materials are all semiconductors with indirect bandgap, and the electronic properties of penta-ptte2 will change from semiconductor to metallic property after applying stress.

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