Transition-Metal-Doped SiP$_2$ Monolayer for Effective CO$_2$ Capture: A Density Functional Theory Study

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ABSTRACT: Two-dimensional materials have exhibited great potential in mitigating climate change through sensing and capturing carbon dioxide. The interaction of CO$_2$ on orthorhombic silicon diphosphide remains unexplored in spite of its interesting properties such as high carrier mobility, piezoelectricity, and mechanical stability. Here, using density functional theory, the adsorption of CO$_2$ on pristine and Ti-, V-, and Cr-doped monolayer SiP$_2$ is investigated. Doped systems exhibited significantly stronger adsorption ($-0.268$ to $-0.396$ eV) than pristine SiP$_2$ ($-0.017$ to $-0.031$ eV) and have the possibility of synthesis with low defect formation energies. Our results on adsorption energy, band structure, partial density of states, and charge transfer conclude that titanium- and vanadium-doped SiP$_2$ monolayers would be promising materials for CO$_2$ capture and removal.

INTRODUCTION

One of the most significant problems countries are facing today is the threat of climate change. Higher sea levels to ocean acidification and global warming have all been documented, where the main cause has been ever-increasing amounts of greenhouse gases in the world since the Industrial Revolution. In particular, the concentration of carbon dioxide experienced a 46% increase from roughly 280 ppm in the late 1700s to 410 ppm in 2019. Substantial efforts have been made by scientists to mitigate climate change by designing materials capable of capturing carbon dioxide. The most mature method is amine scrubbing, where CO$_2$ is absorbed into a liquid solution of monoethanolamine. The CO$_2$–amine solution is then separated under steam, allowing the amine solution to be recycled. However, the process is corrosive, environmentally harmful, and requires a high amount of energy to regenerate the solvent. Therefore, there is a need to search for better methods.

A proposed alternative to the amine process has been to use ionic liquids because they are nonvolatile, stable at high temperatures, and can be tuned to react with CO$_2$. Still, they have not been widely implemented because of their higher price and lower solubility of CO$_2$ compared to other solvents. Within the past few decades, there has been a proliferation of interest in using nanomaterials. Nanomaterials possess a naturally active surface and the ability to be functionalized with other materials, which are favorable properties for gas capture. Metal organic frameworks (MOFs) and zeolites, a subfamily of MOFs, have stood out because of their strong sensitivity, tunability, and broad applicability. Functionalized carbon nanotubes have also held great potential because of their high stability and high adsorption capacity. In recent years, two-dimensional (2D) materials have attracted much attention for CO$_2$ capture because of their extremely high surface area–volume ratio and large reaction sites for capture and permeation.

Promising experimental work on 2D materials for gas capturing confirms the value of its continual theoretical research. MXene 2D nanosheets in a mixed-matrix membrane showed good selectivity toward CO$_2$ and ran with excellent stability over an extended period of time. Similar favorable results for 2D ZnAl and Ni–Al layered double hydroxide nanosheets were found as well. A variety of methods, such as doping, could also be used to manipulate the capture. Wang et al. showed that doping graphene with Cu and Ni increased CO$_2$ adsorption from weak physisorption to chemisorption. In another example, platinum-doped silicene improved its attraction to CO$_2$.

Over the past few years, monolayer SiP$_2$ has attracted much attention over its intriguing properties. Most of the past research focuses on its stability, electronic properties, and potential as a photocatalyst, with limited review of its potential for CO$_2$ capture. When CO$_2$ was adsorbed on the oblique...
form of SiP$_2$, chemical bonds formed and the structure strongly deformed.\textsuperscript{22} Meanwhile, Yu et al. tested the presence of CO$_2$, O$_2$, H$_2$, N$_2$, and H$_2$O molecules on SiP$_2$ to better understand its stability. Their results revealed that SiP$_2$ remained intact, and all the tested gases separated from the substrate.\textsuperscript{17} Notably, there has yet to be research done on the effects of doping to modify the adsorption strength and whether the other SiP$_2$ structures are suitable for CO$_2$ capture.

In this current research, we used first-principles calculations to search for the most stable atomic structure of the SiP$_2$ monolayer. Later, we tested multiple positions to understand the adsorption of CO$_2$ on the SiP$_2$ monolayer. To improve adsorption, we then doped the SiP$_2$ monolayer with titanium, vanadium, and chromium, investigating the band structure, charge transfer, and partial density of states (PDOS).

**METHODS**

**Computations.** We performed first-principles calculations based on density functional theory (DFT) within generalized gradient approximation in the Perdew–Burke–Ernzerhof format\textsuperscript{23} implemented in the ABINIT\textsuperscript{24} suite. For pseudopotentials, we used the projected augmented wave (PAW) method\textsuperscript{25} with projectors generated using ATOMPAW.\textsuperscript{26} The electron configurations used to generate the pseudopotentials are shown in Table 1.

| element    | electron configuration | radius cutoffs (a.u.) |
|------------|------------------------|----------------------|
| silicon (Si)| [Ne]3s$^2$3p$^2$        | 1.91                 |
| phosphorus (P)| [Ne]3s$^2$3p$^3$       | 1.91                 |
| carbon (C) | [He]2s$^2$2p$^2$        | 1.51                 |
| oxygen (O) | [He]2s$^2$2p$^4$        | 1.41                 |
| titanium (Ti) | [Ne]3s$^2$3p$^6$4s$^1$3d$^3$ | 2.3               |
| vanadium (V) | [Ne]3s$^2$3p$^6$4s$^2$3d$^3$ | 2.2               |
| chromium (Cr) | [Ne]3s$^2$3p$^6$4s$^2$3d$^5$ | 2.1               |

In the total energy calculation, the self-consistent field (SCF) will be terminated once the total energy difference is smaller than $1.0 \times 10^{-10}$ Ha for the second time. We then

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**Figure 1.** Top view (first row) and side view (second row) of (a) 3 $\times$ 3 $\times$ 1 oblique SiP$_2$, (b) 3 $\times$ 2 $\times$ 1 Janus SiP$_2$, and (c) 3 $\times$ 1 $\times$ 1 orthorhombic SiP$_2$. The frames in the top view represent the unit cells. Tan atoms represent silicon, and orange atoms represent phosphorus.

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**Figure 2.** Relaxed structure of 3 $\times$ 1 $\times$ 1 SiP$_2$ and six possible adsorption sites of CO$_2$ we analyzed. T denotes that CO$_2$ was placed at the top of an atom, H denotes the placement at the hollow center of the upper hexagon, and B denotes that CO$_2$ was placed at the bond. Oval shapes represent where CO$_2$ was placed horizontally and circles represent where CO$_2$ was placed vertically. Tan and orange atoms denote silicon and phosphorus, respectively.

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**Table 2.** Calculated Lattice Constants of the Three Identified SiP$_2$ Structures and the Theoretical and Experimental Lattice Constants Previously Obtained by Other Researchers\textsuperscript{24}

| structure   | calculated | others | bulk exp | % error |
|-------------|------------|--------|----------|---------|
| oblique     | $a$ (Å)    | 3.73   | 3.71     | 2.2     |
|             | $b$ (Å)    | 3.73   |          |         |
| Janus       | $a$ (Å)    | 3.45   | 3.45     | 17      |
|             | $b$ (Å)    | 6.04   | 6.05     | 0.8     |
| orthorhombic| $a$ (Å)    | 3.47   | 3.44     | 0.86    |
|             | $b$ (Å)    | 10.00  | 10.00    | 0.8     |
|             | $c$ (Å)    |        | 13.97    |         |

\textsuperscript{24}Percent error is determined by calculated and bulk experimental values.
performed convergence with the kinetic energy cutoff, Monkhorst−Pack k-point grids, and vacuum. The dataset will be converged when the total energy difference is less than 0.0001 Ha (0.003 eV) twice consecutively. When performing structural relaxations, the SCF cycle will be terminated once the force difference is smaller than $1.0 \times 10^{-6}$ Ha/bohr twice consecutively. The maximum force tolerance in the relaxation is $5.0 \times 10^{-5}$ Ha/bohr.

Atomic Structure. We examined oblique SiP$_2$ because of its CO$_2$ capture ability, ultrahigh carrier mobility, and stability. We also analyzed the Janus structure because it was determined to have the lowest formation enthalpy compared to the other structures. Orthorhombic SiP$_2$ in the Pbam phase also captured our attention because it was the most widely researched crystal structure of SiP$_2$ and had a lower energy compared to the tetragonal structure. We converged and relaxed the structures using the 3-atom unit cell for oblique, 6-atom cell for Janus, and 12-atom cell for orthorhombic SiP$_2$ (Figure 1). Calculated lattice constants are shown in (Table 2).

After analyzing the pristine SiP$_2$ monolayers, we used orthorhombic SiP$_2$ for CO$_2$ adsorption. We placed the fully relaxed CO$_2$ molecule on the 3 × 1 × 1 SiP$_2$ monolayer at six typical positions, as shown in Figure 2. CO$_2$ is parallel to the

![Figure 3. Atomic structure and band structure of the orthorhombic SiP$_2$ monolayer. (a) Shows the 1 × 1 × 1 unit cell of SiP$_2$, (b) band structure of 1 × 1 × 1 SiP$_2$, (c) 3 × 1 × 1 cell of SiP$_2$, and (d) band structure of 3 × 1 × 1 SiP$_2$. Both structures have a direct band gap of 1.41 eV, as denoted by the blue line. The Fermi level has been set to 0 eV for both graphs. Tan atoms denote silicon, and orange atoms denote phosphorus.](https://doi.org/10.1021/acsomega.2c05532)

**Table 3. Vertical Distance between CO$_2$ and the Substrate Is Represented by $d_{\text{vertical}}$, the Smallest Atom-to-Atom Distance between the Substrate and CO$_2$ Is Denoted by $d_{\text{atom-atom}}$, and the Adsorption Energy of CO$_2$ Is Denoted by $E_{\text{ads}}$.**

|          | T$_0$ | T$_P$ | T$_{2P}$ | 2H | H | B |
|----------|-------|-------|----------|----|---|---|
| $d_{\text{vertical}}$ (Å) | 2.20  | 2.39  | 1.98     | 2.03 | 2.43 | 1.86 |
| $d_{\text{atom-atom}}$ (Å) | 3.83  | 3.99  | 4.04     | 4.12 | 3.86 | 3.96 |
| $E_{\text{ads}}$ (eV)    | −0.028| −0.023| −0.031   | −0.029 | −0.017 | −0.017 |
surface in $T_{Si}$ (on top of a silicon atom), $T_{P}$ (on top of a phosphorus atom), $T_{2P}$ (between two phosphorus atoms in the upper hexagon), and 2H site (on top of the Si–P bond between the lower and upper hexagons). At H (on top of the upper hexagon) and B (on top of the Si–P bond), CO$_2$ is placed vertically to the surface. To calculate the adsorption energies of the various positions, we defined it as

$$E_{ads} = E_{SiP_2+CO_2} - E_{SiP_2} - E_{CO_2}$$  

(1)

where $E_{SiP_2+CO_2}$ is the total energy of the SiP$_2$ monolayer adsorbed with CO$_2$, $E_{SiP_2}$ is that of the pristine monolayer, and $E_{CO_2}$ is that of a single CO$_2$ molecule. A negative $E_{ads}$ denotes that CO$_2$ can be adsorbed on the monolayer and a more negative $E_{ads}$ denotes stronger adsorption. Later, when we substituted titanium, vanadium, and chromium for phosphorus, we calculated defect formation energy as

$$E_f = E_{SiP_2+dopant} - E_{SiP_2} - E_{dopant} + E_{phosphorus}$$  

(2)

where $E_{SiP_2+dopant}$, $E_{SiP_2}$, $E_{dopant}$, and $E_{phosphorus}$ represent the total energy of doped SiP$_2$, pure SiP$_2$, and the chemical potential for Ti, V, and Cr dopant and the removed E$_{phosphorus}$ atom, respectively.

To understand the charge transfer in the doped systems, we used

$$\Delta \rho = \rho(\text{surf} + CO_2) - \rho(\text{surf}) - \rho(CO_2)$$  

(3)

where $\rho(\text{surf} + CO_2)$, $\rho(\text{surf})$, and $\rho(CO_2)$ are the charge density of the CO$_2$–SiP$_2$ system, SiP$_2$ monolayer, and CO$_2$ molecule, respectively.
To plot all the band structures, we used the high-symmetry k-points along Γ(0, 0, 0), Y(0.5, 0, 0), Σ(0.5, 0.5, 0), X(0, 0.5, 0), and S(0, 0, 0).

**RESULTS AND DISCUSSION**

**Outline.** We first analyze the structural and electronic properties of pristine monolayer SiP\(_2\). Next, we examine the adsorption of CO\(_2\) on pristine monolayer SiP\(_2\). Afterward, we discuss the interactions between doped SiP\(_2\) and CO\(_2\) using the band structure, PDOS, and charge transfer.

**Pristine SiP\(_2\).** We determined that the orthorhombic structure is energetically more stable than the oblique and Janus structure by \(-0.895\) and \(-0.003\) eV, respectively. Figure 3b,d shows that the unit cell and 3 × 1 × 1 orthorhombic monolayer SiP\(_2\) are both semiconductors with a direct band gap of 1.41 eV, and the conduction band minimum and valence band maximum are in the \(X−Γ\) path. Although the DFT method is known to underestimate the band gap, the general trend in the unit cell band structure agrees with previously reported findings. 20,21

**CO\(_2\) Adsorption on Pristine SiP\(_2\).** The corresponding adsorption energies, vertical distance of CO\(_2\) to the substrate, and smallest atom–atom distance between CO\(_2\) and SiP\(_2\) are listed in Table 3. Corresponding structures are shown in Figure 4.

As seen in Figure 4a, carbon moved away from T\(_i\), to the center of the lower hexagon with a distance of 3.83 Å to the nearest molecule. When CO\(_2\) was initially placed at T\(_j\), it also moved to the center of the lower hexagon, which can be seen upon comparing the before and after positions in Figure 4b. The energetically most favorable site had an adsorption energy of \(-0.031\) eV at T\(_{2p}\), where CO\(_2\) keeps its initial horizontal position in Figure 4c. In Figure 4d, O rotated from 2H to the center of the lower hexagon with both C atoms near opposite P atoms. The energetically least favorable site occurred at H with an adsorption energy of \(-0.017\) eV (Figure 4e). The O atom closest to the monolayer tilted away from the upper hexagon toward Si, while the other O atom remained at H. When placed vertically at B in Figure 4f, CO\(_2\) tilted toward the substrate and shifted to the edge of the lower hexagon.

In Figure 3, we see how a smaller vertical distance does not correlate with a smaller atom–atom distance and adsorption energy. 2H has the largest atom–atom distance of 4.12 Å; however, its vertical distance is smaller than other positions. T\(_{2p}\) has a larger atom–atom distance than most other positions but the highest adsorption energy. Meanwhile, B has the smallest vertical distance of 1.86 Å, while its adsorption energy is closest to zero. Comparing the positions shown in Figure 4 with the adsorption energy, we find that CO\(_2\) prefers to adsorb parallel at the center of the lower hexagon. As all the adsorption energies are small and there is a large distance from the monolayer at all the positions, pure monolayer SiP\(_2\) is ineffective for CO\(_2\) capture.

**Ti-, V-, and Cr-Doped Monolayer SiP\(_2\).** Finding that the adsorption energies on the pristine SiP\(_2\) monolayer were weak, we substituted Ti, V, and Cr for phosphorus. Doping Ti, V, and Cr resulted in strong adsorption energies of CO\(_2\) compared to other dopants across multiple monolayers. 30–34 Other dopants such as Mn and Fe did also exhibit strong adsorption; however, the strength of their adsorption was not as consistent as Ti, V, and Cr. Since titanium has four valence electrons, 4s\(^2\)3d\(^{3}\), and carbon is an electron acceptor with four valence electrons given by 2s\(^2\)2p\(^2\), we predicted that Ti-doped SiP\(_2\), could adsorb CO\(_2\) through strong ionic bonding between Ti and C. We used the T\(_j\) position for substitutional doping as consistent as Ti, V, and Cr. Since titanium has four valence electrons, 4s\(^2\)3d\(^{3}\), and carbon is an electron acceptor with four valence electrons given by 2s\(^2\)2p\(^2\), we predicted that Ti-doped SiP\(_2\), could adsorb CO\(_2\) through strong ionic bonding between Ti and C. We used the T\(_j\) position for substitutional doping as consistent as Ti, V, and Cr.
We obtained low defect formation energies of 1.288, 1.835, and 1.002 eV for Ti-, V-, and Cr-SiP\(_2\), respectively, by using eq 2 outlined in Methods. With chromium-doped SiP\(_2\), its five electrons in its outer 3d shell can pair with the five valence electrons of phosphorus to form a full 3d orbital, allowing Cr to interact stably with the nearby phosphorus atoms, and support the calculated lowest defect formation energy.

After structural relaxation of Ti-doped monolayer SiP\(_2\), Ti moves to the top of P, expanding the Ti–P–Si angle from 98.8 to 110.8°, as can be seen in the side view of Figure 5a. As can be seen in the side view of Figure 5b, the V–P–Si angle becomes 122.1° and the V–Si distance elongates from 2.34 to 2.48 Å. As shown in Figure 6c, Cr prefers to move above phosphorus with a Cr–P–Si angle of 118.1° and a P–Cr–P angle of 91.6°.

**CO\(_2\) Adsorption on Ti-, V-, and Cr-Doped Monolayer SiP\(_2\).** The adsorption energies, vertical distance, and smallest atom–atom distance between the doped substrates and CO\(_2\) are shown in Table 4. The adsorption energies of CO\(_2\) on the Ti-, V-, and Cr-SiP\(_2\) monolayer are calculated to be –0.396, –0.363, and –0.268 eV, respectively. In all the systems, CO\(_2\) prefers to adsorb vertically above the lower hexagon and form a bond between the dopant and O in the range of 2.22 to 2.28 Å (Figure 6).
Further research should analyze the total adsorption capacity and working capacity of Ti- and V-SiP. We used DFT to study the adsorption of CO and working capacity of Ti- and V-SiP. Figure 8 shows that doped Ti- and V-SiP systems showed significantly higher adsorption energies and their low defect formation energies suggest the feasibility of their synthesis. Band structure, PDOS, and charge transfer calculations were also performed, confirming that CO was strongly adsorbed. Our findings show that doped Ti- and V-SiP hold promise to be used in temperature swing adsorption for CO capture from flue gas. Further research should analyze the total adsorption capacity and working capacity of Ti- and V-SiP to understand their energy penalty and purity of CO capture.

## CONCLUSIONS

In summary, we used DFT to study the adsorption of CO on orthorhombic SiP. Various adsorption sites were considered on pristine SiP, finding small adsorption energies and large adsorption distances unsuitable for gas capture. However, doped Ti-, V-, and Cr-SiP systems showed significantly higher adsorption energies and their low defect formation energies suggest the feasibility of their synthesis. Band structure, PDOS, and charge transfer calculations were also performed, confirming that CO was strongly adsorbed. Our findings show that doped Ti- and V-SiP hold promise to be used in temperature swing adsorption for CO capture from flue gas.

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Notes

The authors declare no competing financial interest.

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