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A novel two-dimensional SiO sheet with high-stability, strain tunable electronic structure, and excellent mechanical properties*

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Using the structure search of particle swarm optimization (PSO) algorithm combined with density functional theory (DFT), we conduct a systematic two-dimensional (2D) material research on the SiO and discover a P2 monolayer structure. The phonon spectrum shows that the 2D P2 is dynamic-stable under ambient pressure. Molecular dynamics simulations show that 2D P2 can still exist stably at a high temperature of 1000 K, indicating that 2D P2 has application potential in high-temperature environments. The intrinsic 2D P2 structure has a quasi-direct band gap of 3.2 eV. The 2D P2 structure can be transformed into a direct band gap semiconductor by appropriate strain, and the band gap can be adjusted to the ideal band gap of 1.2 eV–1.6 eV for photovoltaic materials. These unique properties of the 2D P2 structure make it expected to have potential applications in nanomechanics and nanoelectronics.

Keywords: 2D material, SiO sheet, first-principles method, strain

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1. Introduction

Generally speaking, a two-dimensional (2D) material refers to a material with one or several atomic layers in a certain dimension, and the movement of electrons in this dimension is greatly restricted. Due to the uniqueness of the structure, 2D materials have different electronic, magnetic, and optical properties from three-dimensional (3D) materials, one-dimensional (1D) materials, and zero-dimensional materials,[1,2] In recent years, 2D material has gradually become one of the most attractive research hotspots. With the deepening of research on 2D materials, more and more new 2D materials have been discovered, including metals,[3–7] semi-metals,[8–11] semiconductors,[12–17] and insulators,[18–21] which have application prospects in many fields. These achievements greatly motivate the investigation of other new 2D material.

With the increasing demand for energy, the design and manufacture of high-efficiency photovoltaic devices to convert solar energy into electricity has become an effective way to alleviate the energy crisis. Due to the stability and abundant reserves, traditional silicon-based materials has become the main material of manufacturing solar cells in industry. However, the indirect band gap limits the light absorption and photoelectric conversion efficiency.[22] Because 2D materials have lower dimensions, and also may have adjustable band gaps and excellent mechanical properties, people have turned their attention to 2D photovoltaic systems, making them a new favorite in the photovoltaic field. For an ideal 2D photovoltaic material, it should have a direct band gap and a moderate band gap value about 1.2 eV–1.6 eV.[23] Although many 2D materials have been discovered or predicted in the past, it is very rare to have both properties at the same time. Therefore, looking for new 2D materials with adjustable band gap and excellent mechanical properties will have important research significance.

Here, we conduct a systematic 2D material research on the SiO system and predict a new type of 2D structure P2. The calculation of phonon spectrum shows that the 2D P2 is dynamic stable under ambient pressure. MD simulations show that the structure can still exist stably at a high temperature of 1000 K, indicating that the 2D P2 has application potential in high-temperature environment. The intrinsic 2D P2 structure has a quasi-direct band gap of 3.2 eV. The 2D P2 can be transformed into a direct band gap by a small strain, and has an ideal band gap value about 1.5 eV as a photovoltaic material.

2. Methods

We use the CALYPSO code[24,25] based on particle swarm optimization (PSO) to perform crystal structure search. In order to ensure the accuracy of the search, 2–6 times the chemical formula SiO per unit cell are used. We use the Perdew–Burke–Ernzerhof (PBE)[26] exchange–correlation

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functional and the projector augmented wave (PAW) potential within the Vienna *ab initio* simulation package (VASP) code[27–29] for self-consistent energy calculation and structural optimization. The plane-wave energy cutoff is set to 800 eV. All the geometry structures are fully relaxed until energy and force are converged to 10^{-8} eV and 0.002 eV/Å, respectively. The Brillouin zone is integrated using the tetrahedral method with Blöchl correction. In all calculations, a 15-Å vacuum layer is used. We use the hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE06)[30] method to calculate the band structure to get a more accurate band gap value than PBE method. Phonon dispersion curves are calculated by using a supercell approach as implemented in the Phonopy package.[31] In order to ensure the accuracy of the calculation, a $4 \times 6 \times 1$ supercell of 96 atoms is employed. Convergence criteria employed for the total energy are set to 10^{-8} eV.

3. Result and discussion

Using the CALYPSO code based on the PSO algorithm, we conduct a systematic structure search on the SiO system, and we find a new 2D structure with the space group of P2, as shown in Fig. 1. The structure is composed of many ten-membered rings, and each ten-membered ring is formed by 4 oxygen atoms and 6 silicon atoms. In the 10-membered ring structure unit, 6 Si atoms and 2 O atoms are in one plane, while the other 2 O atoms out of the plane. We have made the electronic localization function (ELF) of the structure, as shown in Figs. 1(c) and 1(d). It can be seen from the ELF data that the protruding plane oxygen atom forms a covalent bond with two adjacent silicon atoms, and two silicon atoms also form a covalent bond with another silicon atom or oxygen atom. The reason why the oxygen atom protrudes from the 2D plane is that the local charge around the oxygen atom and the local charge in the Si–Si bond repel each other. All silicon atoms in the structure form 4-coordination, while oxygen atoms form 2-coordination.

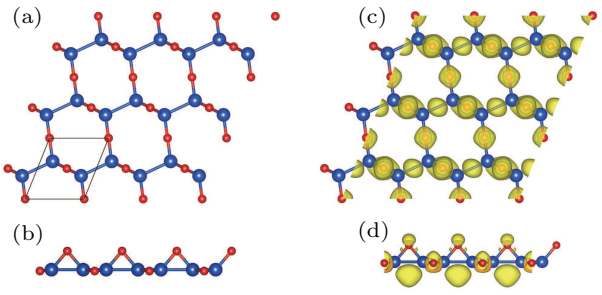


Fig. 1. Equilibrium 2D monolayer SiO of 2D P2 in both top (a) and side (b) views; the calculated ELF of 2D P2 structure [(c)–(d)]. Blue and red balls are Si and O atoms, respectively.

Dynamic stability is an important basis for judging whether a structure can be stable. In order to characterize the dynamic stability of the 2D P2 structure, we use the finite displacement method to calculate the phonon spectrum of the 2D P2 structure. As shown in the Fig. 2, the calculated phonon spectrum has no imaginary frequencies in the Brillouin zone, which shows that the structure has dynamic stability. In order to characterize the relative stability of 2D P2 structure, we calculate its cohesive energy by the expression: $E_{\mathrm{coh}} = (xE_{\mathrm{Si}} + xE_{\mathrm{O}} - E_{\mathrm{SiO}})/2x$. E_{Si}, E_{O}, and E_{SiO} represent the total energies of a single Si atom, a single O atom, and one unit cell of the monolayer, respectively. The x is the number of Si or O atoms in unitcell. The cohesive energy of 2D P2 is positive with 6.29 eV/atom, which suggests that the 2D P2 structure is formed by strongly bonds.

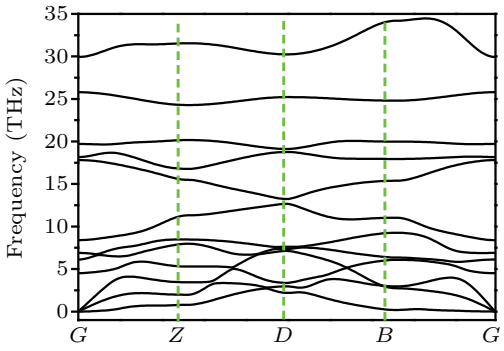


Fig. 2. Phonon dispersions of 2D P2 structure.

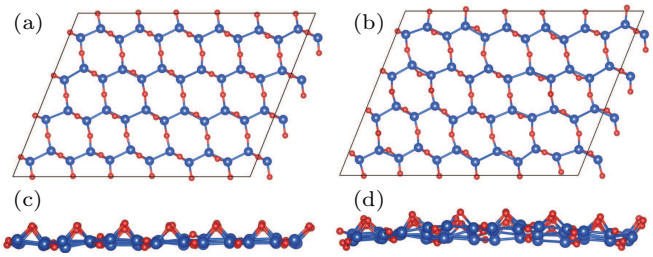


Fig. 3. Snapshots for the equilibrium structures of 2D P2 structure at 300 K [(a) and (b)], 1000 K [(c) and (d)] at the end of 10-ps AIMD simulations.

In order to characterize the thermal stability of 2D P2, we use the NVT ensemble to perform molecular dynamics (MD) simulations of the 2D P2 structure in a temperature range of 300 K–1000 K with a step size of 100 K, as shown in Fig. 3. In the process of calculation, we establish a super cell of $5 \times 7 \times 1$ (140 atoms) as a structural model to ensure the accuracy of MD simulation. Firstly, we calculate the molecular dynamics at 300 K, and the top and side views of the 2D P2 structure as shown in Fig. 3. The results show that each atom oscillates slightly at the equilibrium position and Si–O and Si–Si are still maintained, which indicates that the structure can exist stably at 300 K. As the temperature increases, the wrinkles and deformation of the 2D P2 structure gradually increase. When the temperature rises to 1000 K, Si–O and Si–Si in the P2 structure are still maintained, and no chemical bond breakage occurs. Besides, the curves of total energy *versus* simulation time at 300 K and 1000 K are shown in Fig. S1. The total energy fluctuates around a certain energy value at 300 K and 1000 K, which also shows that the structure can exist stably at 300 K and 1000 K. The above analysis shows that the 2D P2

structure has excellent thermal stability and can remain stable even under high temperature conditions of 1000 K, which also shows that the material has the prospect of application in high temperature environments.

In order to further characterize the electronic properties of the 2D material, we calculate its band structure and DOS, as shown in Fig. 4. First, we calculated the band structure of the 2D P2 structure using the PBE method (the black curve in Fig. 4(a)). From Fig. 4(a), we can see that the bottom of the conduction band and the top of the valence band of 2D P2 structure are located very close in the reciprocal space coordinates, and the band gap value is 2.23 eV. Therefore, this structure can be classified as a quasi-direct band gap semiconductor. Similar band structures have also been reported in other materials.[32,33] In general, the band gap calculated by the PBE method is smaller than the actual band gap value, while the HSE06 method is currently one of the most accurate methods for the calculation of band gap. In order to obtain a more accurate band gap value, we use the HSE06 method to calculate the band structure of the 2D P2 structure, as shown by the red line in Fig. 4(a). The band structure calculated by the HSE06 and PBE methods has a similar shape, except that the bottom of the conduction band shifts upward, and the band gap value is expanded to 3.23 eV. We then calculate the DOS of the 2D P2 material, as shown in Fig. 4(b). The results show that Si p and O p orbitals have similar shapes around the Fermi energy, indicating that the Si p and O p orbitals of this material have a strong coupling effect.

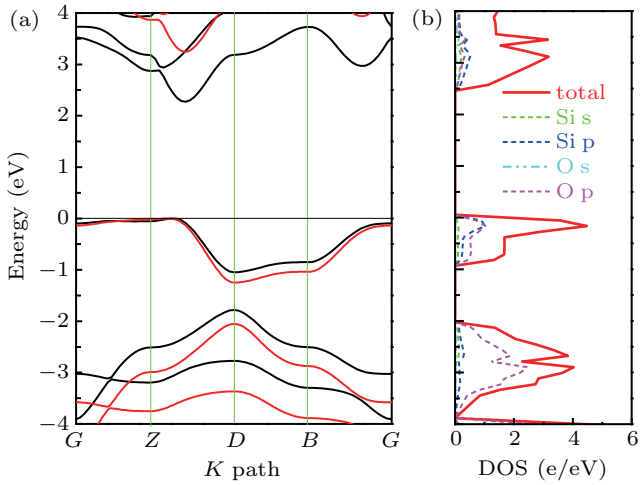


Fig. 4. The calculated (a) band structures of P2 monolayer structure by using PBE (black) and HSE06 (red) methods and (b) density of states (DOS) by using PBE method.

For ideal nano-materials, excellent strain strength is essential, and the stress–strain curve is an extremely important physical quantity that characterizes the mechanical properties of materials. Therefore, we calculate the stress–strain curve of the 2D P2 structure. Since the a and b axes of the 2D P2 structure are not equal, we calculated the uniaxial and biaxial strain curves, and the results are shown in Fig. 5. The strain is defined as $(a-a_0)/a_0$, where a and a_0 are the lattice parameters of the phase with and without strain, respectively. From the figure, we can see that when uniaxial strain is applied to the structure, the strain corresponding to the maximum stress that the structure can withstand is 16%, while for biaxial strain, the corresponding strain value is 10%. When compressive strain is applied, the monolayer can sustain a max stress with the corresponding uniaxial strain of −26% and biaxial strain of −14%, indicating the high mechanical strength of the 2D SiO monolayer. The above data shows that the structure can withstand at least 16% and 10% strain in uniaxial and biaxial directions, which also shows that the structure has very excellent mechanical properties.

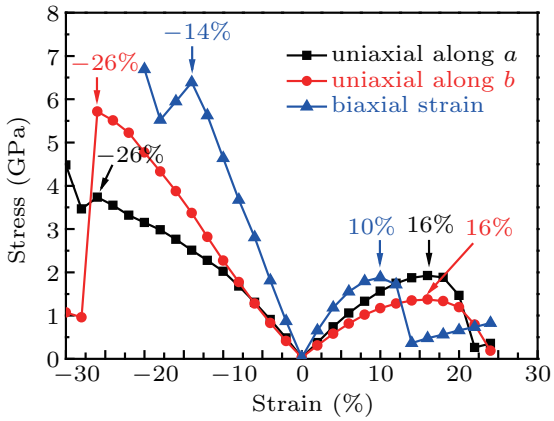


Fig. 5. Stress in the 2D P2 subjected to biaxial and uniaxial strains.

Strain is an effective method to control the electronic properties of 2D materials.[34–39] In order to further study the regulation of strain on the 2D P2, we conduct a study on the regulation of strain on electronic properties. Firstly, we conduct a study on the adjustment of the electronic properties of the 2D structure by uniaxial strain along the a direction, as shown in Fig. 6(a) and Fig. S2. Through the above analysis, the intrinsic 2D P2 structure is an indirect band gap semiconductor. When a tensile strain is applied to the structure along the a-axis direction to 8%, it begins to transform into a direct band gap semiconductor with band gap of 1.65 eV at PBE level and 2.54 eV at HES06 level, and as the tensile strain gradually increases, the band gap gradually decreases. When the increased strain reaches the maximum tensile strain of 16%, the structural band gap is about 0.52 eV using PBE method (1.13 eV using HSE06). When the compressive strain is applied to −8%, the 2D P2 structure can also be transformed into a direct band gap semiconductor with band gap of 2.29 eV at PBE level and 3.30 eV at HSE06 level. The band gap value gradually decreases as the compressive strain gradually increases, and it is about 0.56 eV using PBE method and 1.51 eV using HSE06 at −26%. Subsequently, we conduct a study on the regulation of the band gap by biaxial strain, as shown in Fig. 6(b) and Fig. S2. When a tensile strain of 8% is

applied, the 2D P2 structure undergoes a phase transition from an indirect band gap semiconductor to a direct band gap semiconductor. When compressive strain is applied, the band gap gradually increases. It is worth emphasizing that at a compressive strain of −6%, the band gap has a maximum value, and the 2D P2 structure changes from an indirect band gap semiconductor to a direct band gap semiconductor with band gap of 2.72 eV at PBE level and 3.74 eV at HES06 level. As the compressive strain continues to increase, the band gap value of the 2D P2 structure begins to decrease, and it is about 1.38 eV using PBE method and 2.46 eV using HES06 at −14%. Similarly, we also calculate the uniaxial strain along the *b* direction. There is also a regulation effect of strain on the band gap, but we do not observe the transformation of the structure into a direct band gap. Therefore, the 2D P2 structure can be transformed into a direct band gap semiconductor with appropriate strain, and the band gap value can be adjusted to 1.2 eV–1.6 eV, which is the ideal band gap value for photovoltaic materials. This also shows that the material has potential application in photovoltaic materials.

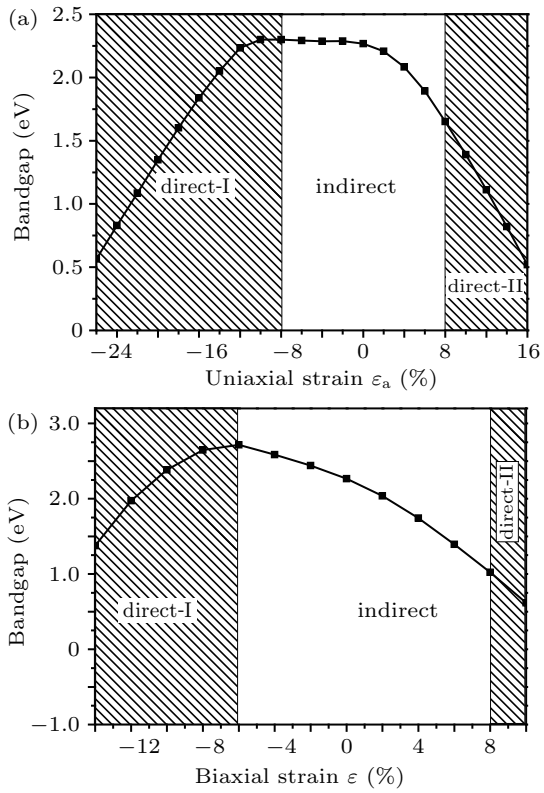


Fig. 6. Variation of band gap with in-plane uniaxial strain along the *a* direction (a) and biaxial strain (b) for the 2D P2 monolayer using the PBE method.

4. Conclusion and perspectives

We conduct a systematic 2D material research on the SiO system and discover a new 2D P2 structure by using the structure search of PSO algorithm combined with DFT. The calculation of phonon spectrum show that the structure have dynamic stability under ambient pressure. Molecular dynamics simulations show that the structure can still exist stably at a high temperature of 1000 K, indicating that the structure has application potential in high-temperature environments. The intrinsic 2D P2 structure has a quasi-direct band gap of 3.2 eV. When appropriate strain is applied, the 2D P2 structure can be transformed into a direct band gap semiconductor, and the band gap value can be adjusted to 1.5 eV, which is the ideal band gap value for photovoltaic materials. These unique properties of the 2D P2 structure make it expected to have potential applications in nanomechanics and nanoelectronics.

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