

## Intergrading effect of investigation of Carbon monoxide adsorbing on Al-doped SiC(001) Surface

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**Abstract:** We study the adsorption integrated effects of CO with different coverage (1/20, 1/10, 3/20, 1/5) on doped-Al-SiC(001) surface by using the generalized gradient approximation (GGA) based on density functional theory (DFT). The PDOS data reveal that p-electrons of Al increase the interfacial activities though Al atoms change the geometrical characteristic of SiC slightly. The changing geometric structure of the adsorbed CO exhibits the integrated effects of the increasing numbers of the adsorbed molecules. The electron density difference shown that the repulsion of the neighbor the same atoms the next-neighbor effect affects the electronic distribution of C and O atoms. The neighbor and next-neighbor effect of the adsorbed CO will change the role of the C atom of CO molecule of acceptor or contributor causing for the change of O-C-Al.

### I. INTRODUCTION

Owing to the wide band gap, high breakdown field, and high heat conductivity, SiC (silicon carbide) has outstanding device potential for high power, high temperature and high frequency application.[1-4] The related chemical and physical properties of SiC are fundamental importance of researchers who devote their efforts to innovative applications. Motivated by chemical and physical important processes such as chemical vapor deposition, doped film growth, interface interaction, formation of stable low dielectric, and accompanied by a more general interest in the effect of adsorbed gas molecules that is applied to research and develop the gas detector for CO, NH<sub>3</sub> and methane in ultra-low concentration and harsh environment,[5] the interaction of inner adsorbed molecules has been studied by using density functional theory (DFT) quite extensively in past.[6-11]

Doping elements is a common method to improve the adsorption performance of semiconductors.[12] The properties of SiC doping have been extensively studied in theory computation. Li [13] has investigated the electronic structure in Al-doped 4H-SiC. They found the Fermi level into the valence band and the energy gap broadening slightly after aluminum atoms doped, which implies that doping can indeed adjust the properties of semiconductor. Dou et al. [14] have studied the electronic properties of SiC doped with different number of Ni. The result shows that a certain number of new impurity energy level is introduced in the energy band gap owing to 3d orbits of Ni, though the analysis of the DOS, electron density difference and Mulliken overlap populations conformed that the Ni atoms are interacting with their neighboring host C atoms. The adsorption of gases on the surface of gas sensors is a complex process, there are many factors affecting the adsorption effect. Fortunately, many researchers have carried on the related investigation in this field. Cheng [15] has researched the CO molecule adsorption on SiC surface. Concluded that CO molecule make SiC exhibits metal characters when it is adsorbed on the surface, this make a clue for the design of gases sensitive device. Zahra [16] suggested that CO interaction amongst themselves (intermolecular) when CO adsorbed on the surface at coverage of 0.5 ML, which arises the interest in the study of the intergrading effects on adsorption properties such as the space geometry, band gap and adsorption energy etc. However, there still lacks of detailed

knowledge of considering the intergrating effect of adsorbed molecules when interacting with aluminum doped interface.

In this work, we will focus our attention on two related effects, doped-Al and the intergrating effect of CO adsorbed. Firstly, in order to understand the mechanism and effect of the atoms doped, we chose nonmagnetic element aluminum doped on 4H-SiC(001) surface to establish the doping model since doped aluminum can form a p-type doped semiconductor which can improve the conductive capacity. Second, polar molecules, CO, with different coverage were chosen to investigate the neighbor effect and the next neighbor effect of absorbed molecule.

## 2. Calculation models and methods

In this paper, the intergrating effect of CO molecule on doped Al-SiC was performed with the program package CASTEP in Materials Studio. As been well known, valence electron configurations of Si, C, O and Al were selected as  $3s^23p^2$ ,  $2s^22p^2$ ,  $2s^22p^4$  and  $3s^23p^1$  respectively. For a better adsorption geometrical structure characters, the generalized gradient approximation (GGA) with the PW91 function for the exchange correlation energy calculation was chosen in this work. [17-19] With the testing experiences, the supercell was set to  $5 \times 4 \times 1$  and the vacuum thickness was set to 12 Å along the Z-axis. For satisfying the requirement of computation, the accuracy of convergence was set to  $1 \times 10^{-5}$  eV/atom, the stress accuracy of convergence in crystal was set to 0.02 GPa and the maximum displacement was set to 0.002 Å with the cut-off energy of plane wave was set to 400 eV in iterative program in this calculation. The optimization step would have stopped until all the convergence conditions were satisfied.

Figure. 1 shows the supercell structure of  $(5 \times 4 \times 1)$  4H-SiC(001) and Al-doped 4H-SiC(001) structure before the optimization. In Figure. 1, the yellow color ball represents silicon atoms, the gray balls are carbon atoms and the pink ones are aluminum atoms respectively. On  $(5 \times 4 \times 1)$  Al-doped 4H-SiC(001) surface, the doping method was that making aluminum atoms replace the silicon atoms on SiC(001) crystal surface forming a substitution type doping. Doping ratio of aluminum and whole atoms on the surface is 1:4.

As shown in Figure 2, we designed the adsorption molecule, CO, with a perpendicular to the interface for a convenient observation on the changing absorbing angles with the intergrating effect.

In Figure. 2, the length of C-O band was set to 1.13 Å and C-Al bond was 1.92 Å which was similar with those parameters. For the sake of discussion, we use the red numbers to mark the CO molecules. [20-22]

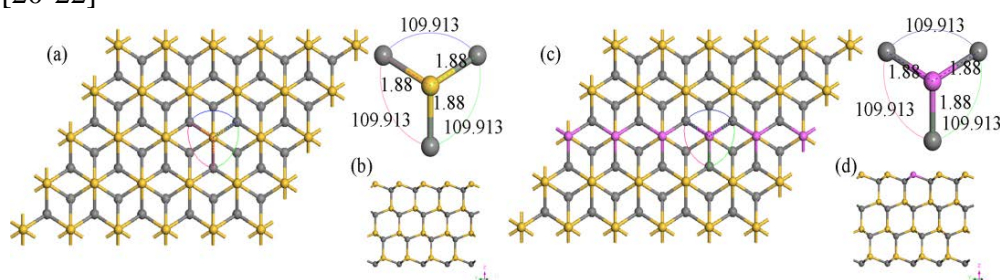


Figure 1. The  $(5 \times 4 \times 1)$  SiC(001) structure and Al-doped 4H-SiC(001) structure: (a) top view of 4H-SiC(001) structure, (b) perspective view of 4H-SiC(001) structure, (c) top view of Al-doped 4H-SiC(001) structure and (d) perspective view of Al-doped 4H-SiC(001) structure.

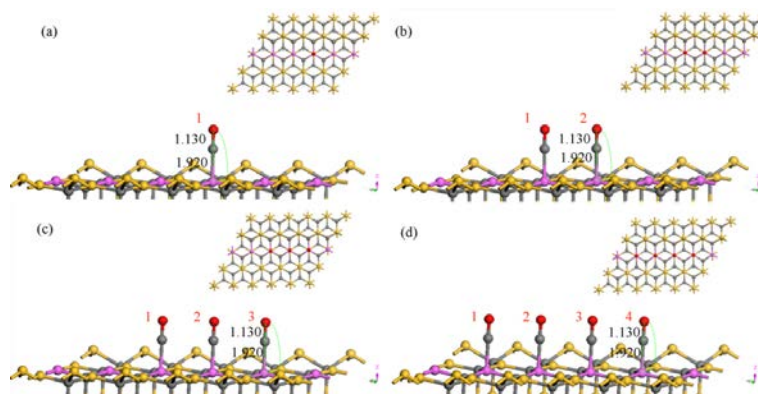


Figure 2. CO adsorbed on different surface at different coverage before optimization: (a) 1 CO on Al-doped 4H-SiC(001) surface, (b) 2 CO on Al-doped 4H-SiC(001) surface, (c) 3 CO on Al-doped 4H-SiC(001) surface, (d) 4 CO on Al-doped 4H-SiC(001) surface.

### 3. Results and discussion

#### 3.1 Structural changes of SiC(001) structure and Al-doped SiC(001) structure.

For convenience of comparison, the structure parameters of 4H-SiC(001) and Al-doped 4H-SiC(001) optimized are shown in Figure 3. As shown in Figure, the length of C-Al bond of Al-doped 4H-SiC(001) structure is longer than the C-Si bond of 4H-SiC(001) structure which means that the weakened bond will drop a hint on the more active interface. The volume of structure changed from 3301.08 Å<sup>3</sup> to 3312.236 Å<sup>3</sup> obtained by calculation, due to the mutual repulsion between the aluminum atoms and the neighboring carbon atoms and the radius of the aluminum atom (1.8 Å) which is larger than the radius of silicon atom (1.1 Å). The total energy of (5×4×1) SiC(001) structure has decreased from 20977.5 eV to 20728.02 eV after doping aluminum atoms. We notice that the lattice parameters of Al-doped SiC(001) optimized were very similar to the structure of SiC(001), which means that the aluminum atoms doped has slightly influence on the structure of SiC(001).

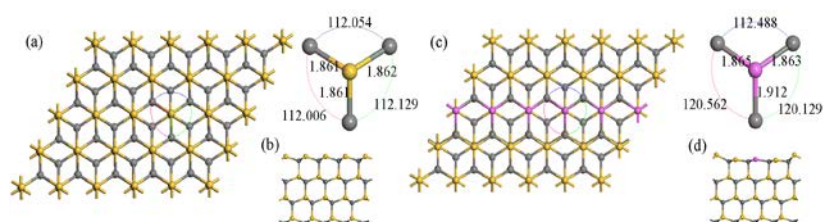


Figure 3. The optimized (5×4×1) SiC(001) structure and Al-doped 4H-SiC(001) structure: (a) top view of optimization 4H-SiC(001) structure, (b) perspective view of optimization 4H-SiC(001) structure, (c) top view of optimization Al-doped 4H-SiC(001) structure and (d) perspective view of optimization Al-doped 4H-SiC(001) structure.

In order to study the electronic structure properties of the aluminum atoms doped clearly, we calculated the partial density of states (PDOS) of (5×4×1) SiC(001) and (5×4×1) Al-doped SiC(001) surface which was illustrated in Figure 4. As can be seen in Figure 4(a), the valence band (VB) of (5×4×1) SiC(001) surface can be divided into two groups: the low energy VB has a width of 5.3 eV, ranging from -16.6 eV to -11.3 eV, mainly originating from C 2s orbital electrons, while high energy VB locates between -9.7 eV to 0 eV primarily from C 2p orbital electrons. The conduction band (CB) ranging from 1.6 eV to 3.5 eV has a width 1.9 eV mainly contributes from Si 3p. Compared Figure 4(a) with Figure 4(b), we find when three aluminum atoms substitute for three silicon atoms, the CB appears a new peak ranging from 0.8 eV to 2.7 eV, which mainly originates from the Al 3p orbits. Thus, the band gap ( $E_g$ ) becomes much narrower, which means that after the aluminum atoms were doped on SiC surface, the surface becomes more active substance for an

adsorption system.

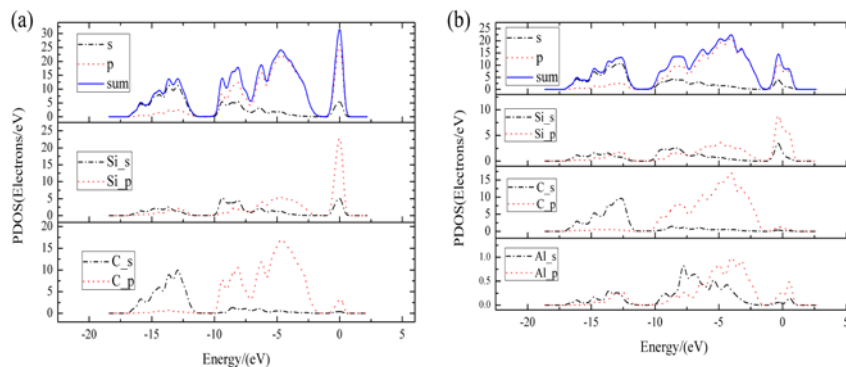


Figure 4. The density of states of supercell: (a)  $(5 \times 4 \times 1)$  SiC(001); (b)  $(5 \times 4 \times 1)$  Al-doped SiC(001).

To further understand how the charge transfers of atoms and the bond situation between atoms, we calculated the electrons difference density of SiC(001) and Al-doped SiC(001) surfaces. The electrons difference density of  $(5 \times 4 \times 1)$  SiC(001) and  $(5 \times 4 \times 1)$  Al-doped SiC(001) surface are showed in Figure. 5. The covalent characteristic can be obviously seen in Figure. 5(a). The nucleus is bound by the density charge shared between silicon and carbon atom. On the Al-doped SiC(001) surface, as is showed in the Figure. 5(b), the electron shifts toward aluminum atoms to compensate for the hole introduced by aluminum doping. The double peaks over Fermi face is from the p orbital of Si and Al, which is mainly from their  $\pi^*$  orbits, as shown in Figure. 4(b). The PDOS data from the Al-doped SiC reveals that the doped aluminum atoms cause for the double peaks of Al-doped SiC, which is a clearly characteristic of delocalized pi-electrons. The electronics density difference of SiC exhibits that Si-C has bonded while Al-C also bonded although it was weakened. An interesting phenomenon is that the doped Al polarized the next neighbor silicon, as shown in Figure. 5(b).

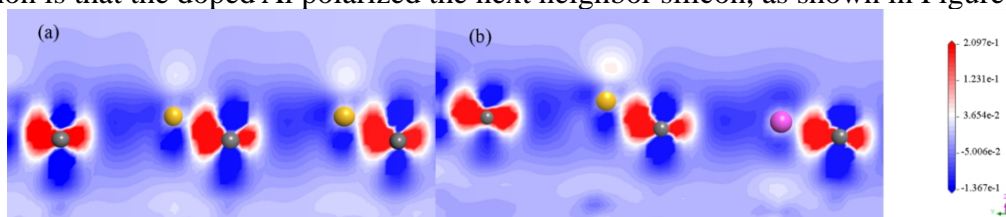


Figure 5. Figureure of electrons difference of each surface: (a) Electrons density difference of SiC(001), (b) Electrons density difference of Al-doped SiC(001).

### 3.2 Adsorption characteristic of different number CO molecules on Al-doped 4H-SiC(001) surface.

To clearly display the spatial change of the adsorbed molecules, the geometric structure for different coverage of CO absorbed on Al-doped SiC(001) surface has been constructed and the bond structure change was showed in Figure. 6. The C-O bond length was  $1.208 \text{ \AA}$ , C-Al bond was  $2.188 \text{ \AA}$  and angle change of O-C-Al decreased  $39.924^\circ$  and C-Al-Si decreased  $43.812^\circ$  at the coverage of 1/20. The bond length of C-O was  $1.174 \text{ \AA}$  to  $1.175 \text{ \AA}$ , C-Al bond was  $2.036 \text{ \AA}$  to  $2.038 \text{ \AA}$ , the angle change of O-C-Al was decreased  $21.613^\circ$  and  $23.189^\circ$  and the angle change of C-Al-Si was decreased  $19.014^\circ$  and  $20.995^\circ$  at coverage of 1/10. The bond length of C-O was  $1.163 \text{ \AA}$  to  $1.177 \text{ \AA}$ , C-Al bond was  $2.005 \text{ \AA}$  to  $2.010 \text{ \AA}$ , the angle change of O-C-Al is decreased  $14.708^\circ$ ,  $10.922^\circ$  and  $22.864^\circ$  and the angle change of C-Al-Si is  $5.646^\circ$ ,  $4.997^\circ$  and  $6.681^\circ$  at coverage of 3/20. The bond length of C-O was  $1.168 \text{ \AA}$  to  $1.176 \text{ \AA}$ , C-Al bond was  $2.041 \text{ \AA}$  to  $2.071 \text{ \AA}$ , the



angle change of O-C-Al is decreased  $22.894^\circ$ ,  $11.181^\circ$ ,  $21.782^\circ$  and  $20.447^\circ$  and the angle change of C-Al-Si is  $22.99^\circ$ ,  $18.558^\circ$ ,  $20.186^\circ$  and  $19.003^\circ$  at coverage of 1/5. In the process of analysis the various of geometry structure, amazingly, we have found some interesting adsorption pattern. In summary, those special parameters of C-O, C-Al and O-C-Al will decrease with the increasing adsorbed CO. We also find an odd-even selective adsorption growing model, i.e. the spatial change with even CO molecules exhibits the same characterization, and geometry will shows different rules with odd molecules adsorbed on the interface. The intrinsic intergrading effect of related electrons will be discussed from the view of electron density difference in the following section.

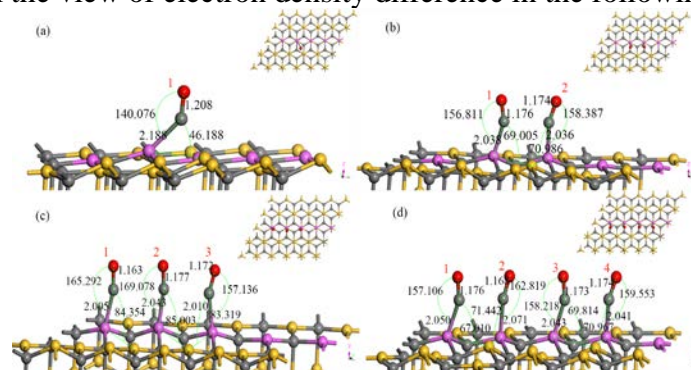


Figure 6. The geometric structure of CO molecules adsorbed on Al-doped SiC(001) surface at different coverages (a) coverage of 1/20 ML, (b) coverage of 1/10 ML, (c) coverage of 3/20 ML and (d) coverage of 1/5 ML.

We would like to calculate the adsorption energy ( $E_{ad}$ ) to verify our conjecture on the role among CO molecules. The adsorption energy of CO on aluminum doped SiC(001) surface can be deduced by Eq (1). [23]

$$E_{ad} = -\frac{1}{N}(E_{SiC.CO} - E_{SiC} - N * E_{CO}) \quad (1)$$

Here, N represents the number of CO molecules adsorbed on SiC or Al-doped SiC surface, The  $E_{ad}$  is the adsorption energy of CO molecules on SiC(001) surface. If the value of  $E_{ad}$  is positive, it means the adsorption is an exothermic reaction, and the bigger the value is, the stronger the reaction is.

With Eq (1), the adsorption energy at different coverage of CO was calculated and displayed in Figure. 7. The adsorption energy of CO on Al-doped SiC(001) surface at coverage of 1/20 ML, 1/10 ML, 3/20 ML and 1/5 are 2.0861 eV, 1.7012 eV, 1.5894 eV and 1.6902 eV, respectively. The calculated  $E_{ad}$  versus the CO coverage for the adsorption of CO on Al-doped SiC(001) surface indicated that the intergrading effect of the adsorbed CO is weakening the interaction of CO with the interface. We found also that there are the optimized coverage for the molecules adsorption system but there are the same adsorption energy for two even molecular adsorption system(i.e.1/10 and 1/5 ML), which was consistent with the structure analysis above.

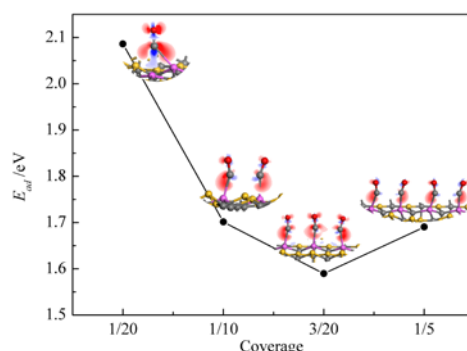


Figure 7. The calculated  $E_{ad}$  versus the CO coverage for the adsorption of CO on Al-doped SiC(001) surface.

PDOS of CO molecules and Al-doped SiC(001) surface with different coverage have been calculated. The results were shown in Figure. 8 and Figure. 9. We can see that the electron peaks of CO molecules at free state are mainly concentrated in -20 eV, -5 eV, 0 eV and 11 eV which are mainly from the p orbital electrons, as shown in Figure. 8(a). The PDOS of CO adsorbed on Al-doped SiC(001) surface is shown in Figure. 8 (b) - (e) corresponding to the coverage at 1/20, 1/10, 3/20 and 1/5 ML, respectively. We find a tend that the electron orbital of CO molecules move to low energy level with the increasing coverage. When the coverage is 1/20 ML, all electron peaks of CO molecule orbital moved 2 eV to low energy levels, the electron peaks of bonding orbital became wider, and peak values reduced. When coverage is 1/10 ML, the extent of movement to lower energy level is the same as coverage is 1/20 ML, but the difference is that the bonding orbital is wider than 1/20 ML and two electron peaks appeared at -11 eV to -9 eV, which means the adsorption is more stable. When coverage is 3/20 ML, the situation becomes different to both of the first two, all electrons orbital shifts 4 eV to lower energy level, and the peaks value becomes higher, due to the neighbor effect among CO molecules. When coverage is 1/5, we find that it's outline of PDOS almost the same as the PDOS of two CO molecule on Al-doped SiC(001) surface, which evidences the selective adsorbing growing model again. From Figure. 9, it can be concluded that PDOS of Al-doped SiC(001) surface changed little with CO molecules adsorbed, the results show that all electron peaks shift to the direction of low energy slightly and some electron peaks appear at -25.5 eV to -22.5 eV. In addition, all the PDOS of CO and Al-doped SiC(001) surface at different coverage shows the CO molecules adsorbed on Al-doped SiC(001) is a chemical adsorption and the neighbor effect among CO molecules exists in the adsorption process.

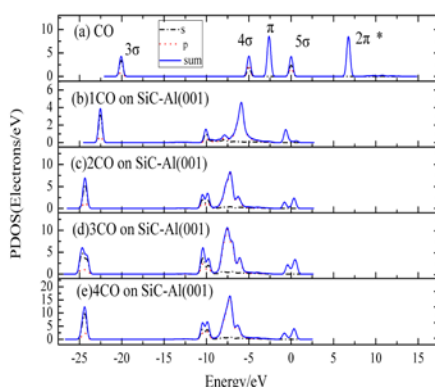


Figure 8. PDOS of CO molecules at different coverage.

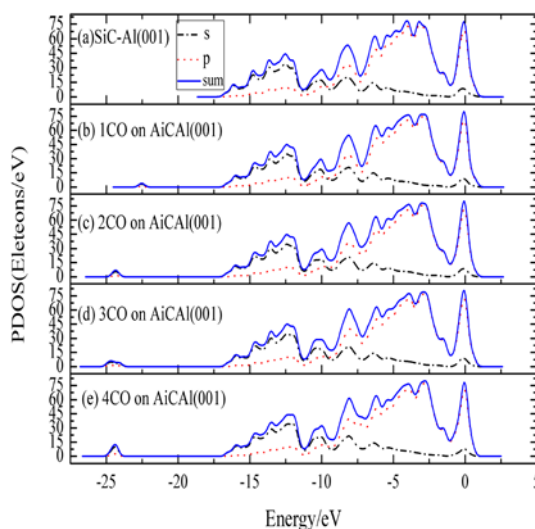


Figure 9. PDOS of Al-doped SiC(001) surface at different coverage.

The electron redistribution and Mulliken charge of related atoms for the adsorption systems are displayed in Figure. 10. When one CO molecule interacted with the interface, its electron density difference exhibited a pretty spatial system a bit like honeybee in Figure. 10(a), which shows special symmetric electronic distribution. The electronic repellant of the same neighbor molecules was clearly seen, at least the increasing distance between O atoms and their electronic cloud is so. From Figure. 10(c), we found some slight torsion occurred to electron clouds among CO molecules with the increasing adsorbing CO molecules, we believe it is for the combination intergrading effects of neighbor and next-neighbor molecules. From Figure. 10(d), although it exhibits a similar electronic distribution as that in Figure. 10(b), the electronic distribution of odd and even CO molecule exhibits respective similarity, which explains mainly the selective odd-even growing model. From the view of electron transferring, O receive -0.41 eV and C atom and Al atom contribute -0.07 eV and 1.32 eV in Figure. 10 (a). The neighbor effect takes significant role in electron transfer when the second CO molecule was designed with a distance about 0.19, as shown in Figure. 10(b). The significant change is that the intergrading effect transfers the role of the two C atom from contribution to receiver, 0.09 and 0.10 eV, respectively, which reveals the cause for O-C-Al decrease in this geometry. The C atoms also become contributor when the third CO molecule was absorbed on the interface. The electron density distribution became more harmony than that in Figure. 10(c), the acceptance and contribution of C and O atoms evidence the analysis above. Interestingly, if we take the four CO adsorbing molecules in Figure.10(d) as two groups, we can see that the neighbor effect phenomenon is more obvious than that in Figure. 10(c). In summary, from these results, we think that the chosen spacial geometries and the decreasing adsorption energy of the adsorption system determined by it's the following features, (1) the repulsion of the neighbor the same atoms is the main factor for its structures and energy, (2) the other factor is from the thickening interaction of C-Si, Si from the interface, (3) the next-neighbor effect affects the electronic distribution of C. with the increasing numbers of CO molecules, the intergrading effect of the neighbor and the next neighbor will be exhibited by the electron state density of C and O atoms, and indirectly displayed by the adsorption energy as discussed above.

The electron redistribution that occurs on adsorption of CO is analyzed through projected density of state diagrams, changes in populations of molecular orbitals and atomic orbitals of the CO adsorbate, and changes in electron populations of atomic orbitals of surface atoms.

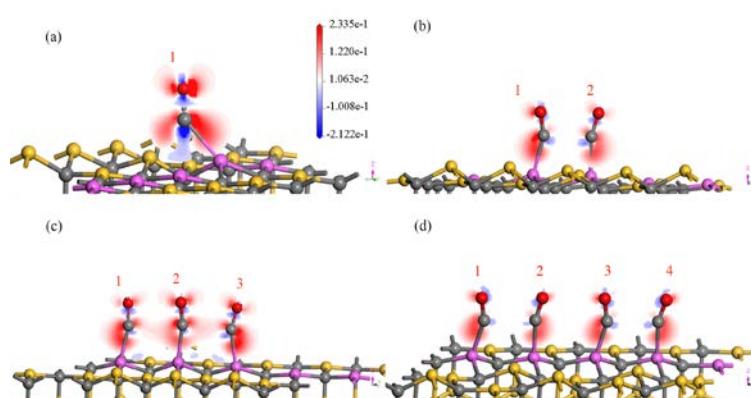


Figure 10. Figure of electron density difference of CO molecules adsorbed on Al-doped SiC(001) surface at different coverage: (a) coverage of 1/20 ML, (b) coverage of 1/10 ML, (c) coverage of 3/20 ML and (d) coverage of 1/5 ML.

#### 4. Conclusion

In this presented study, doped- and no-doped Al SiC(001) interface systems have been investigated and compared by using the first principles DFT-GGA method. It was observed that doped-Al will change the geometry structure of SiC slightly except it will significantly increase the activity of interface, which is the p-electrons of Aluminum atoms increasing the electric content

over the Fermi level cause for the increasing activity. The PDOS data of the Al-doped SiC reveal that the doped Al causes for the double peaks of Si. With the increasing number of the adsorbed CO (1/20, 1/10, 3/20, 1/5), the adsorption energy of adsorption system decrease linearly which means that the adsorption stability of this system is decreasing with the increasing number of the adsorbed molecules. The bond length and bond angle will increase with the adsorbed CO molecule, and the C atom of CO will also transfer its role from acceptor to contributor with the second CO adsorbed. The repulsion of the neighbor the same atoms and the next-neighbor effect cause for the selective growing model of odd and even adsorbed CO adsorbed, which will be investigated in our future works.

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