Adsorption Behavior of $\gamma$-$\text{Al}_2\text{O}_3$ Toward Heptafluoroisobutyronitrile and Its Decompositions: Theoretical and Experimental Insights

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ABSTRACT Heptafluoroisobutyronitrile ($\text{C}_3\text{F}_7\text{CN}$) has received extensive attention for replacing $\text{SF}_6$ in high voltage electrical equipment. It is necessary to assess the suitability of traditional common adsorbent activated alumina ($\gamma$-$\text{Al}_2\text{O}_3$) used in $\text{C}_3\text{F}_7\text{CN}$ based equipment as adsorbent. In this paper, $\text{C}_4\text{F}_7\text{N}/\text{N}_2$ hybrid gas discharge test was carried out on the gas insulation performance test platform, and the decomposition products mainly included $\text{CF}_4$, $\text{C}_2\text{F}_6$, $\text{C}_3\text{F}_8$, $\text{C}_4\text{F}_7\text{CN}$, $\text{C}_2\text{F}_4$, $\text{C}_3\text{F}_6$ and $\text{C}_2\text{F}_5\text{CN}$. Secondly, gas samples were collected at different periods, and the gas before and after being adsorbed by $\gamma$-$\text{Al}_2\text{O}_3$ was analyzed and compared by GC-MS. Finally, based on the density functional theory, the adsorption of gas molecular on the surface of $\gamma$-$\text{Al}_2\text{O}_3$ was studied. The adsorption effect of $\gamma$-$\text{Al}_2\text{O}_3$ to $\text{C}_3\text{F}_7\text{CN}$, $\text{C}_2\text{F}_5\text{CN}$ and $\text{CF}_3\text{CN}$ is very strong, so it is difficult to be used as adsorbing material for $\text{C}_3\text{F}_7\text{CN}$ type gas insulated equipment. However, due to the low cost of $\gamma$-$\text{Al}_2\text{O}_3$, it can be used in waste gas treatment for new environment-friendly insulating gas.

INDEX TERMS $\gamma$-$\text{Al}_2\text{O}_3$, $\text{C}_3\text{F}_7\text{CN}$, $\text{SF}_6$ alternative gas, adsorption, density functional theory.

I. INTRODUCTION
High voltage electrical equipment is widely distributed in power systems around the world. Among them, $\text{SF}_6$ electrical equipment is more and more widely used due to its excellent insulation, arc extinguishing performance and easy maintenance. However, $\text{SF}_6$ gas is recognized as a kind of greenhouse gas with great harm to the atmospheric environment [1]. The Kyoto Protocol clearly listed $\text{SF}_6$ as one of six restricted greenhouse gases in 1997. In North America and Europe, policies and regulations restricting the use and emission of $\text{SF}_6$ have been introduced. China has announced that it will reduce the $\text{SF}_6$ emissions per unit GDP to 55% ~ 60% of the 2005 level by 2019 [2]. It is not difficult to find that the climate deterioration caused by $\text{SF}_6$ has become one of the important roots of the contradiction between power development and environmental protection, and the new environmental-friendly gas insulating high voltage electrical equipment has been trial-operated in many regions around the world [3]. At present, the international investment in alternative gas research is increasing. Alstom and ABB and other electrical equipment manufacturers have successively developed environmental-friendly insulating gas mixtures code-named G3 and Airplus. Their core formulas are $\text{C}_3\text{F}_7\text{CN}$ and $\text{C}_5\text{F}_{10}\text{O}$ of extremely low greenhouse effect and toxicity, respectively. These two types of electronegative gases have received extensive attention due to their superior insulation performance over $\text{SF}_6$ [4], but they must be mixed with buffer gas due to the high liquefaction temperature. $\text{C}_3\text{F}_7\text{CN}$ ($2,3,3,3$-tetrafluoro-2-trifluoromethylpropionitrile) has a relatively low liquefaction temperature and excellent dielectric strength (about 2.74 times that of $\text{SF}_6$ and much higher than that of $\text{C}_5\text{F}_{10}\text{O}$ [5]. When mixed with low boiling point buffer gas (CO$_2$ or N$_2$), the gas mixtures have the potential to reach or approach the same level of $\text{SF}_6$ insulation at the same pressure. The $\text{C}_3\text{F}_7\text{CN}$ gas has performed well in terms of insulation, environmental protection and safety, and has become the most popular potential $\text{SF}_6$ replacement gas.
Relevant institutes and enterprises have conducted research on the development and related technologies of C3F7CN environmentally friendly gas insulation equipment.

In 2015, Kieffel et al. tested the C3F7CN-CO2 gas mixtures in 145kV AC GIS equipment and found that the C3F7CN content of 18%-20% can reach the same insulation strength as pure SF6 [5]. This research center also conducts 100 consecutive breaking performance tests on 4% C3F7CN-96% CO2 gas mixtures, and found that its arcing time is 12ms on average, which is lower than pure SF6 (15ms) and has better arc extinguishing performance [6]. Owens et al. compared the tolerance characteristics of C3F7CN mixed with N2 and dry air respectively at different pressures and C3F7CN contents under 2.5mm plate-plate electrode [7]. Preve et al. conducted a breakdown test after mixing C3F7CN with dry air and found that the insulation withstand voltage is better than SF6 under the impact voltage [8]. Beroual et al. found that the synergistic effect of 3.7% C3F7CN-96.3% CO2 was the strongest by breakdown test under power frequency and impulse voltage [9]. Wang et al. carried out the calculations on the arc extinguishing performance of C3F7CN and its gas mixtures, and confirmed that its decomposition products will reduce the arc extinguishing ability [10]. Zhang et al. combined simulation and experimental research on the decomposition products of C3F7CN and its gas mixtures under discharge, and found that there are toxic gases in the products. These toxic products will cause pollution and damage to the environment in which humans depend, and will also adversely affect the normal operation of electrical equipment and people’s health [11].

In the new environmental-friendly gas insulating electrical equipment, the arc generated by the discharge of the fault or the switch such as the circuit breaker may cause the gas to decompose. How to avoid the accumulation of toxic products becomes a key technical problem that must be solved before the equipment is promoted and applied. SF6 gas also produces many toxic products under high temperature and discharge, so electrical equipment manufacturers generally use adsorbents to adsorb the reaction products and water present in SF6 electrical equipment. Activated alumina (γ-Al2O3) is a porous structure with large surface area, high mechanical strength, good physicochemical stability, high temperature resistance, corrosion resistance and so on becoming the main component of the adsorbent in high voltage electrical equipment [12]. In practical applications, the Al2O3 is required to have high selectivity and high surface activity with effective catalytic action [13], [14]. The adsorbent is widely used in gas insulating equipment to separate the gas mixtures and selectively adsorb the discharge decomposition components, thereby ensuring that the insulating gas is safe, reliable and harmless. What is the adsorption and selectivity of γ-Al2O3 for the environmental-friendly insulating gas C3F7CN and its discharge decomposition products? Can it be used directly in new environmental-friendly gas insulating electrical equipment? It is necessary to carry out experimental research and mechanism analysis.

In this study, the gas discharge as well as the gas adsorption experiments were carried out combined with theoretical density functional theory study. The adsorption effect of γ-Al2O3 on C3F7CN gas and its discharge decomposition products, first of all adsorption decomposition test on C3F7CN gas was carried out, and after discharge to obtain a mixed gas as a test gas for the adsorbent test. In combination C3F7CN is generally used with CO2 or N2 as an environmentally friendly insulating gas. [5], [7]. Under high energy discharge conditions, C3F7CN decomposes and may chemically react with free radicals generated by CO2 and its cracking. The adsorption effect of γ-Al2O3 on C3F7CN gas and its decomposition products was studied. Therefore, N2 gas with less influence on C3F7CN decomposition products was selected as the buffer gas after discharge. Based on considerations of liquefaction temperature, the C3F7CN is generally below 8% in commercial environmentally friendly insulated electrical equipment [6]. The C3F7CN content in the mixed gas tested in this paper is 5%. The test used C3F7CN gas from the NovecTM 4710 model product produced by 3M Company, which is consistent with the application gas of environmental protection gas insulation equipment market. The purity of N2 for mixing is 99.999%.

The C3F7CN/N2 mixed gas was subjected to a power frequency breakdown test using a gas insulation characteristic test platform and the discharge decomposition components were analyzed. The breakdown voltage value in the test is passed through the capacitive voltage divider to transfer the voltage between the electrodes to the readable range of the voltmeter to obtain the test data. The wiring of the test circuit is shown in Figure 1.

The discharge gas chamber was filled with a C3F7CN/N2 mixed gas having a gas pressure of 0.15 MPa and a mixing ratio of 5%. The processing frequency voltage is applied until the ball-ball electrode gap breaks down, causing a severe high-energy discharge. Repeat the above test process 30 times, each time the breakdown test interval is 5 min, provide sufficient time self-recovery and internal gas circulation for the decomposition of local insulating gas caused by severe discharge, and prevent the drop of gas insulation strength in the local area between electrodes due to breakdown affects the test of gas characteristics. In order to prevent the component test from being misaligned due to the operation error,
FIGURE 1. Structure of test platform.

FIGURE 2. Testing device of adsorbing material.

The gas sample after the discharge test was collected for testing and analysis. The gas collected twice was mixed to be the test raw gas of \( \gamma \)-Al\(_2\)O\(_3\) adsorbent and the sealed test chamber is shown in Figure 2 (the internal volume of the chamber was 3 L). The commercial \( \gamma \)-Al\(_2\)O\(_3\) adsorbent has 300 m\(^2\)/g specific surface area. The bulk density is 0.70 g/cm\(^2\) and the compressive strength for every granule is 100 N. The wear rate is less than 0.60. In order to fully prove the adsorption effect of the adsorbent on various gases in a short time, this experiment added 3 g of dry new \( \gamma \)-Al\(_2\)O\(_3\) adsorbent to the cavity and then quickly sealed and vacuumed it. The mixed gas containing the discharge decomposition product obtained after the breakdown test was charged into the can body. In order to simulate the real atmospheric pressure environment inside the tank of the gas-insulated electrical equipment, when the barometer shows that the internal absolute air pressure reaches 0.3 MPa (the gauge pressure is 0.2 MPa), the gas is stopped and the gas circuit is closed. At this time, the C\(_3\)F\(_7\)CN in the mixed gas is about Accounting for 0.015 MPa. The apparatus was placed in a dark room which was dry and kept at a temperature of 20-25\(^\circ\)C for 240 hours. The gas in the tank was again detected by a gas chromatography mass spectrometer to obtain changes in the gases in the mixed gas before and after the adsorption.

B. THEORETICAL SECTION

The adsorption of C\(_3\)F\(_7\)CN and its decomposition products on \( \gamma \)-Al\(_2\)O\(_3\) was all carried out in Dmol\(^3\) [17], [18]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof function (PBE) was adopted [19]. The double numerical plus polarization (DNP) basis set and the DFT semi-core pseudopotential (DSSP) was selected. The DFT-D method was chosen for long range vdW force [20]. The cutoff radius for all atom in all structures was 4.5 Å. All the geometric optimizations were set of \( 1 \times 10^{-5} \) Ha energy convergence, 0.002 Ha/Å force convergence, and 0.005 Å displacement convergence. The k-point was \( 4 \times 4 \times 1 \) and the Gaussian smearing was 0.005 Ha [21].

The adsorption energy of one gas molecule on the surface of \( \gamma \)-Al\(_2\)O\(_3\) is:

\[
E_a = E_{\gamma-Al_2O_3/GAS} - (E_{\gamma-Al_2O_3} + E_{GAS}) \tag{1}
\]

where \( E_{\gamma-Al_2O_3/GAS} \), \( E_{\gamma-Al_2O_3} \) and \( E_{GAS} \) are the calculated energy of \( \gamma \)-Al\(_2\)O\(_3\)/gas adsorption structure, clean \( \gamma \)-Al\(_2\)O\(_3\) surface and gas molecule before adsorption. The charge transfer was based on Hirshfeld (HI) method [22].

We also calculated the density of states of adsorption structures.

For the surface of Al\(_2\)O\(_3\), the \( \gamma \)-Al\(_2\)O\(_3\) (110) was defined and applied for gas adsorption in this study, which proved to have high gas adsorption properties to CO\(_2\) or other kinds of gas molecules [23].

III. RESULTS AND DISCUSSION

A. BREAKDOWN VOLTAGE, DECOMPOSITION COMPONENTS ANALYSIS AND ADSORPTION RESULTS

The variation trend of the breakdown voltage amplitude with the number of test operations is shown in Figure 3. The breakdown voltage is small, distributed between 33 ∼ 34 kV, and its insulation performance basically remains the same level after many severe high-energy discharges. After the discharge
occurs, the product is still relatively small relative to the main insulating gas C₃F₇CN/N₂, and the decomposition products are mainly fluorocarbons. Although the insulation performance is lower than that of C₃F₇CN, it is superior to the general gas. Therefore, the overall insulation effect has not changed significantly.

The product types corresponding to the peaks are obtained by searching for the material standard database. The test results are shown in Fig. 4. The preliminary simulation calculations and experimental tests by the research team at home and abroad found that CF₃, C₂F₆, C₃F₇, CF₃CN, C₂F₅CN, C₃F₆, C₄F₈, C₅F₁₀, C₂N₂ and other decomposition products were produced after C₃F₇CN gas discharge [6], [15]. According to the peak intensity data in the chromatogram, it can be found that the C₃F₇CN/N₂ mixed gas has decompositions mainly composed of CF₃, C₂F₆, C₃F₇, CF₃CN, C₂F₄, C₃F₆ and C₂F₅CN. Other decomposition products have poor stability or very low yield, this study does not consider them temporarily. This is consistent with the description of the main discharge decomposition products produced by conventional discharge faults in [16]–[18], confirming the reliability of the experiment. Among them, C₂F₆ has the highest characteristic peak intensity, indicating that it is the highest among all decomposition products, and it is the most important decomposition product. The contents of CF₃ and CF₃CN are similar, and the contents of C₂F₄, C₃F₆, C₃F₇ and C₂F₅CN are relatively low. In order to verify the non-accidental results of the decomposition, our team repeated the experimental procedure under the same conditions three times, and the chromatogram waveform was basically consistent with Figure 4.

The adsorption test results are shown in Figure 5. By comparison of absorption peaks before and after adsorption in Figure 5, it is found that γ-Al₂O₃ can not only adsorb the main discharge decomposition products of C₃F₇CN, but also adsorb C₃F₇CN itself. The adsorption effect of C₃F₇CN is even stronger than that of other products, C₃F₇CN in the mixed gases are almost fully adsorbed. Because the second most abundant gas C₃F₇CN in the mixed gases is about 0.015 MPa, the absolute pressure is below 0.29 MPa after the adsorption test and before the gasification test (the gage pressure is 0.188 Mpa, and the specific number is shown in Figure 6). According to the experiment results, it is not difficult to find that except for the relatively poor absorption effect of γ-Al₂O₃ to CF₃CN, almost all other decomposition products have good adsorption. In addition, it has strong adsorption properties for the main insulating medium C₃F₇CN. Therefore, it is not suitable for γ-Al₂O₃ to be used as a kind of absorber for C₃F₇CN decomposition products. In order to confirm the reliability of the test results and explore the adsorption principle of γ-Al₂O₃ on C₃F₇CN and its decomposition products, the simulation analysis on the adsorption mechanism by using quantum chemical simulation modeling based on density functional theory was carried out.

**B. ANALYSIS OF ADSORPTION BEHAVIOR OF C₃F₇CN AND ITS DECOMPOSITION PRODUCTS ON THE SURFACE OF γ-Al₂O₃**

We first obtained the geometric structure of C₃F₇CN and its decomposition products in Figure 7. The C₃F₇CN, C₂F₅CN and CF₃CN has a C-N triple bond and the C₂F₄, C₃F₆ has a C-C double bond. The crystal structure of γ-Al₂O₃ was chosen from Digne et al. [16], as seen in Figure 8. The calculated parameters of the crystal were 5.59 Å, 8.41 Å and
8.07 Å with angles of 90°, 90°, and 90.56°. The results are in good agreement of other studies [23], [24]. After obtaining the crystal structure, we chose the surface of γ-Al2O3(110) to adsorb the gas molecules. The surface structure is shown in Fig. 9(a). It can be seen that the surface has several dangling bonds and results in different ligands of atom, including the O(3c), O(2c), Al(4c), Al(3c). Because the surface structure was discussed in detail by other study [23], we will not repeat them. For calculating adsorption structure of one gas molecule adsorbed on the surface, the gas molecule was placed on different adsorption site, such as the top site of O(2c) and Al(3c) with different adsorption direction. We only discussed the adsorption structure with the maximum adsorption energy. To carry out the geometric optimization, three layers in the bottom of the γ-Al2O3(110) was fixed and the atoms could not move when calculation and only the top three layers were experienced fully relaxed. We also calculated the partial density of states (PDOS) of two types of two-fold coordinated oxygen on the surface which proved to be with high activity to adsorbed gas molecule. In Figure 9(c), it can be seen that the states near −18 eV are mainly of 2s orbitals and the states from −9 eV to −1 eV consist of 2p orbitals of oxygen.

We separated the C3F7CN and its decomposition products into three parts, that is, C3F7CN, C2F5CN and CF3CN in one group, C3F6 and C2F4 in another group, C3F8, C2F6 and CF4 in the third group. It should be noted that the group separation was mainly attributed by the different functional groups. The adsorption structure with the maximum adsorption energy for every gas molecule is shown in Figure 10, Figure 11 and Figure 12. Similarity for these three kinds of gas molecule in the first group was that the C-N triple bond experienced dramatic angle change. The original C-N triple bond is about 180° but after adsorption for these three molecules, the sp hybridization of the carbon atom was destroyed and the distance between the C atom and the O1(2c) atom was only from 1.39 Å to 1.41 Å. The adsorption parameters for all gas molecules are shown in Table 1. For C3F7CN, C2F5CN
and CF$_3$CN, the adsorption energy was much larger than that of other gas molecule, from $-3.20$ eV to $-3.23$ eV. We estimated that the relatively larger adsorption energy was attributed by the deformation of C-N triple bond and this process might be an exothermic process. The electron transfer for these three molecules was not very large, from $-0.040$ e to $-0.057$ e. So, the interactions between the C-N triple bond with the surface of $\gamma$-Al$_2$O$_3$ might be very strong and exhibited considerable chemical interactions but the electron transfer was not very obvious. We estimated that there existed new formed covalent bond between the C atom and the O atom but the bonding electron pair was not obviously affiliated with any of these two atoms. To further discuss the chemical interactions between these two atoms, the PDOS was considered in Fig. 13. The overlaps near $-18$ eV were ascribed to the chemical interactions between the C 2s and O 2s orbitals and other overlaps from $-9$ eV to $-1$ eV and $+2$ eV to $+6$ eV were attributed to the chemical interactions between the C 2p and O 2p orbitals. As a result, the chemical interactions between the surface of $\gamma$-Al$_2$O$_3$ and the C-N triple bond was very strong and it was very difficult for the gas molecule desorption from the surface. This phenomenon is according to the experimental results. Thus, the $\gamma$-Al$_2$O$_3$ is very suitable to be adsorbent toward C$_3$F$_7$CN, C$_2$F$_5$CN and CF$_3$CN with strong chemical interactions and difficult desorption process.

For C$_3$H$_6$ and C$_2$H$_4$, the $\pi$ bond from C-C double bond plays an important role. The $\pi$ bond was inclined to be close to the two O(2c) atoms in Fig. 11. However, different from the C-N triple bond, the chemical interactions with the surface of $\gamma$-Al$_2$O$_3$ were quite different for these two kinds of gas molecules. The C$_3$H$_6$ adsorption brought about $-0.94$ eV adsorption energy with relatively larger electron transfer of $+0.210$ e. It can be seen that C$_3$H$_6$ acted as an electron donor. The adsorption distance was about 2.46 Å, much larger than that of the adsorption of C$_3$F$_7$CN, C$_2$F$_5$CN and CF$_3$CN but much smaller than that of C$_2$F$_4$ adsorption. But for C$_2$F$_4$, the interactions with the surface of $\gamma$-Al$_2$O$_3$ was quite smaller. The adsorption energy was only $-0.43$ eV and the electron transfer was only $+0.017$ e. It could be seen that the electron transfer was much smaller.
than that of C$_3$F$_6$ and the adsorption distance was also larger. We also compared the DOS for these two gas adsorptions. For C$_3$F$_6$, state overlaps were mainly near $-9.5$ eV, $-3$ eV and $+2.5$ eV. These overlaps were mainly from the chemical interactions between the C 2p and O 2p orbitals but it was obvious that the degree of overlaps was much weaker than that of the C-N triple bond with the surface. But for C$_2$F$_4$, only very few overlaps could be found near $-8$ eV and $+5$ eV. So, the chemical interactions between C$_2$F$_4$ and the surface of $\gamma$-Al$_2$O$_3$ was weaker than that of the C$_3$F$_6$ adsorption.

For three kinds of perfluorodecalin (C$_3$F$_8$, C$_2$F$_6$ and CF$_4$), the adsorption structure was shown in Figure 12. From the adsorption configurations, the adsorption distance for these three kinds of gas molecule was generally larger than that of the former discussed five molecules. The distance for C$_3$F$_8$ was the shortest and also, the adsorption energy was the largest among these three gases. The adsorption energy was $-0.43$ eV with $+0.101$ e electron transfer from molecule to the surface. For C$_2$F$_6$ and CF$_4$, the adsorption energy was even smaller with smaller electron transfer. So, with the shorten of the carbon chain, the interactions became smaller. We also did not observe obvious state overlaps between the gas molecule and the surface of these three gas adsorptions so we estimated that the chemical interactions were relatively weaker compared to the former discussed five adsorption structures and the vdW force played a leading role. However, because of the high specific surface area of $\gamma$-Al$_2$O$_3$ and the vdW interactions could not be neglected, the adsorption phenomenon of these three kinds of gases still could be observed in the experiment but the effects were generally smaller than other gases.

By comparing the experimental and theoretical result, the adsorption energy highly accords with the height change of the peak of every gas molecule in GCMS in Figure 5. The C$_3$F$_7$CN, C$_3$F$_5$CN and CF$_3$CN adsorptions have the highest adsorption energy, so these gas molecules have strong interactions with Al2O3 and thus, in GCMS, the height of the peaks fallen dramatically for C$_3$F$_7$CN, C$_2$F$_5$CN, CF$_3$CN, C$_3$F$_6$and C$_2$F$_4$. But for CF$_4$, C$_2$F$_6$ and C$_3$F$_8$, the adsorption effect is much lower. For the C$_2$F$_4$ and C$_3$F$_8$, although the adsorption energy is nearly the same, the C$_3$F$_8$ has much larger molecular weight bringing larger vdW force with Al$_2$O$_3$, and thus the chemical interactions is smaller comparing to those of C$_2$N$_4$. In summary, the difference of adsorption energy can explain the different adsorption ability of Al$_2$O$_3$ to different gas molecule in our study to some extent.

We have also calculated the adsorption capacity of $\gamma$-Al$_2$O$_3$ (110) to the insulation medium C$_3$F$_7$N as an example to evaluate the adsorption properties. The calculation was adopted using the Sorption module in Materials Studio. The temperature was set as 298K and the pressure was range from 1bar to 10bar in order to meet with the pressure in GIS. The results are shown in Figure 15. The adsorption capability tends to saturate if the pressure is larger than 200 kPa. As a result, with the increase of the pressure, the final adsorption capability of $\gamma$-Al$_2$O$_3$ to C$_3$F$_7$CN is about $5.03 \times 10^{-6}$ mol/m$^2$.

Although the adsorption properties of $\gamma$-Al$_2$O$_3$ has been studied in this study, there still have several drawbacks of this adsorbent for adsorption of C$_3$F$_7$CN decompositions or other realms. Because the high porosity, large specific surface area and both acidic and basic adsorption sites [23], the properties of selectivity adsorption is poor and because the desorption process happens often higher than 200° C temperature, the working life in engineering proposal is not desired. As a result, new kinds of high-performance adsorbent should be considered in the future.

**IV. CONCLUSION**

This work discussed the adsorption behavior of $\gamma$-Al$_2$O$_3$ to C$_3$F$_7$CN and its decomposition products by experimental and theoretical method. The main conclusions obtained are as follows:

1. After 30 times consecutive breakdown discharges under the quasi-uniform electric field of C$_3$F$_7$CN/N$_2$ mixed gas with a mixing ratio of 5%, the insulation performance remained nearly unchangeable. After discharging process, the decomposition products mainly included CF$_4$, C$_2$F$_6$, C$_3$F$_8$, CF$_3$CN, C$_2$F$_4$, C$_3$F$_6$ and C$_2$F$_5$CN. C$_2$F$_6$ was the main decomposition products. The contents of CF$_4$ and CF$_3$CN were similar and the contents of C$_2$F$_4$, C$_3$F$_6$, C$_3$F$_8$ and C$_2$F$_5$CN were relatively low. Other unstable products and products with very low content were not included in our study.
(2) The experimental results showed that $\gamma$-$\text{Al}_2\text{O}_3$ had strong adsorption on all major decomposition products of C$_3$F$_7$CN and its decomposition products.

(3) Density functional theory study demonstrated that $\gamma$-$\text{Al}_2\text{O}_3$ had much stronger adsorption behavior toward C-N triple bond with larger adsorption and state overlaps. The adsorption of C$_3$F$_6$ and C$_2$F$_4$ which include C-C double bond were relatively weaker and the adsorption of three kinds of perfluorodecalin were ascribed mainly to long range vdW force.

As a result, it is difficult for $\gamma$-$\text{Al}_2\text{O}_3$ to be placed inside the equipment as adsorbent for decomposition products of C$_3$F$_7$CN. However, due to the low cost of $\gamma$-$\text{Al}_2\text{O}_3$, it can be used as an adsorption material for C$_3$F$_7$CN waste gas.

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