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Study of the M-doped Effect (M=Al, Ag, W) on the Dissociation of O_2 on Cu Surface Using a First Principles Method

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The O_2 adsorption and dissociation on M-doped (M=Al, Ag, W) Cu (111) surface were studied by density functional theory. The adsorption energy of adsorbate, the average binding energy and surface energy of Cu surface, and the doping energy of doping atom were calculated. All the doped atoms can be stably combined with Cu atoms and improve the surface activity of Cu surface, while the Al and W atoms would strengthen the bonding effect between the atoms on the Cu (111) slab except Ag doping atom. Due to the different electronegativity of three metals of Al, Ag, W, these doping atoms can resist the dissociation of O_2 by DOS analysis. The potential energy surface was computed, and the result showed that the dissociation reaction of O_2 on the surfaces not only reflected in the barrier energy, but also the reaction energy. Ag atoms had the best resistance effect on the O_2 dissociation comparing with Al and W atoms because of the large barrier energy and reaction energy.

Keywords: *O_2 adsorption, Metal doped, Cu (111), Dissociation.*

1. Introduction

The reaction of gas molecule and metal is under study both experimentally and computationally for metal Cu, as it is related to many processes such as catalysis, deposition, coating, corrosion or oxidation[1,2]. Among them, oxidation of Cu and Cu-based alloy surfaces is both common and important phenomenon because the oxide film formed in air protects the surface against further reaction and corrosion. The steps in the oxidation process involve dissociative adsorption of O_2 on Cu-based alloy surfaces, migration of O into the surfaces, and then oxide formation. However, the initial reaction mechanism has not been well understood, and the energy barrier of the initial oxidation are still under debate.

The adsorption and reaction of O_2 on Cu surface has been studied for years by experimental technologies. The interaction of Ni/Fe-covered Cu (100) surfaces with O_2 were studied by x-ray photoelectron spectroscopy (XPS). The authors pointed that the composition and coverage of the oxides of Fe and Ni are related to the concentration of O_2 and the exposure time[3]. Then A. R. Balkenende and collaborators found the exposure of O_2 to Cu (100) and Cu (110) surfaces leads to dissociative adsorption and the dissociation on Cu (110) surface is about an order of magnitude faster than on Cu (100) surface[4]. Dissociative chemisorption of O_2 on Cu (100), S/Cu (100) and Ag/Cu (100) surface alloy were investigated by Auger electron spectroscopy (AES). It is concluded that at very low Ag coverages, the reduced reactivity of Ag/Cu (100) towards O_2 dissociation is primarily due to the steric blocking of the surface defects and that any electronic effects are only secondary and present only at higher Ag coverages[5]. An energy selective molecular beam surface scattering experiments revealed a defect induced low-barrier dissociation pathway leading to enhanced dissociation of O_2 molecules on Cu surface with translational energy up to 60 meV[6]. These qualitative and quantitative results are mainly due to the analysis of energy oscillation spectroscopy, without directly observing the microscopic process of the initial stage of O_2 adsorption and dissociation on Cu surface.

In contrast, theoretical simulation work is more suitable for directly obtaining microscopic information such as the structure, energy, transition state, and potential energy surface of O_2 adsorption and dissociation on Cu surface. Because O atoms exhibit insignificant selectivity with respect to positions and coverages on Cu surface. For examples, based on density functional theory (DFT) calculations, people found that on Cu (211) surface the step microfacets are very reactive and the dissociation of the O_2 molecule at room temperature occurs mostly on those sites[7]. First principles simulations based on DFT were used to determine absorption energies and pathways to dissociation of O_2 at finite temperature on the Cu (110) surface. The results suggested that adsorption kinetics play an important role in determining the mechanism of dissociation[8]. Another work showed that the expansive strain parallel to the surface plane could enhance the binding of atomic and molecular oxygen on Cu (111) surface as well as to decrease the transition state energy of O_2 dissociation[9]. However, the theoretical sticking probability of O_2 dissociation on Cu (100) is found non-activated and topology of the potential energy surface is very open in entrance channels[10]. The previous work mentioned above show that the micro-mechanism of

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dissociation and adsorption of O_2 on Cu surface is a very important research topic.

Dissociation of O_2 on Cu (111) has been described as both a direct process and one mediated by a molecular precursor. The steering effect plays an important role in the oxygen molecule dissociative process. The potential-energy hypersurface (PES) for O_2 on Cu (111) is of key importance to assess dissociative phenomena. However, the surface doped elements are also an important factor affecting the dissociation of adsorbates. The doping atom could penetrate the substrate actively, change the surface activity and affect the dissociation of adsorbate on the surface[11-13]. Some metals, such as Al, Ag, W, are common elements in electrical engineering materials, and their presence has an important effect on the performance of Cu wires. Therefore, studying the microscopic process of O_2 dissociation by the doping atoms on the Cu surface will provide a direct help in understanding the oxidation and protection mechanisms of Cu-based products.

2. Computational Details

First principles calculations based on density functional theory (DFT)[14,15] were used to investigate O_2 adsorption and dissociation on the Al, Ag and W doped Cu (111) surface in the CASTEP code[16]. The ultrasoft pseudopotential[17,18] was used to describe electron-ion interaction for all atoms. The generalized gradient approximation-Perdew-Wang 1991 (GGA-PW91)[19,20] was used to describe the exchange and correlation functional. In our calculations, the cutoff energy of 500 eV was employed for plane wave expansions. The Brillouin zone is sampled by using a 10 × 10 × 10 Monkhorst-Pack k-point grid[21] for the Cu bulk lattice constant. The energy difference, the residual force, the maximum stress and the displacement of each atom were set as 10^{-5} eV/atom, 0.03 eV/Å, 0.05 GPa and 0.001 Å during the optimization to ensure the convergence of the self-consistent field calculations[22]. The climbing image nudged elastic band (CI-NEB) Method[23] was used to estimate transition state and final state structures.

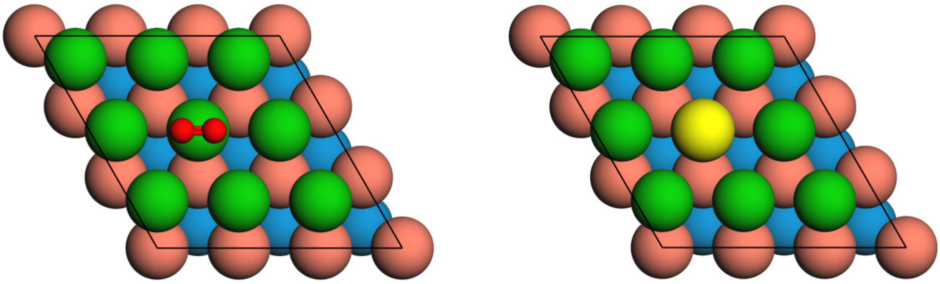
In order to check the validity of our methodology, the lattice parameter of bulk Cu which has a three-dimension primitive cell with bcc symmetry was computed. Our calculated value (3.491 Å) has a difference less than 3.5% compared to the experimental value of 3.615 Å[24] and theoretical value of 3.607 Å[25]). The surface size was modelled by using super approach with periodic boundary conditions. A vacuum layer of 20 Å was found to be sufficient to prevent the interactions between the periodic images. We used the slabs consisting of 7-layer, and relaxed the first 3 layers including doping atoms and the bottom 4 layers. By using a 3 × 3 × 1 Monkhorst-Pack k-point grid, the surface structural relaxation and the total energy calculation were performed in our study. Besides, the *p*(3x3) super cell was used to study the properties of O_2 adsorption and dissociation on the pristine/doped Cu (111) seeing in Figure 1.

The adsorption energy (E_{ads}) of adsorbate, the average binding energy (E_b) and surface energy (γ) of Cu surface, and the doping energy (E_{im}) of doping atom are calculated. The four kinds of energies are calculated in following equations 1-4.

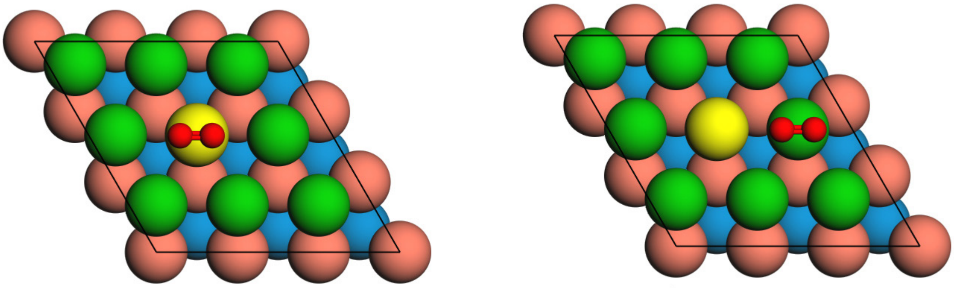
$$E_{ads} = (E_{total} - E_{slab} - E_{O2})\ /\ 2 \tag{1}$$

$$E_b = \ (E_{slab} - (n-m)E_{Cu} - mE_m)\ /\ (n+m) \tag{2}$$

$$\gamma = (E_{slab} - (n-m)E_b{}^{Cu}\ /\ 4\ - mE_b{}^{m}\ /\ 4)\ /\ 2A \tag{3}$$



(a) O2 adsorption (b) M-doped



(c) M_1NN (d) M_TOP

Figure 1. The initial structures of O_2 adsorption pristine/doped Cu (111) surface. (a) is the O_2 adsorption pristine surface. (b) is the M-doped surface. (c) is O_2 adsorption on TOP-type doped surface. (d) is the O_2 adsorption on 1NN-type doped surface. The green, bronzing and blue particles denote the first, second, third layers of Cu atoms. The oxygen and doping atoms are shown in red and yellow color, respectively.

$$E_{im} = E_{slab} - E_{slab}^{\ Cu} - E_m \tag{4}$$

where E_{total} is the total energy of the surface system, E_{slab} is the energy of pristine/doped Cu surface, $E_{slab}^{\ Cu}$ is the energy of Cu surface with the doping atom removed, and *n* and *m* denote the number of Cu and metal atoms, respectively. The E_{Cu} and E_m denote the atomic energy of Cu and metal atoms, respectively. E_{O2} is the energy of the isolated O_2 in gas phase, while $E_b^{\ Cu}$ and $E_b^{\ m}$ are the bulk energy of *fcc*-type crystal of Cu and metals, respectively.

The energy barrier (E_B) and reaction energy (E_R) are defined in equation 5 and equation 6.

$$E_B = E_{TS} - E_{IS} \tag{5}$$

$$E_R = E_{FS} - E_{IS} \tag{6}$$

The E_{IS}, E_{TS}, and E_{FS} are the energies of the initial state, transition state, and the final state of the configuration, respectively.

3. Results and Discussions

3. 1. Al, Ag, W doped Cu (111) surface

The effect of doping atoms (Al, Ag, W) on the surface binding and stability are studied firstly. We replace one Cu atom of the first layer with the metal atom to get a M-doped (M= Al, Ag, W) Cu (111) surface. We optimize the stoichiometric geometries of M-doped Cu (111) surface until the external and internal degree of freedom can relax to the force and stress vanished in the bulk calculations. The lattice constants change after metal atoms have been doped on the Cu (111) surface. The relaxed structure of the M-doped Cu (111) surfaces are shown in Figure 2. All the doping atoms can be stably combined with Cu atoms, while being slightly embedded in the surface to a certain depth. The new lattice constants for M-doped Cu surfaces are 7.617 Å, 7.632 Å, 7.638 Å, respectively, which are all slightly larger than those of pristine Cu (111) surface (7.611 Å) because of larger radius of the doping atoms. The average bond length between Cu-Cu atoms in the first layer of pristine surface is 2.537 Å. While the average bond length between Al-Cu, Ag-Cu, W-Cu atoms in the first layer of doped surfaces are 2.543 Å, 2.582 Å, 2.554 Å, respectively, which means the doping atoms make the surrounding Al atoms slightly excluding to them. This repulsion effect enhances the bonding between surface atoms and improves the energy stability of the doped Cu surfaces.

The doping energy (E_{im}), binding energy (E_b) and surface energy (γ) of pristine/doped Cu surface are listed in Table 1. It is clear seen that all the doping atoms can be stably combined with Cu atoms due to the negative values of E_{im}. The W-doped surface has the lowest E_{im} with -7.614 eV than Al-doped and Ag-doped surfaces because W atom has more valence electrons that can be transferred to and from Cu atoms. Then we compared and analyzed the change of E_b and γ between the doped surface and the pristine surface. In this paper, the E_b reflects the strength of the bonding between atoms in the slab. The E_b of pristine Al surface is -3.628 eV and lower than the E_b of Al-doped and W-doped surfaces, so the binding energy data confirms that the Al and W atoms will strengthen the bonding effect between the atoms on the Cu (111) slab. But on the Ag-doped surface, the result is exactly the opposite. In addition, the γ of pristine Al surface (3.6451 J/m^2) is lower than Al-doped and W-doped surfaces. That means Al and W atoms improves the surface activity of Cu surface, which may be more favorable for small molecules. In the same situation, Ag-doped surface has lower γ than the pristine Cu surface. Based on above results, Ag atom reduces the surface activity of Cu and inhibit the reaction between Cu surface and oxygen molecules.

3.2. O_2 adsorption on pristine/doped Cu (111) surface

It is known that O_2 prefer to adsorb at the top site of metal surface. In this work, there are one site for O_2 adsorption on pristine Cu (111) surface and two sites for O_2 adsorption on doped surface. Figure 3a shows the optimized O_2 adsorption on pristine Cu surface, and Figure 3b are the optimized O_2 adsorption on the top site of doped Cu surfaces (TOP-type) which named Al_TOP, Ag_TOP, W_TOP, respectively, and Figure 3c are the optimized O_2 adsorption on the 1st near-neighbor top site of doped Cu surface (1NN-type) which named Al_1NN, Ag_1NN, W_1NN, respectively. For all kinds of doped surfaces, it should be pointed out that the O_2 molecules prefer to adsorb in a parallel to the TOP-type surfaces, and they adsorb with a little tilt angle related to the 1NN-type surfaces. This difference is mainly caused by different atomic radii and different surface flatness under the adsorbate.

We calculated the adsorption energy (E_{ads}) of O_2 on the pristine/doped surfaces to obtain the most stable adsorption configurations. As is shown in Table 1, for the M-doped

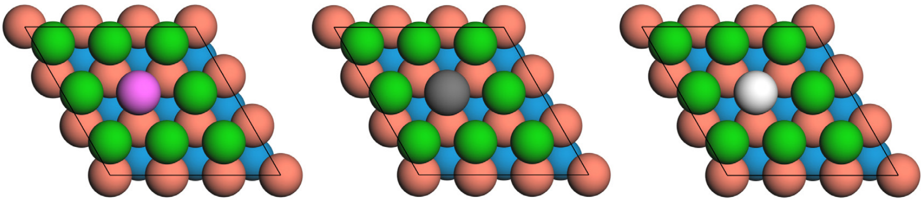

Al-doped Ag-doped W-doped

Figure 2. The top view of optimized structure of the M-doped Cu (111) surfaces. The purple, dark brown and white particles denote the Al, Ag and W atoms.

Table 1. The calculated the doping energy (E_{im}), binding energy (E_b), adsorption energy (E_{ads}) and surface energy (γ) of pristine/doped and O_2 adsorption Cu surface.

Al (111) surface	E_b (eV)	E_{im} (eV)	E_{ads} (eV)	γ (J/m^2)
Pristine	-3.628	--	--	3.645
Al doped	-3.644	-5.555	--	3.655
Ag doped	-3.610	-3.555	--	3.607
W doped	-3.708	-7.614	--	3.670
O_2 adsorption	-3.647	--	-0.589	3.641
Al_Top	-3.676	-7.577	-1.011	3.656
Al_1NN	-3.661	-6.617	-0.531	3.649
Ag_Top	-3.619	-3.996	-0.276	3.591
Ag_1NN	-3.628	-4.569	-0.562	3.597
W_Top	-3.777	-9.964	-2.175	3.770
W_1NN	-3.759	-8.833	-1.609	3.742

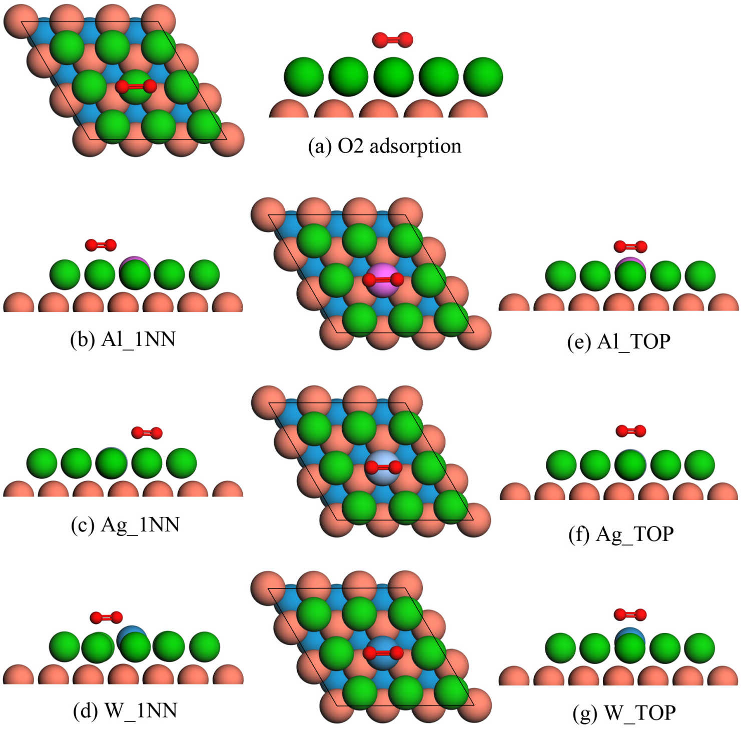


Figure 3. The top view of optimized structure of O_2 adsorption on the pristine/doped Cu surfaces. The white, maroon and brown particles denote the Al, Ag and W atoms.

surfaces, we found that most TOP-type surfaces are more stable than pristine surface for O_2 adsorption. The E_{ads} of Al_TOP, W_TOP and W_1NN surfaces are -1.011 eV, -2.175 eV and -1.609 eV, which are still much lower than pristine surface (-0.589 eV). The reason is that the distance between adsorbates and top-site Cu is smaller than these of top-site Al and W atoms. In another word, Al and W atoms embedded in the surface increase the internal binding of the system, and weaken the adsorption effect with the adsorbate. In addition, the O atom prefers to adsorb on the top of the doping atom rather than on the top site of Cu atom, because the 1NN-type surfaces have higher values of E_{ads} than TOP-type surfaces. However, the results of Ag-doped surfaces are opposite to those of other surfaces. Because of the inhibition effect of Ag atoms, the E_{ads} on both types of Ag-doped surfaces is lower than that of pristine surface. Besides that, we also computed the E_{im}, E_b and γ of O_2 adsorption on the M-doped Cu surfaces and shown the data in Table 1. After O_2 adsorption, the values of E_{im} and E_b of pristine/doped surfaces are lower than before except Ag-doped surfaces, but the values of γ of pristine/doped surfaces are higher than the clean surfaces except W-doped surfaces. The reason for our analysis is that the adsorption of O_2 causes the doping atoms to be further embedded in the surface, which increases the doping energy. This conclusion is consistent with the result of adsorption energy we mentioned above. As the doping atoms continue to penetrate into the Cu surface, the space between the Cu atoms is reduced, thereby increasing the binding energy inside the material. The reason for the increase in surface energy is also due to the presence of adsorbates. However, since the radius of Ag atom is much larger than that of Cu atom, the obvious repulsion effect causes the weak bonding between surface atoms to no longer follow the above rules.

To further explore the interaction between the substrate, doping atom and adsorbate, we introduced the electron density of states (DOS) for O_2 adsorbed pristine/doped Cu surfaces. As shown in Figure 4, we plotted the DOS of one doping atoms, two oxygen atoms and two kinds of Cu atoms, one is the Cu atom just below the adsorbed O atoms and the other one is the nearest neighbor to both the doping atom and the adsorbed O atom. We can see that the contribution of Cu-*d* elctorns to the DOS is obviously large, although the Cu-*s* and Cu-*p* electrons have hybridization and little contributions in the energy range of -10 eV to + 10 eV. Among them, the number of *d*-electrons of Cu atoms on the pristine surface is higher than that of O adsorbed surfaces. In another word, the Cu-*d* orbital electrons in the former are concentrated in the high energy region (-5 eV to 0 eV), while O-*p* orbitals in the latter are concentrated in wider energy level range of -7 eV to +2 eV. At the same time, the O-*s* and O-*p* orbital electrons have obvious peaks in the energy range of -7 eV to + 10eV, which indicates that after O adsorption, an interaction occurs between O-Cu, and some electrons are transferred from Cu atom to O atom, which in turn causes the remaining electrons of Cu atom to move to a lower

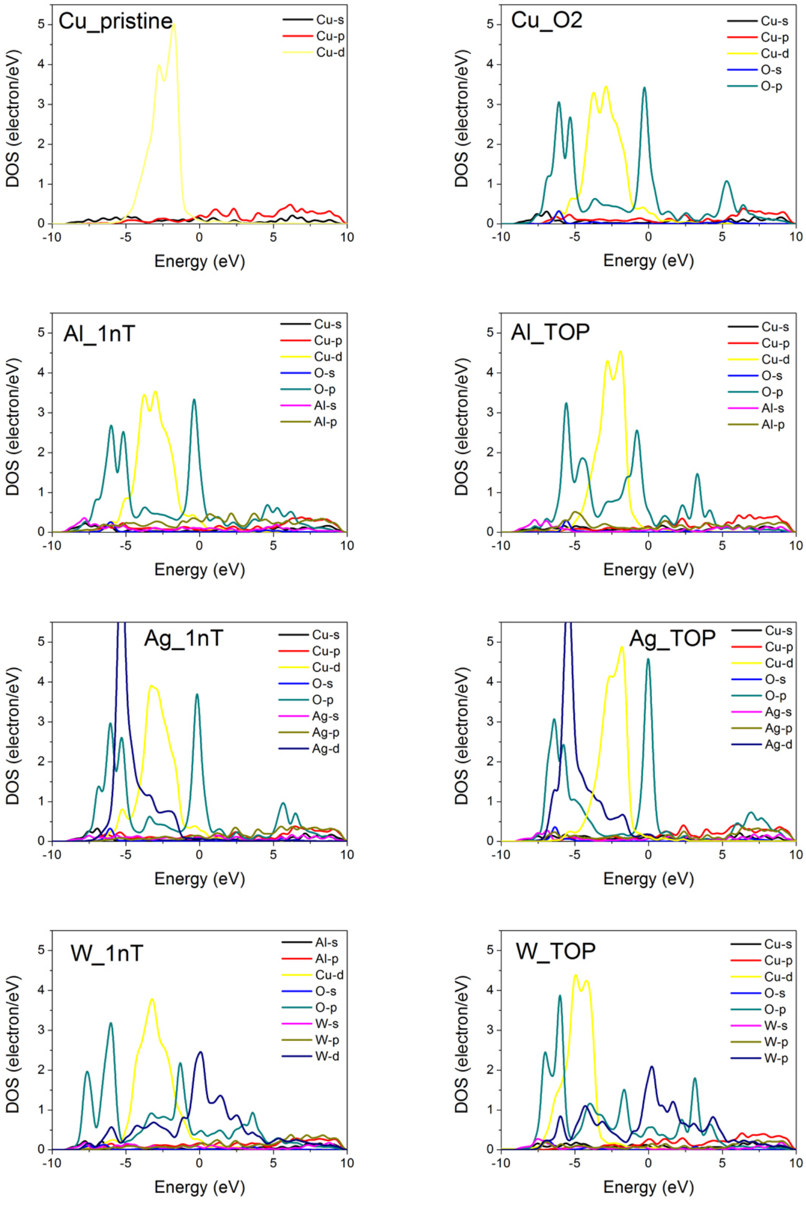


Figure 4. The DOS of O_2 adsorbed the pristine/doped Cu surfaces.

energy level and improves the bonding between the inner atoms in the Cu surface, and finally shows the effect on the value of the binding energy. However, O atoms and doping atoms contribute significantly to the DOS, especially the O-*p* orbital electrons and the *d* orbital electrons of doping atoms. Due to the different electronegativity of three metals Al, Ag, W, the hybridization rules of the electron orbitals on the three doped surfaces are different. The Al-*p* orbital peaks and O-*p* orbital peaks have overlap in a wide energy range, but there are nearly not hybridization peaks between Cu-*d* and Al-*p* orbits. The hybridization of the peaks of the Ag-*d* orbit and O-*p* orbit is affected by the O adsorbed sites and appears to overlap at high and low levels, respectively. But Ag-*d* orbit has the highest peak at low energy level of all the three doping atoms. The W-*d* orbital and O-*p* orbital have a broad peak hybridization only at high energy levels, but the number of electrons of these overlapping peaks is the smallest of the three doped metals. The analysis of the electronic structure shows that the difference in energy calculated in Table 1 is not only influenced by the orbital hybridization between the adsorbate and the surface atoms, but also related to the electronegativity and the orbital energy level of the doping atoms. In one sense, our results provide fundamental insights into O_2 impossible dissociative adsorption on these M-doped Cu surfaces.

3.3. O_2 dissociation on pristine/doped Cu (111) surface

In this section, we mainly investigate the O_2 dissociative processes ($O_2 \rightarrow O + O$) on the pristine/doped Cu surface. We computed the initial state (IS) and final state (FS) in order to obtain the potential energy surface (PES). Then we obtained the intermediate states using a linear interpolation. At last, we used the same convergence criteria of force and energy as the whole simulation process. The energy barrier (E_B) and reaction energy (E_R) and structure parameters of O_2 are listed in Figure 5 and Table 2.

It is seen that the degree of O_2 dissociation is related to the doping atoms on Cu surfaces. This result is as similar as our previous calculations[11,12] that pointed that the precovered-atoms affect the subsequent H_2O dissociation. The E_B is 0.405 eV on the pristine Cu surface. Except W_TOP surface, the value is lower than the E_B on other M-doped surfaces. It shows that the doping atom can resist the dissociation of O_2. Further studying the data, we found that the E_B on three kinds of Al_Top, Ag_1NN and W_1NN surfaces are 0.505 eV, 0.905 eV and 0.814 eV, respectively, which are much larger than other surface models. This seems to indicate that the adsorbed O_2 in a certain range near the doping atoms has good effect of accelerated dissociation. However, by analyzing the reaction energy, we found that the dissociation reaction of O_2 on the surfaces is not only reflected in the barrier energy, but the reaction energy can be also an important index. The E_R are -5.355 eV, -6.426 eV, -5.771 eV, -6.113 eV, -5.386 eV, -7.191 eV, -5.356 eV for pristine, Al_Top, Al_1NN, Ag_Top, Ag_1NN, W_Top, W_1NN surfaces, respectively. The results show that the O_2 can be dissociated more easily on the M_1NN surfaces than that of M_Top surfaces. We found that the reaction energy of O_2 on the pristine Cu surface is larger than that of all doped surfaces, and the E_R of O_2 at the M_TOP surface is also low. For the previous results, we believe that the doping Ag atoms actually resist the dissociation of O_2. The results of bond length (L_{O-O}) also prove our inference, because the value of L_{O-O} for Ag doped surfaces are smaller than that on the pristine Cu surface. Therefore, Ag atoms have the best resistance effect on the O_2 dissociation comparing with Al and W atoms because of the large barrier energy and reaction energy.

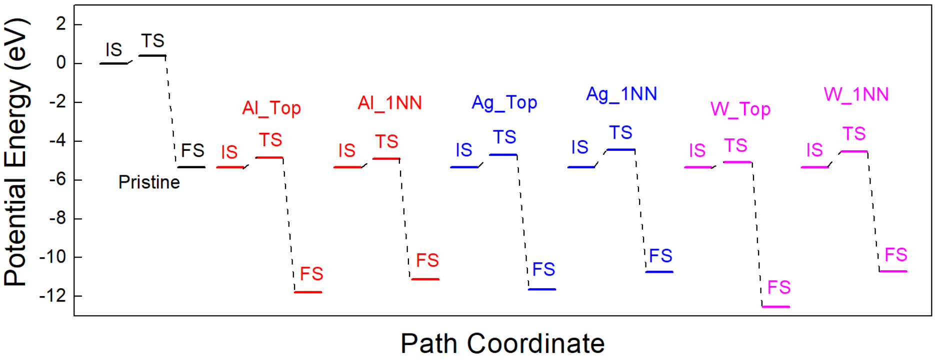


Figure 5. The potential energy surface for O_2 dissociation on the pristine/doped Cu surfaces. The initial state (IS), transition state (TS) and final state (FS) are shown as solid lines.

Table 2. The bond length of O atoms (L_{O-O}), the energy barrier (E_B) and reaction energy (E_R) of O_2 dissociation on the pristine/doped Cu surfaces.

	Pristine	Al_Top	Al_1NN	Ag_Top	Ag_1NN	W_Top	W_1NN
L_{O-O} (Å)	1.409	1.558	1.424	1.334	1.384	1.495	1.478
E_B (eV)	0.405	0.505	0.434	0.635	0.905	0.273	0.814
E_R (eV)	-5.355	-6.426	-5.771	-6.113	-5.386	-7.191	-5.356

4. Conclusions

The O_2 adsorption and dissociation on the pristine/doped Cu (111) surface were studied by density functional theory. The Al, Ag and W atoms were doped on the surface to study the interaction between O_2 and Al. All the doped atoms could be stably combined with Cu atoms, while being slightly embedded in the surface to a certain depth. The E_b of pristine Al surface is lower than that of Al-doped and W-doped surfaces, so the binding energy data confirms that the Al and W atoms would strengthen the bonding effect between the atoms on the Cu (111) slab except Ag doping atom. The O atom prefers to adsorb on the top of the doping atom rather than on the top site of Cu atom. However, Ag atom reduces the surface activity of Cu and inhibit the reaction between Cu surface and oxygen molecules. Due to the different electronegativity of three metals Al, Ag, W, the hybridization rules of DOS for O_2 adsorbed pristine/doped Cu surfaces are different. After O adsorption, an interaction occurs between O-Cu, and some electrons are transferred from Cu atom to O atom, but the doping atom can resist the dissociation of O_2. Moreover, we computed the initial state and final state in order to obtain the PES. The result shows that the dissociation reaction of O_2 on the surfaces not only reflected in the barrier energy, but the reaction energy can be also an important index. Ag atoms have the best resistance effect on the O_2 dissociation comparing with Al and W atoms because of the large barrier energy and reaction energy.

5. Acknowledgements

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