

# The Partial Density of States of CO<sub>2</sub> Molecules Adsorption on the Fe (111) Surface

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**Abstract.** The state of CO<sub>2</sub> molecules adsorption on Fe (111) surface is studied by simulation with the software, the partial density of states the adsorption is obtained. Through the graphical distribution, the pseudogap and the partial density of states at the Fermi level of the CO<sub>2</sub> molecules adsorption on the Fe (111) surface is analyzed and compared. The key mechanism of CO<sub>2</sub> molecules adsorption on the Fe (111) surface is revealed. The results showed that the CO<sub>2</sub> molecules adsorption on the bridge position of Fe (111) surface is stable. The main reason of O atom and Fe atom combining with the bonding is that the resonance of the density of states happened between the O 2p orbital and Fe 3d orbital.

## 1. Introduction

In solid-state and condensed matter physics, the density of states (DOS) and the partial density of states (PDOS) of a system describe the number of states per interval of energy at each energy level that are available to be occupied [1]. A high DOS of molecules at energy level means that there are many states available for occupation. The zero DOS means that there are no states can be occupied at the energy level. In general the DOS is an average occupied by the system over the time and space domains. The DOS is the main index of adsorptions' properties, the DOS is defined as follows [2]:

$$\text{DOS}(E) dE = \text{number of levels between } E \text{ and } E + dE \quad (1)$$

$E$  is the energy. The DOS for CO<sub>2</sub> adsorption on Fe (111) surface are obtained by the different position adsorption on Fe (111) surface [3,4].

## 2. Model building

The figure 1 is the unit cell structure of CO<sub>2</sub> molecule, the length of the cell is  $a=b=c=8.00 \text{ \AA}$ , the bond length of C-O is  $1.16 \text{ \AA}$  in the CO<sub>2</sub> molecule, the bond angle is  $180^\circ$ .



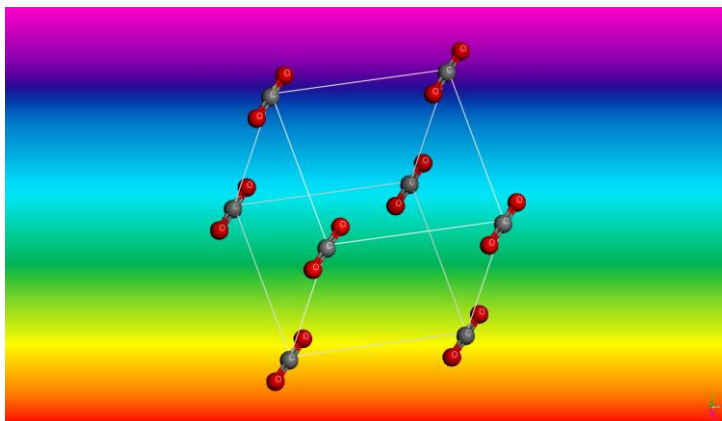


**Figure 1.** The unit cell structure of CO<sub>2</sub> molecule.

The unit cell structure of Fe is the figure 2, the length of the cell is  $a=b=c=2.8664 \text{ \AA}$ .

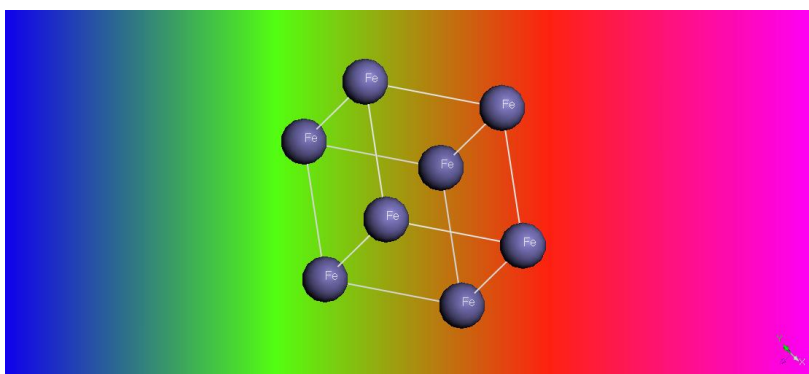


**Figure 2.** The unit cell structure of Fe.

The figure 3 is Fe (111) surface, the fractional top is  $1.5 \text{ \AA}$  and the thickness is  $1.5 \text{ \AA}$ , the vacuum thickness is  $10 \text{ \AA}$ .

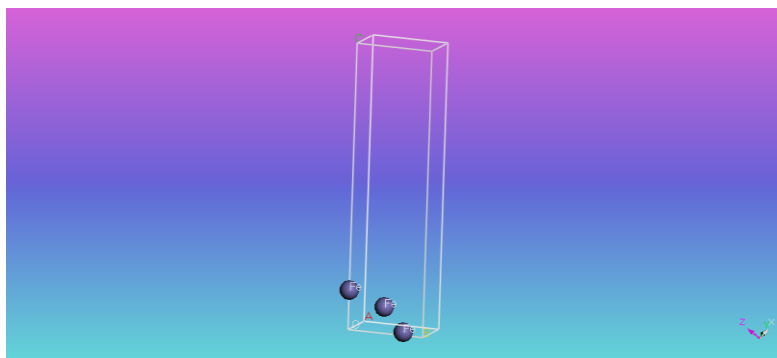


**Figure 3.** The Fe (111) surface.

The bond length of Fe-O is  $1.887 \text{ \AA}$ , the coordinates of O atom are  $x=1.8152$ ,  $y=0.3077$ ,  $z=2.9512$ . The 3D model of the CO<sub>2</sub> molecule adsorption on the Fe (111) surface is figure 4, the figure 4 (a) and the figure 4 (b) are different angles of the Fe (111) surface.

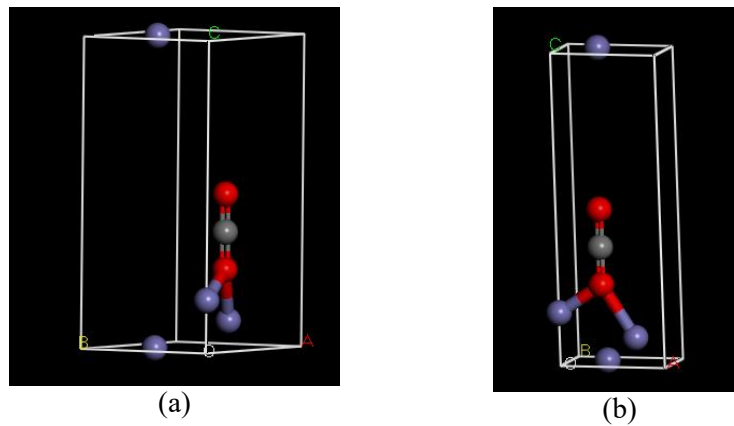


**Figure 4.** The Fe (111) surface.

The PDOS of  $\text{CO}_2$  molecule is figure 5:

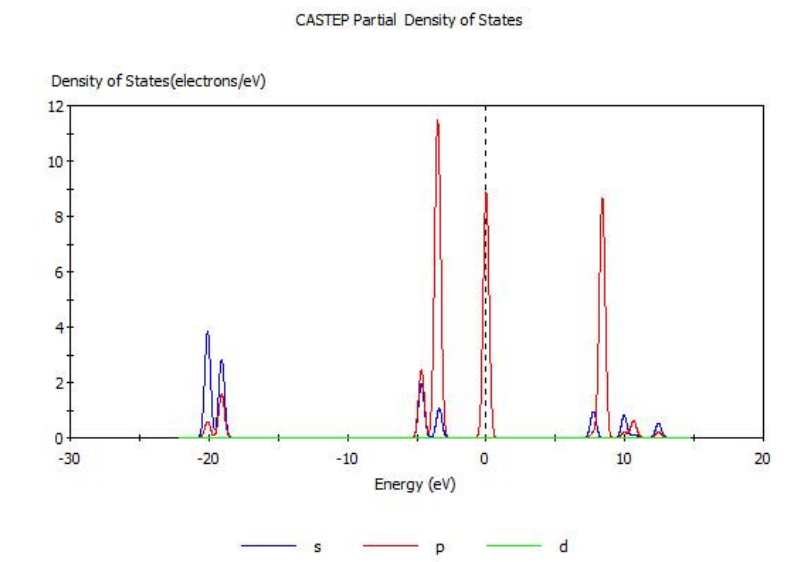


**Figure 5.** The PDOS of  $\text{CO}_2$  molecule.

The figure 6 is the PDOS of Fe (111) surface:

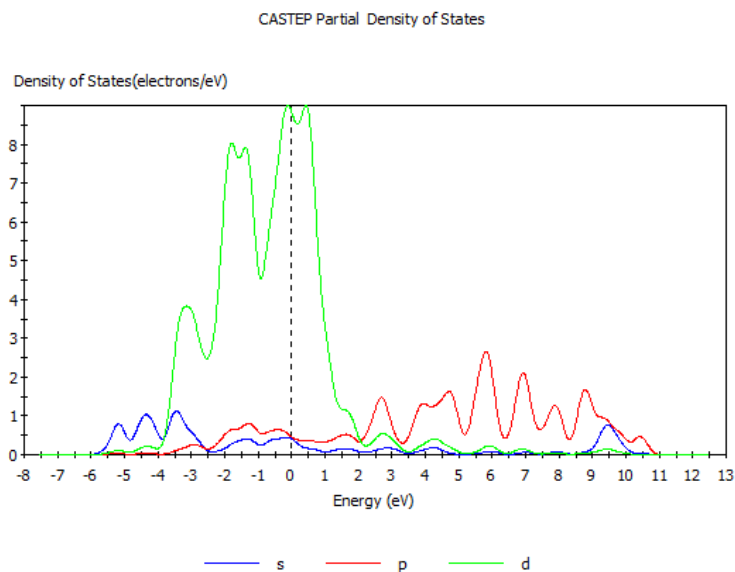


**Figure 6.** The PDOS of Fe (111) surface.

The figure 7 is the PDOS of CO<sub>2</sub> molecule adsorption on the Fe (111) surface:

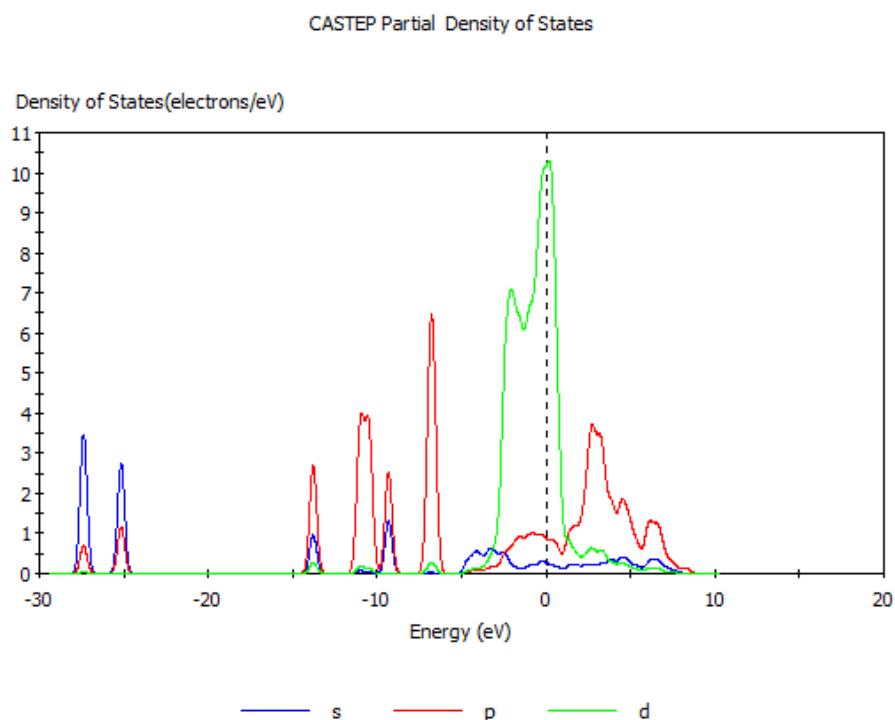


**Figure 7.** The PDOS of CO<sub>2</sub> molecule adsorption on the Fe (111) surface.

The figure 8 is the PDOS of CO<sub>2</sub> molecule after adsorption on the Fe (111) surface:

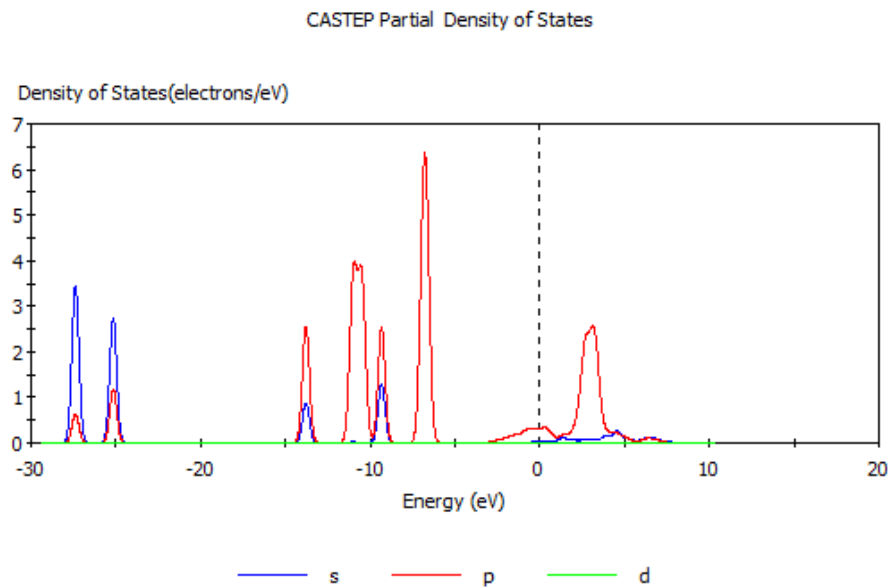


**Figure 8.** The PDOS of CO<sub>2</sub> molecule after adsorption.

The figure 9 is the PDOS of Fe after adsorption:

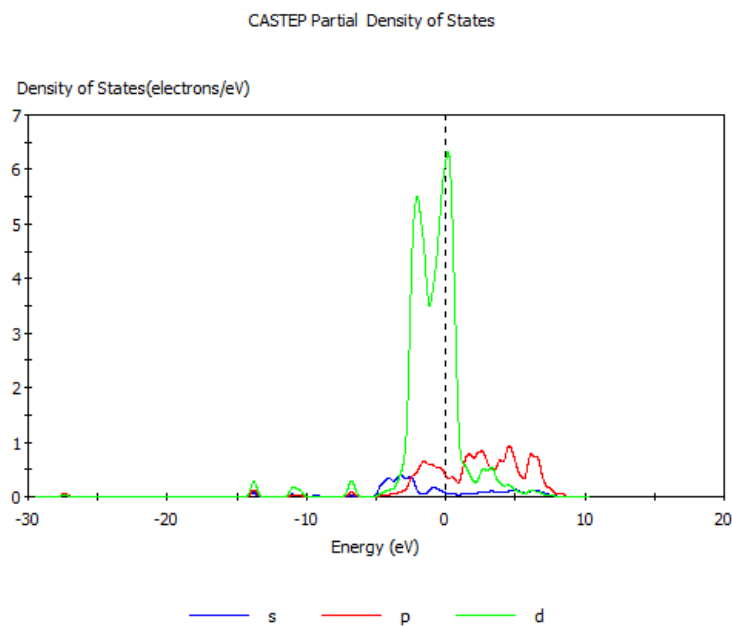


**Figure 9.** The PDOS of Fe after adsorption.

### 3. Results and discussions

The dotted line is the Fermi level in figure. From the figure 7, the DOS is very uneven in the whole energy interval distribution, it shows that the delocalized properties of electronic are very weak [5]. The values of PDOS in Fermi level are not zero, there are partial wave DOS across the Fermi level. These characteristics indicate that the system is analogous metal conductor. Atom Fe is itself a metal, the nature of the metal is due to the surface state of the Fe. In the Fig.7, there have respectively two peaks on both sides of the Fermi level [6,7]. The DOS between the two peaks is not zero. The energy discrepancy between the two peaks is 5.57eV, that is the pseudogap.

From the figure 5 and figure 8, the s orbital and p orbital of CO<sub>2</sub> move toward to low energy level. From the figure 6 and figure 9, the PDOS of the 3p orbital, 4s orbital and 3d orbital for atom Fe

decreases. From the PDOS, the 4s orbital and 3d orbital of atom Fe contribute to the PDOS of O 2s for CO<sub>2</sub> near the -25eV. The 3d orbital of Fe and O 2p orbital of CO<sub>2</sub> resonate at the -14eV, -10eV, -7eV.

#### 4. Conclusions

By simulation the CO<sub>2</sub> molecule adsorption on the Fe(111) surface, the CO<sub>2</sub> molecule adsorption on the Fe(111) surface. The pseudogap is 5.57eV in the PDOS of the CO<sub>2</sub> molecule adsorption on the Fe(111) surface. From the PDOS of the CO<sub>2</sub> molecule adsorption on the Fe(111) surface, the bond is strong covalent, the CO<sub>2</sub> molecule adsorption on the Fe(111) surface is stable. The values of PDOS in Fermi level are not zero, there are partial wave DOS across the Fermi level. These characteristics indicate that the system is the analogous metal conductor. The PDOS of the 3p orbital, 4s orbital and 3d orbital for atom Fe decreases. From the PDOS, the 4s orbital and 3d orbital of atom Fe contribute to the PDOS of O 2s for CO<sub>2</sub> near the -25eV. The 3d orbital of Fe and O 2p orbital of CO<sub>2</sub> resonate at the -14eV, -10eV, -7eV.

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