Interactions of $C_5F_{10}O$ Molecule With Cu (1 1 0) and (1 0 0) Surfaces Based on Density Functional Theory

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ABSTRACT This paper based on density functional theory (DFT) investigate the interaction of C5-PFK molecule with Cu (110) and (100) surfaces, in order to analyze the chemical compatibility of Cu metal in the environment of $C_5F_{10}O$ (C5-PFK) insulation gas. The frontier molecular orbital theory implies that the $C = O$ group in the C5-PFK molecule can interact strongly with the Cu surfaces. The results show that both Cu (110) and (100) surfaces have strong interactions with the C5-PFK molecule, showing chemisorption of the molecule, with E_{ad} of -1.17 and -1.03 eV, respectively. Meanwhile, the C5-PFK molecule performs strong electron-accepting behavior in the interactions, which captures 0.262 and 0.204 e from the Cu (110) and (100) surface, respectively. Even though, the geometric and electronic properties of Cu surface are not largely impacted, as supported by the basically unchanged morphologies and DOS curves of Cu surfaces before and after gas adsorption. These findings manifest the favorable stability and compatibility of Cu metal in the C5-PFK environment. Our work uncovers the safe operation of C5-PFK immersed insulation devices with Cu-based generatrix and shell in a long running, which is of great significance to guarantee the safe operation of the power system.

INDEX TERMS C5-PFK, Cu metal, compatibility, DFT method.

I. INTRODUCTION

Sulfur hexafluoride (SF_6) has been applied as an insulation medium in the electrical engineering for a long time due to its extraordinary insulating and arc-extinguishing performances [1]–[3]. However, SF_6 is quite a strong greenhouse gas with the Global Warming Potential (GWP) value up to 23500 and has an atmospheric lifetime of 3200 years [4]. In the meanwhile, SF_6 in a long running equipment will decompose in the presence of trace water and oxygen into many toxic chemicals [5]–[7], weakening its insulation behavior, threating the safe operation of the power system, and making it more difficult to recycle the pure SF_6 from the high-voltage devices. Therefore, some authorities have issued related policies to restrict the use of SF_6 in the electrical equipment, aiming at proceeding the green development of the power industry [8]. Also, scholars in this fields emphasize on exploring novel and environmental-friendly insulation

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candidate for application in the medium-voltage and high-voltage devices to replace SF_6.

With the developing progress of exploring novel SF_6 alternative gases, the C5 perfluorinated ketone (C5-PKF, $C_5F_{10}O$) has been studied as a promising candidate in recent years [9]. As reported, the insulation performance of C5-PFK is twice stronger than that of pure SF_6, with GWP value of only 1 [10]. And the gas toxicity of C5-PFK within an internal arc is close to air, indicating its non-hazardous property and good security for the maintenance personnel compared with SF_6 [11]. Therefore, C5-PFK has strong potential for use in middle-voltage gas insulated switchgear or some switch cabinet employing C5-PFK as the insulating medium in 2015 and initiate a long-term field experience program in Netherlands [12].

On the other hand, the carbonyl group ($C = O$) in the C5-PFK molecule has been predicted with strong chemical reactivity, which may interact with the metal-based generatrix or the shell of the high-voltage devices [13]. Thus, the compatibility between C5-PFK and some frequently used metals

in the electrical equipment is significant to verify the possible application of C5-PFK as the insulation medium and the safe operation of the power system in a long running. For this end, Li *et al.* theoretical studied the interaction between the C5-PFK molecule and the Cu (111) surface to illustrate its compatibility with Cu metal [14]. However, the Cu (110) and (100) surfaces are also quite active ones with strong chemical reactivity upon the surroundings [15], which should also be characterized as representative interfaces simulating their interactions with C5-PFK molecule to fully understand the compatibility between them. To this end, we investigate the interaction between C5-PFK molecule and Cu (110) and (100) surfaces using density functional theory (DFT) method in this paper. At the same time, the frontier molecular orbital theory is carried to illustrate the possible interaction group in the C5-PFK molecule [16]. Based on the relaxed structure of C5-PFK molecule and Cu surfaces, the possible adsorption configurations are established and optimized. Subsequently, the adsorption parameters and electronic behaviors are fully analyzed to understand the compatibility between C5-PFK and Cu metal. Also, our calculations can provide guidance for a prediction of the lifetime of the electrical equipment using C5-PFK gas.

II. COMPUTATIONAL DETAILS

The whole calculations in this paper were obtained within the DMol^3 package of the Materials Studio, which adopts the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) exchange correlation functional [17]. The Semi-core Pseudopots is chosen as the core treatment, and the DFT-D2 method proposed by Grimme was employed to better address the Van der Waals force and Long-range interactions in gas adsorption [18]. Double numerical plus polarization (DNP) was selected as the atomic orbital basis set, and DFT semi-core pseudopotential (DSSP) method was employed to dissolve the relativistic effect of the Cu atoms [19]. The Brillouin zone sampling was calculated using a Monkhorst-Pack grid with k-point mesh of $6 \times 6 \times 1$ for both geometric optimizations and electronic calculations [20]. The displacement, energy tolerance accuracy and maximum force were defined as 5×10^{-3} Å, 10^{-5} Ha and 2×10^{-3} Ha/Å, respectively [21]. For the static electronic structure calculations, the self-consistent loop energy of 10^{-6} Ha and global orbital cut-off radius of 5.0 Å were set respectively to ensure the high accuracy of the total energy [22].

The Cu (110) and (100) surfaces were modeled by a five-layered 3×4 supercell including 84 Cu atoms and a four-layered 4×4 supercell including 82 Cu atoms, respectively, with a vacuum layer of 20 Å to prevent the interaction between adjacent units [23]. The calculated constant lattice of bulk Cu was obtained as 3.62 Å, in agreement with the previous theoretical [24] and experimental [25] results. The adsorption energy (E_{ad}) is defined to evaluate the binding force between the C5-PFK molecule and Cu surfaces, calculated as: $E_{ad} = E_{Cu-C5} - E_{Cu} - E_{C5}$, wherein E_{Cu-C5},

E_{Cu} and E_{C5} signify the energy of C5-PFK/Cu system, related Cu surfaces and isolated C5-PFK molecule, respectively. Besides, the Hirshfeld method was considered to analyze the charge-transfer (Q_T) in gas adsorption, based on which the negative values indicated the electron-accepting behavior of the analytes.
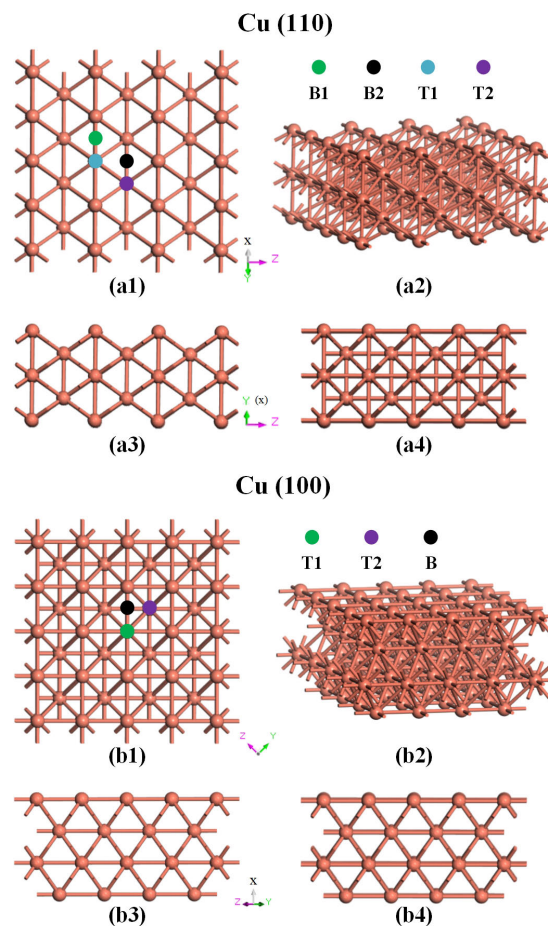

FIGURE 1. Optimized structures of Cu (110) surface (a1)-(a4) and Cu (100) surface (b1)-(b4) with possible adsorption sites.

III. RESULTS AND DISCUSSION

A. ANALYSIS OF Cu SURFACES AND C5-PFK MOLECULE

The optimized Cu (110) and (100) surfaces are exhibited in Figure 1. The Cu-Cu bond lengths are measured as 2.56 Å, consistent with the previous report [24]. For Cu (110) surface, there are four possible adsorption sites, traced as B1 (bridge site of the upper Cu atoms), B2 (bridge site of the lower Cu atoms), T1 (top site of the one upper Cu atom) and T2 (top site of one lower Cu atom); while for Cu (100) surface, there are three possible site for gas adsorption, traced as T1 (top site of one upper Cu atom), T2 (top site of one lower Cu atom) and B site (bridge site of upper Cu atoms). These adsorption sites are also noted in Figure 1 for better observation. We only analyze the properties of the most adsorption configuration (MSC)

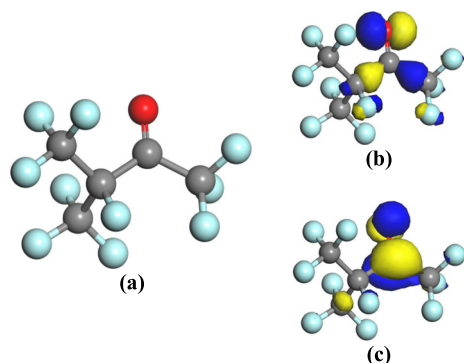for C5-PFK adsorption on Cu (110) and (100) surfaces in the following parts.

FIGURE 2. Geometry (a) and HOMO (b) & LUMO (c) of C5-PFK molecule.

Figure 2 depicts the optimized C5-PFK molecule and relevant frontier molecular orbitals (FMO), including the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). In the C5-PFK molecule, the C-C bond and C-F bond are measured in average as 1.57 and 1.35 Å, respectively, while the $C = O$ bond is measured as 1.20 Å. Based on Hirshfeld analysis, the O atom is negatively charged by 0.147 e, and the bonded C atom is positively charged by 0.122 e which is larger than that C atom in the C-F group (0.053 e) but is smaller than those C atoms in the CF_3 groups (0.233 e); on the other hand, all the F atoms are negative charged by about 0.073 e. These findings are consistent with [26] published elsewhere. From the distributions of FMO, one can see that HOMO and LUMO are dominantly localized on the $C = O$ bond. Since such two orbitals are the most active for interactions with the impurities in the surroundings, it could be assumed that $C = O$ group has suitable reactivity to interact with the Cu surfaces in this study [27]. Although there also exist somewhat HOMO and LUMO distributions on the CF and CF_3 groups, they are quite inert compared with the $C = O$ group. Thus, we will not highlight their interaction with the Cu surface in the following sections.

B. ADSORPTION OF C5-PFK ON Cu (110) SURFACE

For C5-PFK adsorption onto the Cu (110) surface, the $C = O$ group is approaching to the labelled possible adsorption sites of the Cu (110) surface for interactions and to identify the MSC. Figure 3(a1)-(a4) present the considered possible sites for adsorption of C5-PFK molecule, and after geometric optimization Figure 3(b)-(c) present the MSC in different views with corresponding charge deformation density (CDD) in Figure 3(d) to illustrate the charge-transfer behavior during gas adsorption. From Figure 3, one can find that, the MSC for C5-PFK molecule on the Cu (110) surface is through the B1 site, wherein the E_{ad} is calculated as -1.17 eV determining the chemisorption of this system [28] and indicating the strong interaction between $C = O$ group and Cu (110) surface. Also, the E_{ad} here is larger than that of 0.84 eV for
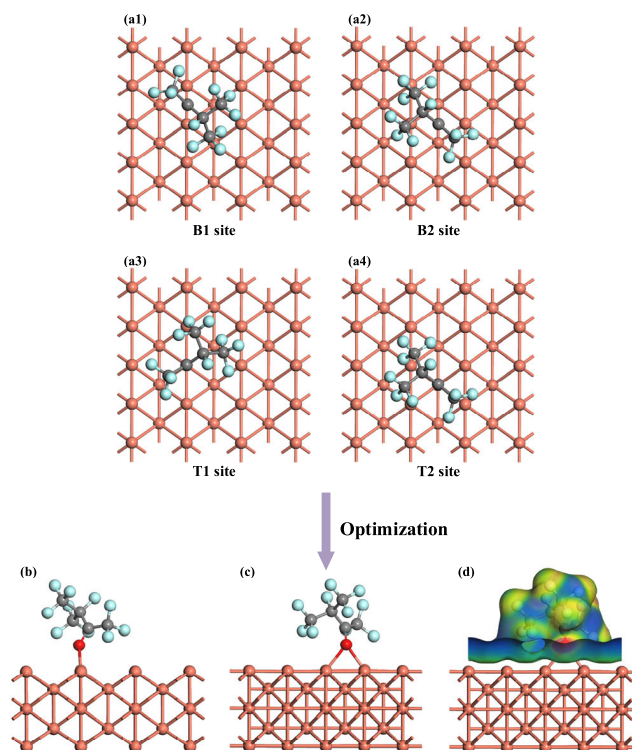

FIGURE 3. Possible adsorption structures (a1)-(a4) and MSC (b) as front view and (c) as side view with CDD (d) for C5-PFK adsorption onto Cu (110) surface (B1 site). In CDD, the red areas are electron accumulation and the blue areas are electron depletion, with the isosurface set as 0.03 e/Å³.

C5-PFK adsorption onto the Cu (111) surface [14], indicating the better performance of Cu (110) surface upon C5-PFK adsorption and the stronger interaction between Cu atoms and $C = O$ group in this system. After adsorption, the O atom of the $C = O$ group is trapped by two Cu atoms of the first Cu lattice layer, with the newly-formed Cu-O bonds measured to be 2.09 and 2.19 Å, respectively. It is worth noting the Cu-O bond lengths here are longer than that of 1.86 Å in bulk CuO and Cu_2O structures [29], indicating the relatively weaker binding force of Cu-O bonds in this work in compared with that in the copper oxides. Besides, the $C = O$ bond is elongated to 1.29 Å compared with that of 1.20 Å in the gas phase of C5-PFK molecule, indicating its geometric activation in the surface interaction. Apart from these local geometry changes, the geometries of Cu (110) and C5-PFK molecule suffer little deformation in adsorption, wherein the C-C and C-F bonds in C5-PFK molecule and Cu-Cu bonds in Cu (110) surface elongate within 0.04 Å. In other words, Cu (110) has good geometric stability upon C5-PFK adsorption. Moreover, it is interesting to add when putting the C5-PFK molecule on the B2 and T1 sites of the Cu (110) surface, it experiences remarkable displacements and also anchors on the B1 site after optimization, with close amount of E_{ad} obtained. On the other hand, when putting the C5-PFK molecule on the T2 site of the Cu (110) surface, the $C = O$ has quite weak interaction with the Cu surface, in which the nearest Cu-O distance is

measured as 2.57 Å with the E_{ad} obtained as -0.45 eV, which indicates the physisorption of Cu (110) surface upon C5-PFK molecule at this site. All these findings confirm the preferred configuration through B1 site.

Based on the Hirshfeld analysis, the C atoms in the C5-PFK molecule are all positively charged whereas the O and F atoms are all negatively charged after adsorption; and from the molecular point of view, the C5-PFK molecule is negatively charged by 0.262 e after adsorption, implying its electron-accepting behavior when interacting with the Cu (110) surface. From the CDD, the electron accumulation is mainly localized on the O atom of the C = O group, followed by the F atoms, while the electron depletion is localized on the C atoms, which manifests the electron-accepting behavior of C5-PFK molecule, consistent with the Hirshfeld analysis. Moreover, the work function (WF) of Cu (110) is increased by 0.25 eV from that of 4.27 eV in its pure phase, suggesting that the adsorption of C5-PFK molecule could impede the electron-dislodging behavior of the Cu metal. Therefore, we assume that the charge-transfer behavior from the Cu (110) surface to the C5-PFK molecule might be weakened as the number of adsorbed C5-PFK molecule increases [30]. Besides, we perform the adsorption of two C5-PFK molecules on the Cu (110) surface, which shows that the charge-transfer of 0.258 and 0.196 e from the Cu (110) surface to two C5-PFK molecules, which to some extent verify our hypothesis. Also, this result expounds the good compatibility between Cu metal and C5-PFK in a long running.

The density of state (DOS) analysis is conducted to elaborate the electronic behavior of Cu (110) surface upon adsorption of C5-PFK molecule, as displayed in Figure 4. From Figure 4(a) where the total DOS is shown, one can see that the DOS curves of Cu (110) with C5-PFK molecule adsorbed is basically overlapped with those of the pure counterpart around the Fermi level. This finding implies that the electronic property of Cu (110) is basically unchanged after adsorption of C5-PFK molecule. Although there are somewhat deformations at level below -5 eV, we assume that the states in the deep valence band cannot exert large impact on the electronic behavior of the whole system. Thus, it could be determined that C5-PFK adsorption has quite small effect on the electronic behavior of Cu (110) surface. In Figure 4(b), it is found that the Cu $3d$ orbital is somewhat hybrid with that of O $2p$ orbital at around -4.8, -3.8, -1.5 and 0.2 eV, which manifests the formation of newly Cu-O bond during gas adsorption. And through the orbital hybridization between Cu and O atoms, the charge-transfer between the Cu (110) surface and C5-PFK molecule is identified. However, the orbital interaction around the Fermi level is not strong enough to realize the sufficient deformations for the electronic behavior of the whole system, thus leading to the quite feeble change in the total DOS of Cu (111)/C5-PFK system [31].

In short, the Cu (110) surface behaves chemisorption upon C5-PFK molecule with strong binding force with the C = O group, deforming the C = O bond to some extents.
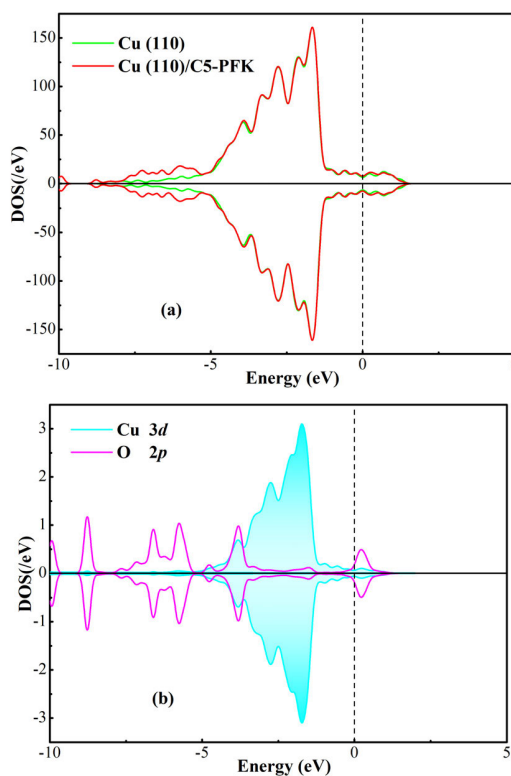

FIGURE 4. Total DOS (a) and atomic DOS (b) of C5-PFK adsorption on Cu (110) surface. The dash line is Fermi level.

However, such adsorption has not transformed the geometric and electronic properties of the Cu (110) largely, as supported by the basically unchanged geometry and DOS of Cu (110) with C5-PFK molecule adsorbed.
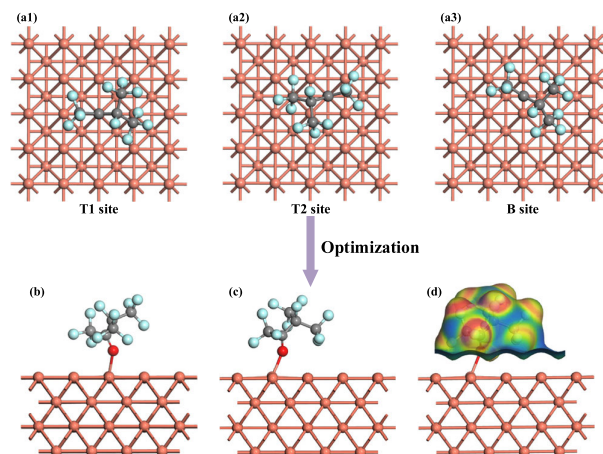

FIGURE 5. Possible adsorption structures (a1)-(a4) and MSC (b) as front view and (c) as side view with CDD (d) for C5-PFK adsorption onto Cu (100) surface (B site). In CDD, the red areas are electron accumulation and the blue areas are electron depletion, with the isosurface set as 0.03 e/Å³.

C. ADSORPTION OF C5-PFK ON Cu (100) SURFACE

When it comes to interaction of C5-PFK molecule with the Cu (100) surface, three possible sites could be traced, as exhibited in Figure 5(a1)-(a3); while after fully optimization, the MSC as depicted in Figure 5(b)-(c) expounds that

the C5-PFK molecule prefers to be adsorbed on the Cu (100) surface through the B site. One can find that the O atom in the C = O group is captured by one Cu atom standing on the right-top of the Cu-Cu bond. Also, on the B site, only one Cu atom is bonded with the O atom forming a Cu-O bond measured as 2.05 Å; while the other Cu atom has the atomic distance of 2.75 Å with the O atom suggesting their weak binding force. Since the C5-PFK molecule prefers to be trapped on the Cu (110) and (100) surfaces through the Cu-Cu bridge site, we can presume from this aspect that the binding force between Cu (100) surface and C5-PFK molecule is weaker than that between Cu (110) surface and C5-PFK molecule. Apart from that, the bond elongation of the C = O group on the Cu (100) surface by 0.05 Å is not as obvious as that on the Cu (110) surface by 0.09 Å, which could also identify the weaker interaction in the Cu (100)/C5-PFK system. On the other hand, the similarity for C5-PFK molecule adsorption on the Cu (110) and (100) surfaces is that the Cu surfaces undergo little geometric deformation after C5-PFK adsorption, and the morphology of C5-PFK itself suffers small deformation as well. These findings imply the desirable structural stability of Cu (100) surface upon interaction with C5-PFK molecule.

According to the definition of E_{ad}, it is calculated as -1.03 eV, which again verifies the weaker performance of Cu (100) surface in comparison with Cu (110) surface upon C5-PFK adsorption. Therefore, the adsorption performance of Cu surfaces to C5-PFK molecule is in order as (110) > (100) > (111), which verifies the desirable behavior of Cu (110) and (100) surface upon C5-PFK adsorption. At the same time, chemisorption could be identified as well in this system give the large value of $E_{ad.}$ [32]. From the Hirshfeld analysis, we find that there are 0.204 e transferring from the Cu (100) surface to the C5-PFK molecule, confirming the electron-accepting behavior of C5-PFK when interacting with the Cu metal. Similarly, the charge-transfer here is also smaller than that in the Cu (110)/C5-PFK system. From the CDD in Figure 5(d), the electron accumulation is largely localized on the O atom of the C = O group, and the F atoms are also surrounded by the electron accumulation to a large extent, whereas the electron depletion is mainly localized on the C atoms. These phenomena are consistent with the Hirshfeld analysis which indicates that the O atom is negatively charged by 0.191 e, all the F atoms are negatively charged ranging at 0.071~0.094 e, while all the C atoms are positively charged at 0.037~0.233 e. Compared the WF of the pure Cu (100) surface (4.51 eV) with that with C5-PFK molecule adsorbed (4.65 eV), our results expound that the contact barrier of the Cu (100) surface will be enhanced with the increasing number of the adsorbed C5-PFK molecule. Accordingly, it can deteriorate the electron-overflow behavior of Cu (100) surface to the vacuum level in the C5-PFK environment [33]. That is, the Cu (100) will gradually become chemical inert and interact weaker and weaker with the C5-PFK molecules, which ensures the chemical compatibility of Cu metal in the C5-PFK insulation environment.

It is worth noting that the calculated WF of Cu (110) and (100) surfaces are close to those in [24], in which the WF are obtained as 4.18 eV for the Cu (110) surface and 4.39 eV for the Cu (100) surface respectively, confirming the good accuracy of our calculations. Moreover, the growing WF in the Cu (110) and (100) surfaces after adsorption of C5-PFK molecule support the decreased electron mobility of Cu metal in the surrounding of C5-PFK in a long running. This is beneficial for using C5-PFK as an insulation media in a Cu-based generatrix or device [34]. Although C = O group remains good reactivity with the Cu (100) surface, it is not comparable with that on the Cu (110) surface. While there has little deformation on the electronic behavior of the Cu (110) surface with C5-PFK molecule adsorbed, it is necessary to investigate the electronic behavior of the Cu (100) surface upon adsorption of C5-PFK molecule.
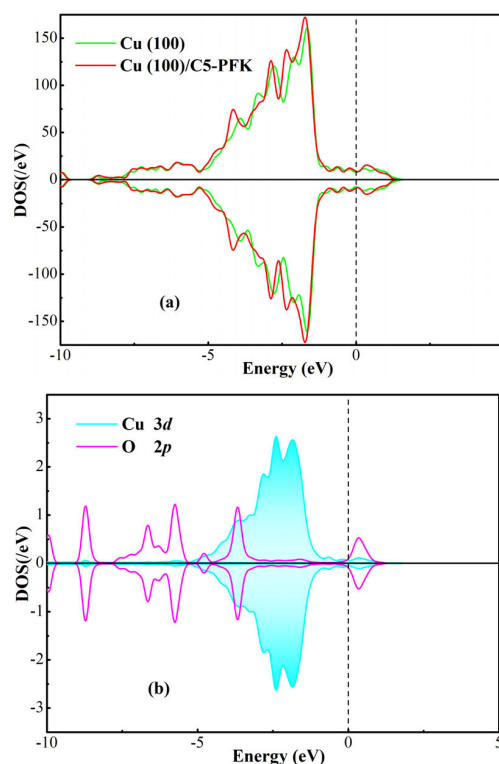

FIGURE 6. Total DOS (a) and atomic DOS (b) of C5-PFK adsorption on Cu (100) surface. The dash line is Fermi level.

Figure 6 portrays the DOS distributions of the Cu (100)/C5-PFK system. From the total DOS in Figure 6(a), one can observe that there has little difference between the DOS states of the pure Cu (100) surface and that of the C5-PFK molecule adsorbed system, especially at the places around the Fermi level where the DOS peaks of such two systems are basically overlapped. In other words, the electronic property of Cu (100) surface will not largely affected by C5-PFK adsorption, indicating the good stability in physicochemical properties of Cu (100) in interacting with C5-PFK molecule. Regarding the atomic DOS in Figure 6(b), the Cu 3d orbital is mainly hybrid with O 2p orbital at about -4.8, -3.6 and 0.3 eV. These orbital hybridizations not only

account for the formation of the new Cu-O bond, but also support the charge-transfer during orbital interaction [35]. However, there has little orbital hybridization around the Fermi level, suggesting that the contributions from the impurity states to the whole system is not strong enough. This may be cause resulting in the basically unchanged DOS states of Cu (100)/C5-PFK system compared with that of the pure Cu (100) surface around the Fermi level [36].

In the Cu (100)/C5-PFK system, chemisorption could be identified as well given the large value of E_{ad}. However, the geometric and electronic property of Cu (100) surface is not afflicted with significant deformation after adsorption of C5-PFK molecule, suggesting its good compatibility in the surrounding of C5-PFK. Thereby, it is predictable that in a long running, the chemical reactivity of Cu (100) will gradually decrease and its inert behavior would play the dominate role in interacting with the C5-PFK molecule.

From the above analysis, one can infer that both Cu (110) and (100) surfaces behave desirable adsorption performance upon C5-PFK molecule. Nevertheless, the physicochemical properties of the Cu surfaces are not largely impacted, which manifests the favorable stability and compatibility in the C5-PFK environment. Combined with the study by Li *et al.* [14], it could be concluded that Cu metal could stably exist in the insulation device using C5-PFK as the insulation medium. In summary, this work sheds light on the fundamental insight into the compatibility of Cu metal in the C5-PFK environment, and puts forward that the C5-PFK immersed insulation devices can work safely in a long running with Cu-prepared generatrix or the shell of the devices, which is advantageous for the safe operation of the power system.

IV. CONCLUSION

In this work, we using density function theory (DFT) method investigate the interaction between C5-PFK molecule and Cu (110) & (100) surface in order to analyze the compatibility and stability of Cu metal in the environment of such insulation gas. We first based on frontier molecular orbital theory illuminate the distribution of HOMO and LUMO of the C5-PFK molecule and point out the strong chemical reactivity of C = O group. Then we highlight the adsorption of C5-PFK molecule through the C = O group onto the Cu (110) and (100) surfaces. The E_{ad} and Q_T are obtained as -1.17 eV and -0.262 e for the Cu (110)/C5-PFK system, whereas are obtained as -1.03 eV and -0.204 e for the Cu (100)/C5-PFK system. These adsorption parameters indicate that both Cu (110) and (100) surfaces behave chemisorption with strong electron-releasing property upon adsorption of C5-PFK molecule. And the adsorption performance of Cu surfaces to C5-PFK molecule is in order as (110) > (100) > (111). On the other hand, the geometric and electronic properties of Cu surface experience little deformation upon C5-PFK adsorption. These findings show the favorable stability and compatibility of Cu metal in the environment of C5-PFK insulation gas, as supported by the basically unchanged morphologies and overlapped DOS curves of Cu

surfaces after gas adsorption. Our work would be meaningful to set forth the fundamental information of using Cu-based generatrix and shell for the C5-PFK immersed insulation devices in the power system, which can guarantee their safe operation in the long running.

V. ACKNOWLEDGMENT

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