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Theoretical Study on the Compatibility Between HFO-1234ze(E) Gas and Ag (1 1 1) Surface

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Abstract

In gas-insulated equipment, the Ag surfaces of silver-plated contacts are directly exposed to the insulating gas. Poor compatibility between the gas and Ag may therefore compromise the insulation performance and operational reliability of the equipment. To investigate the gas–solid compatibility between the environmentally friendly insulating medium HFO-1234ze(E) and Ag components, the interactions between HFO-1234ze(E) and the Ag (1 1 1) surface were examined at the microscopic level using density functional theory (DFT). First, the reactive regions of HFO-1234ze(E) were identified through frontier molecular orbital and electrostatic potential analyses. Subsequently, the adsorption energies, charge transfer, charge density difference distributions, and other microscopic parameters were calculated and compared for HFO-1234ze(E) and SF₆ adsorbed on pristine Ag (1 1 1). Molecular dynamics simulations and activation barrier calculations for representative bond dissociation pathways were then performed to evaluate the dynamic and kinetic stability of the adsorption system. Finally, the effects of a Ag vacancy defect on the adsorption characteristics were investigated. The results show that the interaction of HFO-1234ze(E) with pristine Ag (1 1 1) is substantially weaker than that of SF₆ with the same surface. HFO-1234ze(E) remains structurally stable throughout the molecular dynamics simulations. The vacancy defect only enhances the adsorption strength and interfacial electronic interactions. These findings indicate that HFO-1234ze(E) exhibits favorable initial adsorption compatibility with Ag (1 1 1) under the computational conditions considered.

Keywords: HFO-1234ze(E) gas; Ag (1 1 1); density functional theory; compatibility



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1. Introduction

Sulfur hexafluoride (SF₆) is widely used in the power industry owing to its outstanding dielectric strength and arc-quenching capability [1]. Nevertheless, it has an extremely high global warming potential (GWP), approximately 23,900 times that of CO₂, with an atmospheric lifetime of up to 3200 years, making it one of the most potent greenhouse gases [2–4]. The Paris Agreement, which entered into force in 2016, established a global framework for reducing greenhouse gas emissions. This framework has intensified efforts to reduce reliance on gases with high GWP values, such as SF₆. Consequently, there is an urgent need to identify an environmentally friendly gaseous insulating medium as an alternative to SF₆ [5–9].

Trans-1,3,3,3-tetrafluoropropene (HFO-1234ze(E)) is considered a promising alternative to SF₆ for electrical equipment operating at medium and low voltages [10–12]. It has a GWP of 6, an atmospheric lifetime of less than 10 days, zero ozone depletion potential (ODP), and low toxicity.

In recent years, considerable research has focused on HFO-1234ze(E). Chachereau et al. [13] measured the swarm parameters of pure HFO-1234ze(E) and its gas mixtures using pulsed Townsend experiments together with models of attachment kinetics. They analyzed electron attachment behavior and derived the corresponding ionization and attachment coefficients. Their results showed that the effective ionization coefficient decreased with increasing HFO-1234ze(E) concentration and pressure. The dielectric strength of pure HFO-1234ze(E) at 130 kPa approached that of SF₆. Tian et al. [14] investigated the power-frequency breakdown characteristics of HFO-1234ze(E)/CO₂ mixtures through experiments and simulations. Their results showed that the insulation performance improved with increasing gas pressure and HFO-1234ze(E) mixing ratio. They suggested that a mixing ratio of 20–25% at 0.3 MPa was suitable for equipment operating at medium and low voltage levels. The mixture also exhibited favorable self-recovery performance.

Nevertheless, the engineering application of gases proposed as alternatives to SF₆ requires not only favorable insulation performance but also adequate compatibility between the gaseous media and solid materials [15]. Density functional theory calculations are currently widely used to predict the structural, electronic, mechanical, and thermodynamic properties of various materials, thereby providing theoretical guidance for materials design [16,17]. In studies of environmentally friendly insulating gases, the authors of [18] used density functional theory (DFT) and variational transition-state theory (VTST) to investigate the decomposition and recombination pathways of HFO-1336mzz(E) under discharge conditions over a temperature range of 300–1500 K. The results supported its potential application as an alternative to SF₆. However, the study considered only gas-phase decomposition under thermal and electrical stresses and did not account for the influence of solid interfaces. The adsorption characteristics of C₅F₁₀O on Cu (1 1 0) were calculated in [19]. The adsorption of C₅F₁₀O was weaker than that of SF₆, supporting its potential as an SF₆ alternative. However, only adsorption energy and charge transfer were calculated, which were insufficient for a comprehensive assessment of gas–solid compatibility. Using first-principles calculations, the study in [20] investigated the gas–solid compatibility of the environmentally friendly insulating medium CF₃SO₂F with representative surfaces used in electrical equipment. CF₃SO₂F exhibited high stability and compatibility with the investigated surfaces, and both properties were comparable to those of SF₆. However, the study did not consider unavoidable metallic surface defects, such as vacancies and dislocations, which may influence gas–solid compatibility under practical operating conditions [21].

In gas-insulated equipment, in addition to commonly used conductive materials such as copper and aluminum, silver is widely employed as a coating material for electrical contacts. Because the silver coating is directly exposed to the insulating gas, their gas–solid compatibility can directly affect contact reliability and the long-term operational stability of the equipment [22,23]. Previous experimental studies have investigated the interactions of SF₆ and several organofluorine compounds with silver surfaces. Using a combination of infrared laser photoacoustic spectroscopy and X-ray photoelectron spectroscopy, the submonolayer adsorption of SF₆ on silver films was directly characterized at 90 K [24]. Temperature-programmed experiments combined with quantitative gas-phase analysis further demonstrated that SF₆ can undergo conversion reactions on silver electrodes, with a conversion efficiency approximately 30% higher than that on copper electrodes under the same high-temperature conditions [25]. Moreover, temperature-programmed desorption and photoelectron spectroscopy measurements revealed that the adsorption

of CF_3I on Ag (1 1 1) is strongly dependent on surface coverage and can proceed through both molecular and dissociative adsorption. The dissociation process primarily involves cleavage of the C–I bond, whereas the C–F bonds remain intact [26]. These findings indicate that silver surfaces are not completely inert toward fluorinated gases and that interfacial behavior may be strongly influenced by molecular structure and adsorption conditions. Existing compatibility studies of HFO-1234ze(E), however, have focused mainly on copper and aluminum. Reference [27] experimentally and theoretically investigated the compatibility of HFO-1234ze(E) with these two metals at 100–200 °C. The results showed no appreciable decomposition of HFO-1234ze(E) within this temperature range and good compatibility with aluminum; however, above 150 °C, the gas may chemically interact with copper and cause surface corrosion. Nevertheless, to the best of our knowledge, no direct experimental study has specifically examined the interaction between HFO-1234ze(E) and silver surfaces. The compatibility of HFO-1234ze(E) with Ag surfaces remains to be systematically investigated.

To address this gap, this study uses DFT to calculate the adsorption energy, charge transfer, and charge density difference distributions of HFO-1234ze(E) on pristine Ag (1 1 1). SF_6 is included as a reference gas to compare the interfacial interaction strengths. The interaction mechanisms are analyzed in terms of energy and electronic structure, while molecular dynamics simulations and bond-dissociation barrier calculations are performed to evaluate the dynamic and kinetic stability. Finally, the effects of a surface Ag vacancy on the adsorption characteristics are investigated, and the underlying physical mechanisms are clarified. This study provides theoretical support for evaluating the compatibility between HFO-1234ze(E) and Ag (1 1 1) during initial adsorption.

2. Methods and Structural Models

2.1. Methods

All calculations were performed using the DMol³ module within the density functional theory (DFT) framework. Electron exchange and correlation effects were described using the Perdew–Burke–Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). Weak van der Waals interactions were accounted for using the Grimme DFT-D2 dispersion correction. Convergence tests were performed for the k-point mesh and numerical basis set, as shown in Figure 1. Based on the test results, a $4 \times 4 \times 1$ k-point mesh was used to sample the Brillouin zone. The electronic wave functions were expanded using the double numerical plus polarization (DNP) basis set. Relativistic effects for Ag were treated using the DFT semicore pseudopotential (DSPP), with a global orbital cutoff radius of 4.5 Å. A dipole correction was applied along the surface normal direction (z direction) to reduce spurious interactions arising from slab asymmetry. Numerical atomic-orbital basis sets implemented in DMol³ have been reported to reduce basis set superposition error (BSSE) relative to conventional Gaussian-type basis sets [28]. Therefore, no counterpoise correction for BSSE was applied in this study. The present analysis focused on relative molecule–surface interaction trends at the electronic energy level. Therefore, zero-point energy (ZPE) and finite-temperature corrections were not included. Geometry optimization was considered converged when the energy change, maximum force, and maximum displacement were below 1.0×10^{-5} Ha, 0.002 Ha Å^{−1}, and 0.005 Å, respectively. Molecular dynamics simulations were performed to evaluate the dynamic stability of the gas–surface system. The simulations were conducted in the canonical (NVT) ensemble at 400 K for 10 ps, using a time step of 1 fs. The transition states of the investigated reaction pathways were searched using the complete linear synchronous transit and quadratic synchronous transit method (LST/QST) implemented in DMol³. Vibrational frequency calculations were

subsequently performed for the obtained transition-state structures. Each transition state was characterized by a single imaginary frequency.

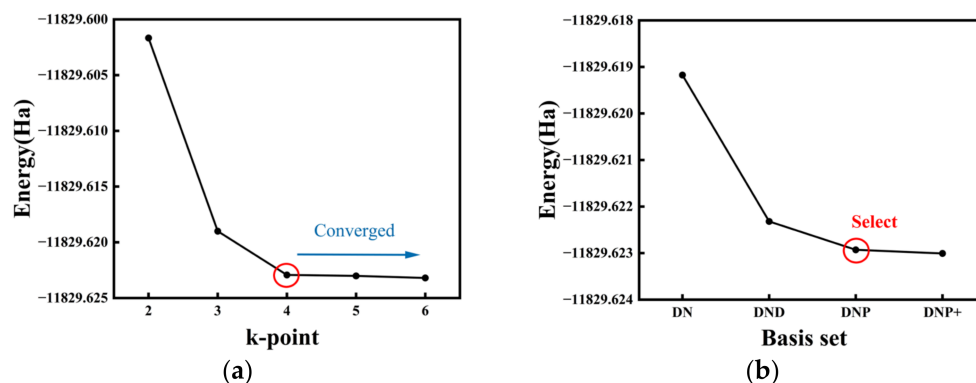


Figure 1. Convergence tests: (a) the k-point mesh and (b) basis set.

2.2. Model Construction

2.2.1. Molecular Configuration and Properties of HFO-1234ze(E)

HFO-1234ze(E) is an insulating gas with a low global warming potential, and its molecules consist of carbon, fluorine, and hydrogen atoms. Under specific test conditions, its dielectric strength can approach that of SF₆ [29]. The optimized molecular structure and corresponding geometric parameters are presented in Figure 2 and Table 1, respectively.

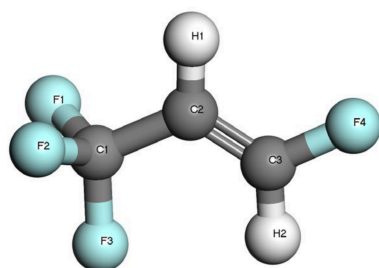


Figure 2. HFO-1234ze(E) molecular structure.

Table 1. HFO-1234ze(E) Structure Parameters.

Bond	Length (Å)	Angle	Value (°)	Angle	Value (°)
C1-C2	1.486	F1-C1-F2	106.335	H1-C2-C3	122.015
C1-F1	1.371	F1-C1-F3	107.203	C2-C3-H2	125.883
C1-F2	1.372	F2-C1-F3	107.126	C2-C3-F4	121.168
C1-F3	1.367	F1-C1-C2	111.290	H2-C3-F4	112.948
C2-H1	1.088	F2-C1-C2	111.331		
C2-C3	1.332	F3-C1-C2	113.191		
C3-H2	1.090	C1-C2-C3	121.518		
C3-F4	1.353	C1-C2-H1	116.464		

Before constructing the adsorption configurations, the reactive regions of HFO-1234ze(E) were examined to guide the selection of candidate initial adsorption orientations. According to frontier molecular orbital theory, the highest occupied molecular orbital (HOMO) indicates regions are more likely to donate electrons. In contrast, the lowest unoccupied molecular orbital (LUMO) indicates regions that are more likely to accept electrons [30]. Molecular electrostatic potential (MEP) analysis identifies regions of relatively negative and positive electrostatic potential, thereby providing insight into possible

electrostatic interactions between the molecule and the surface [31]. Therefore, the HOMO, LUMO, and MEP distributions of HFO-1234ze(E) were calculated, as shown in Figure 3.

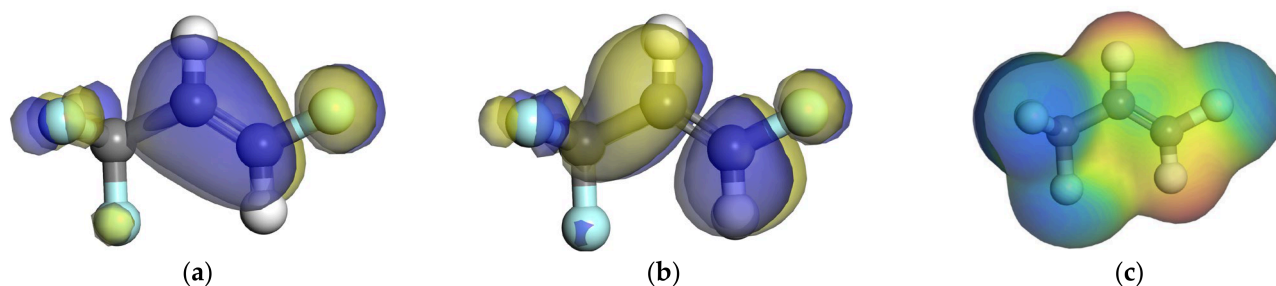


Figure 3. Frontier molecular orbital isosurfaces and molecular electrostatic potential map of HFO-1234ze(E). (a) HOMO, (b) LUMO, and (c) molecular electrostatic potential map.

As shown in Figure 3a,b, the HOMO and LUMO distributions of HFO-1234ze(E) are mainly localized around the C=C bond and the H1, H2, and F4 atoms. This orbital localization suggests that these regions may preferentially participate in electron donation or acceptance during interactions with the Ag surface. Figure 3c shows pronounced regions of negative electrostatic potential around the CF₃ group and the F4 atom, indicating electron-rich regions that may contribute to electrostatic interactions with the metal surface [32]. Based on the combined frontier molecular orbital and MEP analyses, initial adsorption configurations with the C=C bond, H1, H2, F4, and CF₃ group oriented toward the Ag surface were constructed for subsequent adsorption calculations.

2.2.2. Geometric Configuration and Adsorption Sites of Ag (1 1 1)

The bulk Ag unit cell was obtained from the Materials Studio crystal database and fully optimized, as shown in Figure 4. The optimized lattice constant was 4.14 Å. Among the low-index Ag surfaces, Ag (1 1 1) has lower surface energy than Ag (1 0 0) and Ag (1 1 0), indicating its greater thermodynamic stability [33]. Ag (1 1 1) is also a commonly exposed facet of face-centered cubic Ag and therefore provides a representative model for the stable regions of silver-plated contacts. Accordingly, the Ag (1 1 1) surface was selected for the microscopic compatibility analysis. As shown by the convergence tests in Table 2, the calculated surface energy essentially converged when a four-layer slab and a 20 Å vacuum region were used. Therefore, the Ag (1 1 1) surface was modeled using a four-layer 4 × 4 slab with a 20 Å vacuum region.

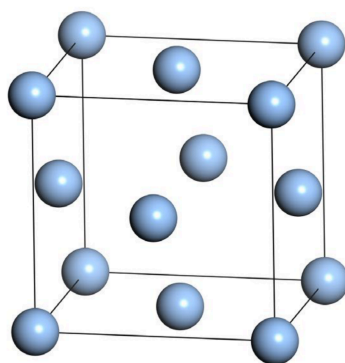
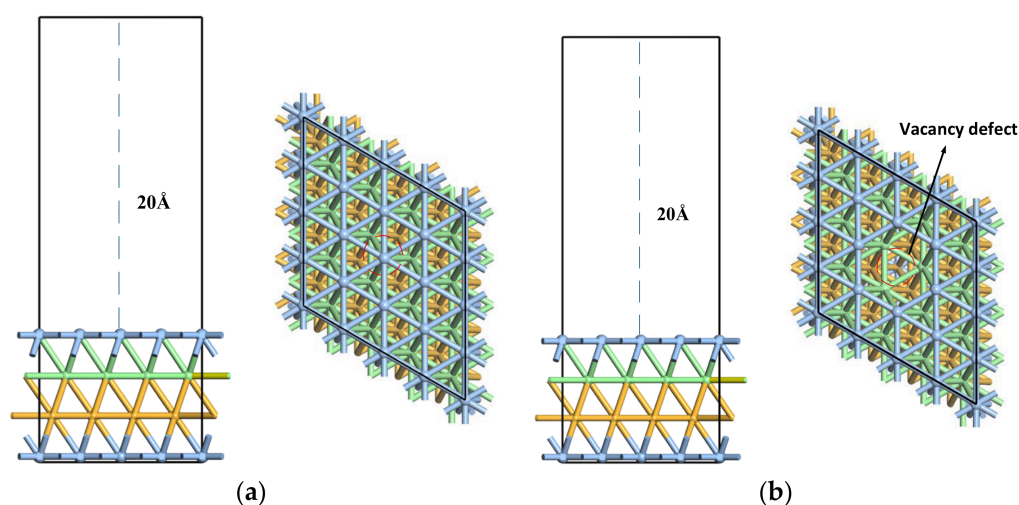


Figure 4. Bulk Ag unit cell.

Table 2. Ag (1 1 1) Surface Model Layer Number and Vacuum Layer Thickness Test.

Vacuum (Å)	Layers	Surface Energy (J/m ²)	Layers	Vacuum (Å)	Surface Energy (J/m ²)
20	2	1.024	4	10	1.032
20	3	1.039	4	15	1.039
20	4	1.048	4	20	1.048
20	5	1.051	4	25	1.050
20	6	1.053	4	30	1.051

A single Ag vacancy was introduced by removing one Ag atom from the topmost layer of the four-layer Ag (1 1 1) slab. During geometry optimization, the bottom two Ag layers were fixed at their bulk-truncated positions, whereas the upper two layers were fully relaxed. The optimized pristine and vacancy-containing Ag (1 1 1) models are shown in Figure 5.

**Figure 5.** Side and top views of the four-layer Ag (1 1 1) slab models with a 20 Å vacuum region: (a) pristine surface and (b) vacancy-containing surface.

Four adsorption sites were considered on the pristine Ag (1 1 1) surface: the top, bridge, hcp hollow, and fcc hollow sites, as illustrated in Figure 6. Five molecular regions, namely the CF₃ group, F4 atom, H1 atom, H2 atom, and C=C bond, were selected to define the initial adsorption orientations. Each molecular region was directed toward each of the four surface sites, yielding 20 initial adsorption configurations. The initial vertical separation between the molecule and the topmost Ag layer was set to 2.5 Å for all configurations. Each configuration was then optimized using the slab constraints described above. The resulting adsorption structures and energies were compared to identify the energetically favorable configurations.

The initial adsorption configurations on pristine Ag (1 1 1) were labeled using the notation X-S, where X identifies the molecular region facing the surface and S identifies the surface adsorption site. The identifiers C, F4, H1, H2, and CF₃ represent the C=C bond, F4 atom, H1 atom, H2 atom, and CF₃ group, respectively. The adsorption sites were labeled Top, Bridge, Fcc, and Hcp. For example, C-Fcc denotes the configuration with the C=C region oriented toward the fcc hollow site, whereas F4-Top denotes the configuration with the F4 atom oriented toward the top site.

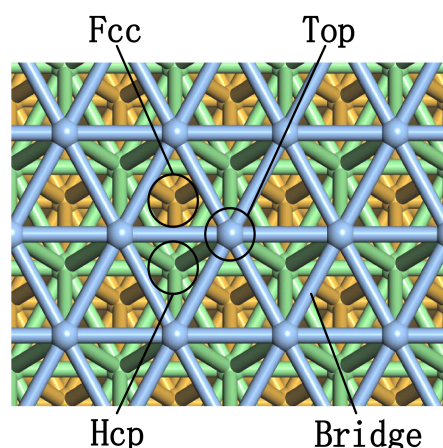


Figure 6. Ag (1 1 1) surface adsorption sites.

For the vacancy-containing Ag (1 1 1) surface, the prefix V was added, giving the notation V-X-S. For example, V-F4-Top denotes the configuration in which the F4 atom faces the top site on the vacancy defective surface. The four SF₆ adsorption configurations were denoted as SF₆-S, where S identifies the adsorption site. For example, SF₆-Top denotes the configuration in which one F atom of SF₆ faces the top site of pristine Ag (1 1 1).

3. Calculation Results and Analysis

Because practical gas–solid compatibility is governed by numerous factors, this study is limited to evaluating the initial adsorption compatibility between HFO-1234ze(E) and Ag (1 1 1). The evaluation considers adsorption energetics, interfacial electronic interactions, and dynamic stability over the simulated timescale.

3.1. Adsorption Energy

To compare the adsorption strengths of HFO-1234ze(E) and SF₆ on pristine Ag (1 1 1), the adsorption energies of all optimized configurations were calculated. The adsorption energy (E_{ad}) was calculated as follows:

$$E_{ad} = E_{gas/metal} - E_{metal} - E_{gas} \quad (1)$$

where $E_{gas/metal}$ is the total energy of the optimized gas–surface system, E_{metal} is the energy of the Ag (1 1 1) surface, and E_{gas} is the energy of the isolated gas molecule. All energies were calculated using the same computational settings. A negative E_{ad} indicates exothermic adsorption, whereas a positive value indicates an endothermic and energetically unfavorable process. For negative values, a larger $|E_{ad}|$ generally indicates a stronger adsorption interaction [34].

The calculated adsorption energies of HFO-1234ze(E) on pristine Ag (1 1 1) are listed in Table 3 and range from −0.316 to −0.719 eV, indicating relatively weak adsorption according to the qualitative criterion introduced above. The optimized adsorption configurations are presented in Figure 7. Among them, the C-Fcc configuration exhibits the most negative adsorption energy of −0.719 eV and is therefore identified as the most energetically favorable configuration. For SF₆, the adsorption energies of the four configurations are listed in Table 4. The SF₆-Top configuration is the most favorable, with an adsorption energy of −2.16 eV. Its magnitude is substantially larger than those calculated for all HFO-1234ze(E) configurations. As shown in Figure 7f, S–F bond cleavage occurred after SF₆ adsorption on the Ag (1 1 1) surface. All six S–F bonds in gas-phase SF₆ had a length of 1.613 Å, whereas two of them were elongated to 2.334 and 2.675 Å after adsorption, indicating that the corresponding bonds had been cleaved. Meanwhile, the distances between the

two dissociated F atoms and the neighboring surface Ag atoms were 2.334 and 2.342 Å, respectively, indicating the formation of distinct Ag–F interactions. Therefore, the configuration shown in Figure 7f was identified as partially dissociative adsorption of SF₆ on Ag (1 1 1). Previous studies reported a high-pressure-limit apparent activation energy of approximately 4.45 eV for the gas-phase unimolecular dissociation of SF₆ via S–F bond cleavage [35]. By comparison, transition-state calculations yielded a barrier of only 0.19 eV for the initial S–F bond cleavage of SF₆ on Ag (1 1 1) [1]. Although these two energy values differ in their definitions and computational conditions, their large contrast qualitatively suggests that the Ag (1 1 1) surface substantially facilitates S–F bond activation and cleavage. Therefore, under identical computational conditions, the adsorption of HFO-1234ze(E) on pristine Ag (1 1 1) is substantially weaker than that of SF₆.

Table 3. Adsorption Energy and Charge Transfer of HFO-1234ze(E) on the Pristine Ag (1 1 1) Surface.

Configuration	E_{ad} (eV)	Mulliken Charge (e)	Hirshfeld Charge (e)
C-Top	−0.680	0.023	−0.043
C-Bridge	−0.505	0.012	−0.052
C-Fcc	−0.719	0.026	−0.042
C-Hcp	−0.619	−0.018	−0.055
F4-Top	−0.509	−0.017	−0.076
F4-Bridge	−0.316	−0.001	−0.008
F4-Fcc	−0.324	0.001	−0.048
F4-Hcp	−0.328	−0.001	−0.039
H1-Top	−0.685	0.024	−0.040
H1-Bridge	−0.544	−0.015	−0.070
H1-Fcc	−0.559	−0.011	−0.080
H1-Hcp	−0.515	−0.011	−0.076
H2-Top	−0.488	−0.010	−0.075
H2-Bridge	−0.510	−0.019	−0.081
H2-Fcc	−0.516	−0.017	−0.084
H2-Hcp	−0.565	−0.016	−0.074
CF ₃ -Top	−0.514	0.012	0.012
CF ₃ -Bridge	−0.439	0.014	0.017
CF ₃ -Fcc	−0.440	0.016	0.019
CF ₃ -Hcp	−0.421	0.010	0.013

Table 4. Adsorption Energy and Charge Transfer of SF₆ on the Pristine Ag (1 1 1) Surface.

Configuration	E_{ad} (eV)	Mulliken Charge (e)	Hirshfeld Charge (e)
SF ₆ -Top	−2.16	−1.031	−0.794
SF ₆ -Bridge	−0.925	−0.212	−0.228
SF ₆ -Fcc	−0.867	−0.231	−0.228
SF ₆ -Hcp	−0.899	−0.240	−0.232

3.2. Charge Transfer and Charge Density Difference

Net charge transfer provides a complementary measure of the electronic interaction between an adsorbate and a surface. Because Mulliken population analysis is sensitive to the basis set, Hirshfeld population analysis was also performed to cross-check the charge transfer trends for all optimized configurations. A positive charge transfer value denotes electron transfer from the gas molecule to the surface, whereas a negative value indicates transfer in the opposite direction [36].

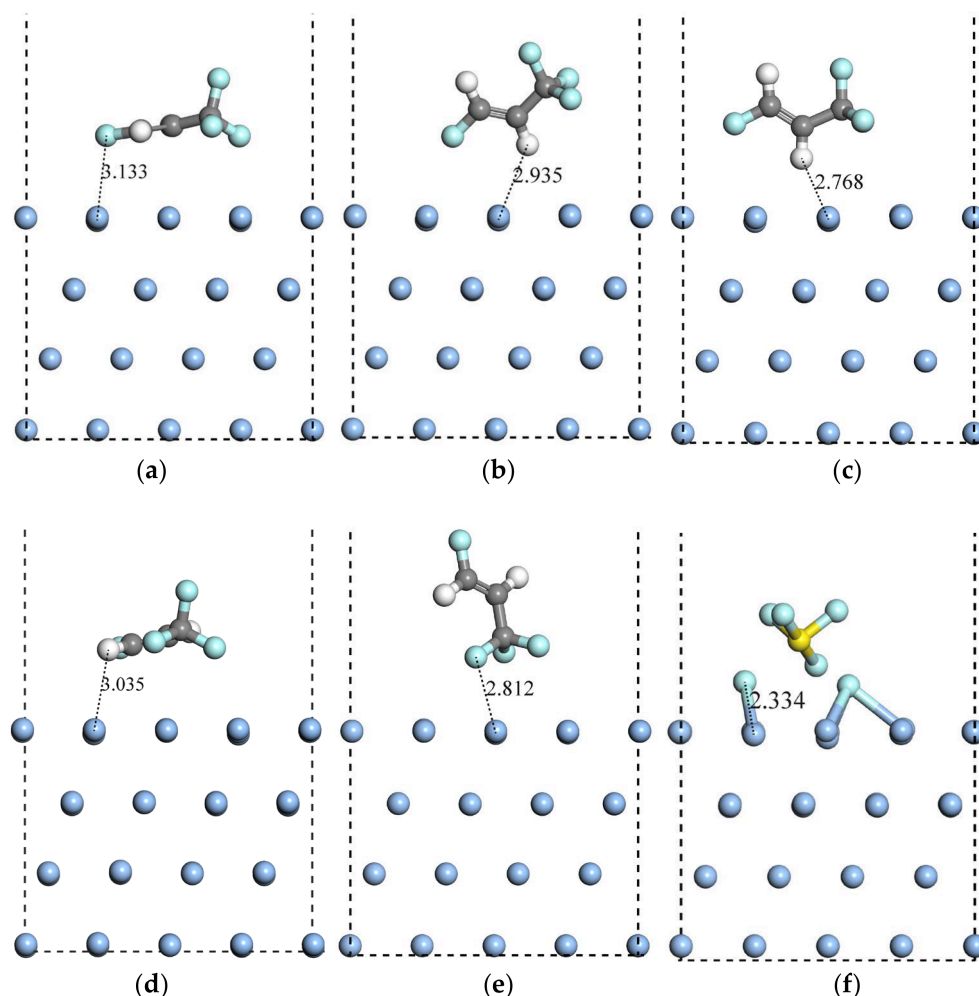


Figure 7. Most energetically favorable configurations on pristine Ag (1 1 1). (a) C-Fcc, (b) F4-Top, (c) H1-Top, (d) H2-Hcp, (e) CF₃-Top, and (f) SF₆-Top.

According to Tables 3 and 4, the absolute Mulliken charge transfer values for HFO-1234ze(E) on pristine Ag (1 1 1) range from 0.001 to 0.026e. The corresponding Hirshfeld values range from 0.008 to 0.084e. These relatively small values, together with the low adsorption energy magnitudes, indicate limited electronic interactions consistent with predominantly physical adsorption. In comparison, the absolute Mulliken and Hirshfeld charge transfer values for the SF₆ systems range from 0.212 to 1.031e and from 0.228 to 0.794e, respectively. Both analyses therefore indicate substantially stronger electronic interactions for SF₆ than for HFO-1234ze(E).

Charge density difference calculations were performed to examine adsorption-induced charge redistribution in the most energetically favorable HFO-1234ze(E) and SF₆ configurations. The corresponding maps for the C-Fcc and SF₆-Top configurations are presented in Figure 8. According to the color convention used in the figure, the yellow and blue regions represent charge depletion and accumulation, respectively. As shown in Figure 8a, no pronounced charge accumulation occurs in the interfacial region between HFO-1234ze(E) and Ag (1 1 1), providing no clear evidence of interfacial chemical bond formation. In contrast, Figure 8b shows substantial charge redistribution between SF₆ and the surface. Charge accumulation is concentrated between the interfacial F and adjacent Ag atoms, indicating pronounced Ag–F electronic coupling and possible chemical bond formation. This observation is consistent with the adsorption energy and charge transfer results. The

stronger redistribution in the SF₆ system may be associated with the strong electronegativity of F and enhanced polarization at the Ag–F interface.

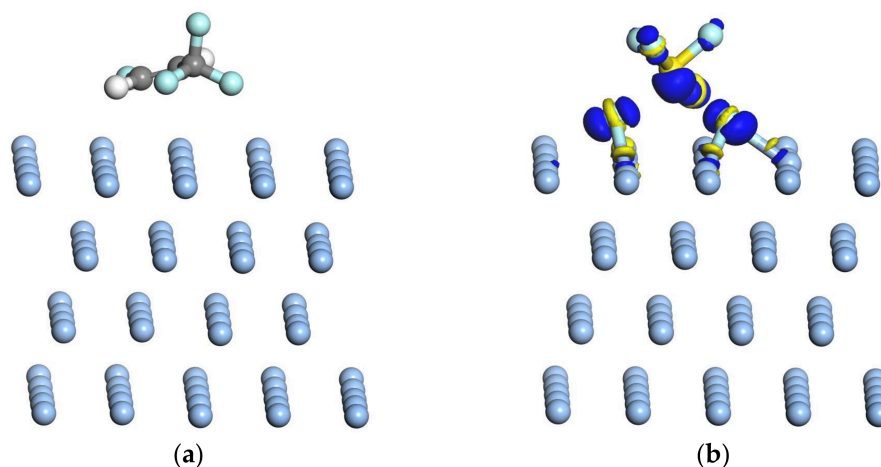


Figure 8. Charge density difference of HFO-1234ze(E) and SF₆ adsorbed on pristine Ag (1 1 1) surface (a) HFO-1234ze(E); (b) SF₆ (the isosurface is 0.05 eÅ^{−3}).

3.3. Work Function

The work function (WF) is the minimum energy required to transfer an electron from the Fermi level to the vacuum level. It therefore characterizes the energy barrier for electron emission [37]. It was calculated as

$$\Phi = E_{\text{vacuum}} - E_{\text{fermi}} \quad (2)$$

where E_{vacuum} and E_{fermi} denote the vacuum-level and Fermi-level energies, respectively. Gas adsorption can modify the surface dipole and electrostatic potential through interfacial charge redistribution. Therefore, the work function change provides a measure of the perturbation of the surface electronic environment induced by adsorption [38].

The calculated work functions and corresponding changes for the most energetically favorable HFO-1234ze(E) and SF₆ adsorption systems are listed in Table 5. The work function of pristine Ag (1 1 1) is 4.194 eV. After HFO-1234ze(E) adsorption, it increases slightly to 4.215 eV, corresponding to a change ($\Delta\Phi$) of 0.021 eV. This small change indicates that HFO-1234ze(E) adsorption only weakly perturbs the surface electronic environment. In contrast, SF₆ adsorption increases the work function to 4.785 eV, giving a substantially larger $\Delta\Phi$ of 0.591 eV. This larger change indicates a stronger surface dipole and more-pronounced interfacial charge redistribution induced by SF₆ adsorption.

Table 5. Work Function Modification of Gas Molecules Adsorbed on the Pristine Ag (1 1 1) Surface.

System	Φ (eV)	$\Delta\Phi$ (eV)
Ag (1 1 1)	4.194	—
C-Fcc	4.215	0.021
SF ₆ -Top	4.785	0.591

The larger work function increase following SF₆ adsorption is consistent with electron redistribution toward the electronegative F atoms at the interface. The resulting interfacial dipole has its negative end oriented toward the adsorbate, raising E_{vacuum} relative to E_{fermi} and thereby increasing Φ . This interpretation is consistent with the charge transfer and charge density difference results.

3.4. Density of States

To examine the changes in the electronic structure of Ag (1 1 1) induced by adsorption, the total density of states (TDOS) and projected density of states (PDOS) were analyzed for the most energetically favorable HFO-1234ze(E) and SF₆ configurations. All energies were referenced to the Fermi level, which was set to 0 eV.

The TDOS curves of pristine Ag (1 1 1) and the two adsorption systems are presented in Figure 9a,b. The corresponding PDOS results for the interfacial atoms are shown in Figure 9c,d. For the C-Fcc configuration, the PDOS was projected onto the C atom closest to the surface and its nearest Ag atom. For the SF₆-Top configuration, it was projected onto the interfacial F atom and its nearest Ag atom. As shown in Figure 9a, HFO-1234ze(E) adsorption increases the TDOS mainly within the energy range from −15 to −7 eV, whereas only minor changes occur at other energies. Figure 9c shows that the additional states in this energy range originate mainly from the C-2s and C-2p orbitals. Limited spectral overlap occurs between the C-2p and Ag-5s states near −5.38 eV and between the C-2p and Ag-4d states near −3.71 eV. These limited overlaps indicate weak interfacial orbital coupling and only a minor perturbation of the electronic states of Ag (1 1 1). For the SF₆ system, the TDOS also changes noticeably within the energy range from −7 to −3 eV, as shown in Figure 9b. The PDOS results in Figure 9d indicate that these changes arise mainly from the F-2p and Ag-4d states. Pronounced spectral overlap between the F-2p and Ag-4d states occurs near −4.73 eV, indicating stronger orbital hybridization and electronic interaction between F and Ag. Together with the adsorption energy, charge transfer, charge density difference, and work function results, these findings support predominantly physical adsorption of HFO-1234ze(E) on pristine Ag (1 1 1). In contrast, SF₆ interacts substantially more strongly with the surface and exhibits more-pronounced chemisorption characteristics under identical computational conditions.

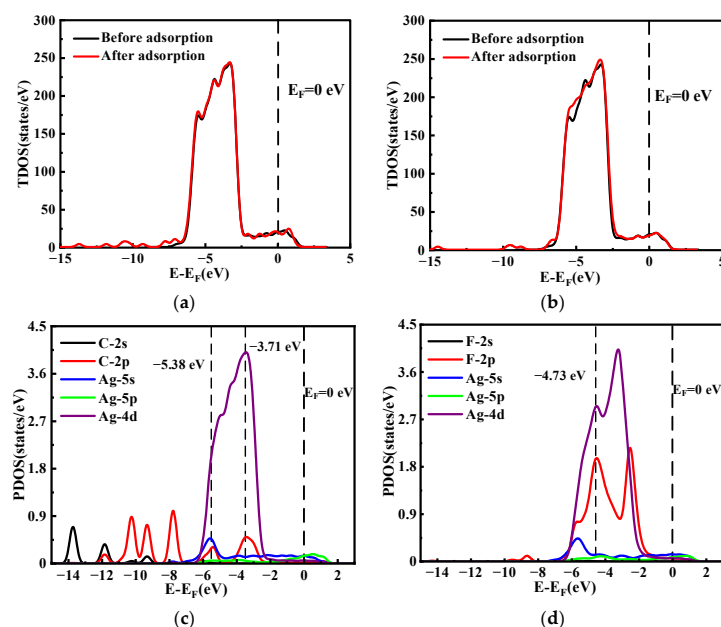


Figure 9. TDOS and PDOS of HFO-1234ze(E) and SF₆ adsorbed on pristine Ag (1 1 1). (a) HFO-1234ze(E) TDOS, (b) SF₆ TDOS, (c) HFO-1234ze(E) PDOS, and (d) SF₆ PDOS.

3.5. Dynamic and Kinetic Stability Analysis

Following the static adsorption analysis, the stability of HFO-1234ze(E) on pristine Ag (1 1 1) was evaluated from both dynamic and kinetic perspectives. First, a molecular dynamics simulation was performed to evaluate the dynamic stability of HFO-1234ze(E) on pristine Ag (1 1 1) over a short timescale. The Electric Power Research Institute recommends

a temperature range of 100–200 °C for material compatibility testing [39]. Accordingly, the simulation temperature was set to 400 K (approximately 127 °C), which lies within the recommended range and represents an elevated compatibility test temperature.

The most energetically favorable configuration of HFO-1234ze(E) on Ag (1 1 1) was used as the initial structure. The temperature and total energy profiles over the 10 ps simulation are presented in Figure 10a,b, respectively. The temperature fluctuates around the target value of 400 K, indicating effective temperature control. Meanwhile, the total energy exhibits bounded fluctuations without abrupt changes, suggesting that no major structural reconstruction or reaction occurs during the simulation. The variations in the bond lengths of HFO-1234ze(E) as a function of time were extracted from the MD trajectory and are presented in Figure 11. The results show that all molecular bond lengths exhibit only limited thermal fluctuations around their equilibrium values, without persistent elongation or abrupt changes indicative of bond cleavage. Meanwhile, the distance between the selected C3 atom and the Ag (1 1 1) surface gradually increases during the simulation, indicating that HFO-1234ze(E) tends to move away from the Ag (1 1 1) surface.

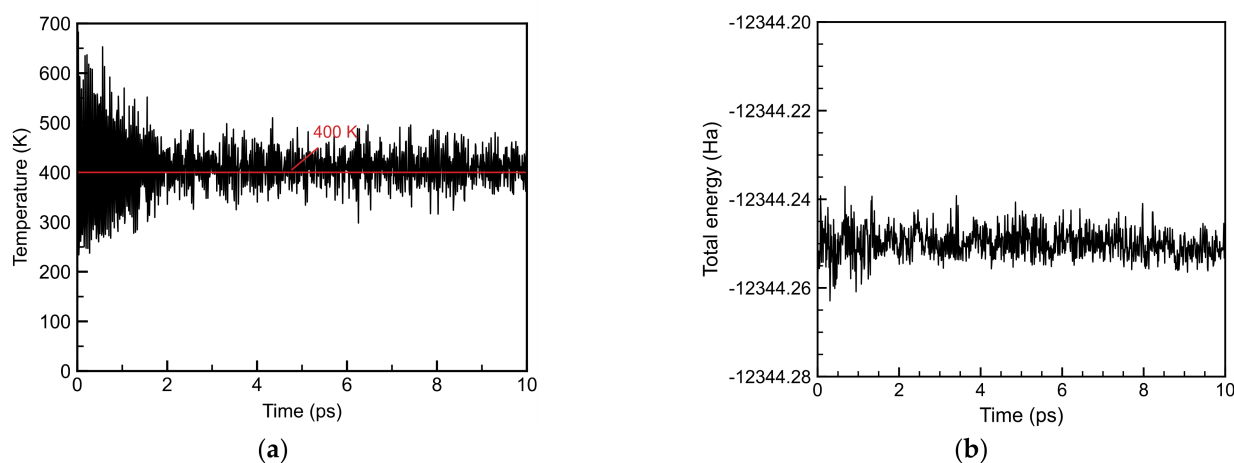


Figure 10. Time evolution of temperature and total energy during the 10 ps molecular dynamics simulation of HFO-1234ze(E) on pristine Ag (1 1 1) at 400 K. (a) temperature; (b) total energy.

Because a 10 ps MD trajectory may be insufficient to sample reactions involving relatively high activation barriers, the absence of bond cleavage during the trajectory alone cannot be interpreted as evidence of general chemical inertness. Therefore, using the most stable C-Fcc adsorption configuration as the initial state, transition-state searches and activation barrier calculations were performed for the cleavage of the C1–F1, C2–H1, C=C, C3–H2, and C3–F4 bonds. As shown in Figure 12, the activation barriers of pathways R1 to R5 are 2.98, 1.75, 1.74, 1.33, and 1.93 eV, respectively. The transition-state and final-state structures of the HFO-1234ze(E) decomposition reactions on the Ag (1 1 1) surface are shown in Figure 13. Even the lowest barrier, corresponding to pathway R4, reaches 1.33 eV, whereas it has been confirmed that the gas–solid system is unlikely to provide energy to cross the energy barrier higher than 0.5 eV [40]. This result explains why no decomposition event was observed during the 10 ps MD trajectory and indicates that the dissociation of HFO-1234ze(E) on Ag (1 1 1) is kinetically hindered under the present simulation conditions.

Taken together, the MD trajectory and reaction barrier calculations indicate that, within the present computational model and simulation timescale, HFO-1234ze(E) retains its molecular integrity during its interaction with the pristine Ag (1 1 1) surface and exhibits both short-term dynamic stability and kinetic stability.

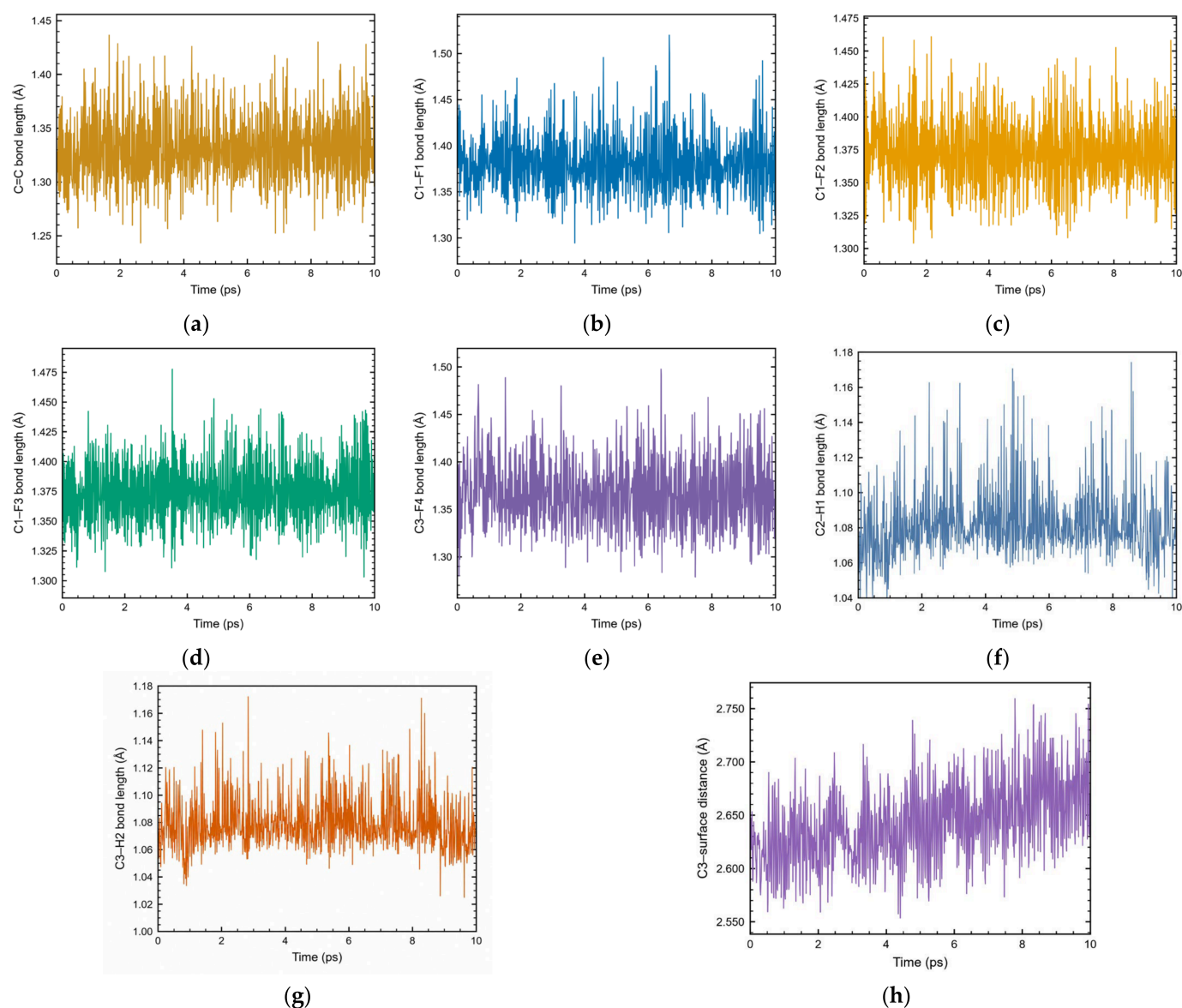


Figure 11. Time evolution of the bond lengths of HFO-1234ze(E) and the distance between the C3 atom and the Ag (1 1 1) surface during the 10 ps MD simulation at 400 K. (a) C=C; (b) C1-F1; (c) C1-F2; (d) C1-F3; (e) C3-F4; (f) C2-H1; (g) C3-H2; (h) C3-surface.

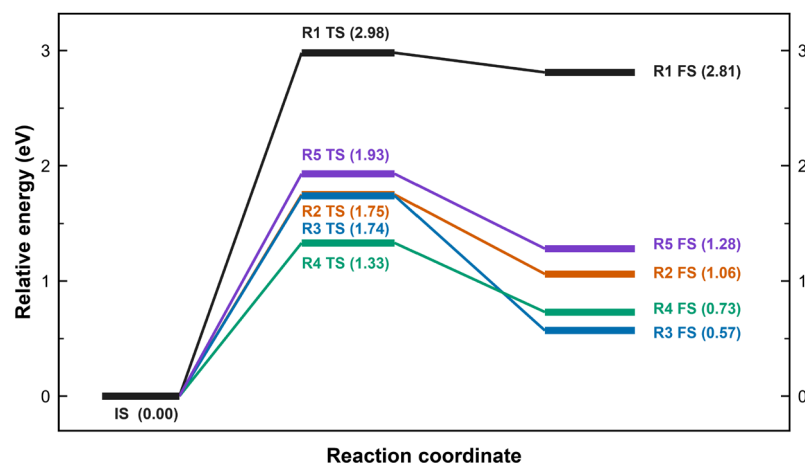


Figure 12. Relative energy profiles of five representative bond dissociation pathways for HFO-1234ze(E) on Ag (1 1 1).

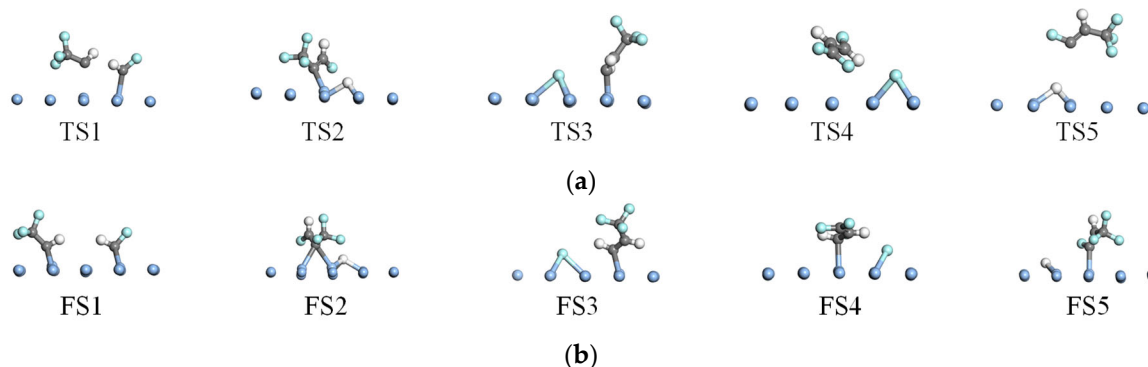


Figure 13. Transition-state and final-state structures of HFO-1234ze(E) decomposition reactions on the Ag (1 1 1) surface. (a) Transition-state; (b) Final-state.

4. Vacancy-Defect Effects on Compatibility

A surface Ag vacancy was introduced to represent an undercoordinated site on silver-plated contacts, thereby modifying the local coordination and electronic structure. Its effects on HFO-1234ze(E) adsorption were evaluated through adsorption energy, charge transfer, and density of state calculations using the same molecular orientations and adsorption sites as those on pristine Ag (1 1 1).

4.1. Adsorption Characteristics Analysis

As shown in Table 6, the adsorption energies of HFO-1234ze(E) on vacancy-containing Ag (1 1 1) range from -0.603 to -0.964 eV. The optimized adsorption configurations are presented in Figure 14. For the corresponding configurations, the adsorption energy magnitudes are higher than those on pristine Ag (1 1 1), indicating that the surface vacancy enhances the adsorption interaction. The V-C-Fcc configuration exhibits the most negative adsorption energy of -0.964 eV and is therefore the most energetically favorable configuration on vacancy-containing Ag (1 1 1).

Table 6. Adsorption Energy and Charge Transfer of HFO-1234ze(E) on Vacancy-Containing Ag (1 1 1).

Configuration	E_{ad} (eV)	Mulliken Charge (e)	Hirshfeld Charge (e)
V-C-Top	-0.755	0.026	-0.056
V-C-Bridge	-0.834	0.039	-0.057
V-C-Fcc	-0.964	0.033	-0.066
V-C-Hcp	-0.948	-0.042	-0.062
V-F4-Top	-0.890	0.027	-0.088
V-F4-Bridge	-0.603	-0.010	-0.017
V-F4-Fcc	-0.610	0.008	-0.053
V-F4-Hcp	-0.714	0.031	-0.060
V-H1-Top	-0.759	-0.033	-0.068
V-H1-Bridge	-0.655	-0.023	-0.088
V-H1-Fcc	-0.832	-0.025	-0.095
V-H1-Hcp	-0.840	-0.035	-0.097
V-H2-Top	-0.723	-0.013	-0.083
V-H2-Bridge	-0.655	-0.033	-0.098
V-H2-Fcc	-0.761	0.020	-0.089
V-H2-Hcp	-0.760	-0.021	-0.088
V-CF ₃ -Top	-0.881	0.035	0.029
V-CF ₃ -Bridge	-0.728	0.022	0.020
V-CF ₃ -Fcc	-0.768	-0.028	-0.048
V-CF ₃ -Hcp	-0.787	-0.023	-0.038

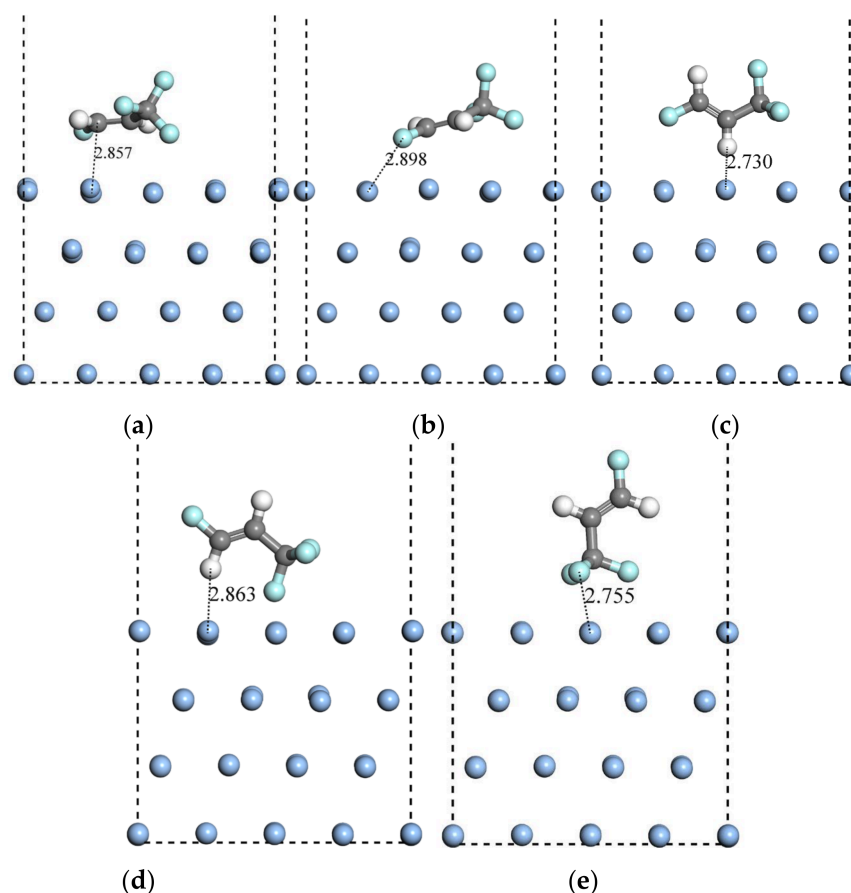


Figure 14. Most energetically favorable structures of HFO-1234ze(E) on vacancy-containing Ag (1 1 1) surface. (a) V-C-Fcc, (b) V-F4-Top, (c) V-H1-Hcp, (d) V-H2-Fcc, and (e) V-CF₃-Top.

The absolute Mulliken and Hirshfeld charge transfer values range from 0.008 to 0.042e and from 0.017 to 0.098e, respectively. Although these values are slightly higher than those obtained for pristine Ag (1 1 1), their magnitudes remain relatively small. These results indicate that the increase in interfacial charge transfer caused by the vacancy remains modest. The charge density difference distribution of the most stable V-C-Fcc configuration is presented in Figure 15. Compared with the corresponding configuration on pristine Ag (1 1 1), the vacancy-containing system exhibits slightly more-pronounced electron accumulation and depletion at the adsorption interface, consistent with the calculated charge transfer results. Nevertheless, the interfacial charge redistribution remains limited and localized, and no pronounced continuous electron-accumulation region indicative of strong covalent bonding is observed between HFO-1234ze(E) and the surface Ag atoms. Therefore, the adsorption characteristics are assessed by considering the optimized geometry, DOS and charge density difference results together with the adsorption energy and charge transfer, rather than using the adsorption energy alone.

4.2. Adsorption-Strength Mechanism

The TDOS and PDOS results for the most energetically favorable HFO-1234ze(E) configuration on vacancy-containing Ag (1 1 1) are presented in Figure 16. All energies are referenced to the Fermi level, which is set to 0 eV. The PDOS was projected primarily onto the C atom closest to the surface and the Ag atom adjacent to the vacancy, denoted as Ag_{vac}, with particular attention given to their C-2p and Ag_{vac}-4d states. Figure 16a shows only minor changes in the TDOS peak intensities after adsorption. As shown in Figure 16b, the Ag_{vac}-4d states exhibit a new shoulder and a slight increase in the main peak intensity

compared with the Ag-4d states on pristine Ag (1 1 1). These changes indicate that the vacancy modifies the local electronic structure of neighboring Ag atoms. The new shoulder lies close in energy to a C-2p feature, but the degree of spectral overlap between them remains limited. This limited overlap indicates only a modest increase in the coupling between the C-2p and Ag_{vac}-4d orbitals, rather than strong orbital hybridization. Taken together, the vacancy-induced enhancement is mainly attributed to strengthened local interfacial interactions rather than adsorption dominated by strong chemical bonding.

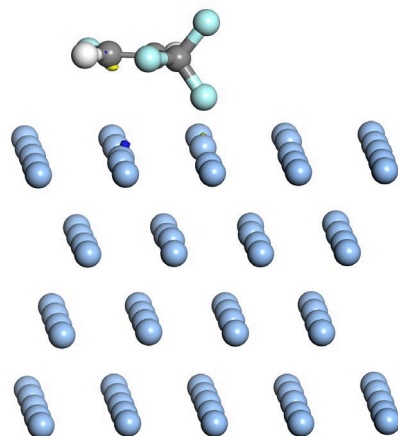


Figure 15. Charge density difference of HFO-1234ze(E) on vacancy-containing Ag (1 1 1) surface.

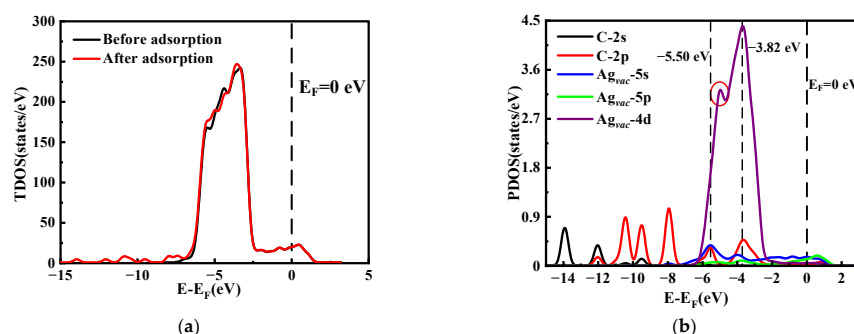


Figure 16. TDOS and PDOS of HFO-1234ze(E) adsorbed on vacancy-containing Ag (1 1 1). (a) TDOS and (b) PDOS.

5. Conclusions

In this study, the microscopic interactions of HFO-1234ze(E) with pristine and vacancy-containing Ag (1 1 1) surfaces were investigated using density functional theory. The main conclusions are as follows:

- (1) The frontier molecular orbital and molecular electrostatic potential analyses indicate the C=C bond, H1, H2, F4, and CF₃ group are potential interaction regions. These regions were therefore used to construct the initial molecular orientations for the adsorption calculations.
- (2) On pristine Ag (1 1 1), HFO-1234ze(E) exhibits smaller adsorption energy magnitudes and lower charge transfer values than SF₆. The electronic structure results reveal only limited orbital coupling and no clear evidence of interfacial chemical bond formation. During the 10 ps molecular dynamics simulation at 400 K, HFO-1234ze(E) moved away from the surface while retaining its molecular structure, and no decomposition was observed. Furthermore, the calculated activation barriers for five representative bond-cleavage pathways range from 1.33 to 2.98 eV, indicating that molecular dissociation is kinetically hindered under the investigated conditions.

- (3) The surface vacancy increases the adsorption energy magnitude and interfacial charge transfer of HFO-1234ze(E). The new shoulder in the $\text{Ag}_{\text{vac}}\text{-4d}$ states indicates that the vacancy modifies the local electronic structure of neighboring Ag atoms. However, the charge transfer and spectral overlap between the C-2p and $\text{Ag}_{\text{vac}}\text{-4d}$ states remain limited. Taken together, these results indicate that the surface vacancy only modestly enhances the local interfacial interaction without producing adsorption dominated by strong chemical bonding.

Overall, HFO-1234ze(E) exhibits favorable initial adsorption compatibility with Ag (1 1 1) under the computational conditions considered. These results characterize only the initial interfacial interaction and molecular stability over the 10 ps simulation period. Moreover, the favorable compatibility of the parent HFO-1234ze(E) molecule does not necessarily guarantee the compatibility of its decomposition products generated under electrical discharge. Reactive products such as HF and other fluorinated fragments may interact more strongly with the Ag surface and potentially affect the chemical stability, corrosion behavior, and electrical contact performance of the silver plating. Therefore, the present results do not establish compatibility over extended periods of operation in actual electrical equipment. Further investigation is required to evaluate the interactions of both HFO-1234ze(E) and its major decomposition products with Ag surfaces under realistic pressure, impurity, electric-field, and discharge conditions.

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