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Mechanism of ultralow friction in fluorinated stanene/graphene heterostructures

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ABSTRACT

First-principles calculations were employed to investigate the ultralow friction of stanene/graphene systems based on a combined strategy of heterostructure construction and fluorination. The potential energy surfaces (PES) and sliding energy barriers of six configurations were analyzed. Heterostructure formation primarily reduced friction by suppressing interlayer charge redistribution, while fluorination further lowered friction by smoothing the PES and inhibiting charge rearrangement due to the strong electron-withdrawing effect of fluorine. Under external load, the collapse and reversal of the PES were governed by the competition between interlayer van der Waals and Coulomb interactions. Among all systems, StaF/Gr showed the lowest sliding barrier and achieved the minimum friction coefficient of 0.0012, maintaining stable ultralow friction over a wide load range, whereas Sta/Gr only exhibited such behavior under low loads. These results clarified the mechanisms of the heterostructure-fluorination strategy and demonstrated the potential of fluorinated stanene/graphene for low-dissipation nano- and micro-scale applications.

1. Introduction

Friction-induced energy dissipation accounts for nearly 30% of the global energy consumption, and the associated direct economic loss amounts to approximately 5% of the total social productivity each year [1,2]. In engineering area, nearly 80% of mechanical component failures originate from lubrication failure at contact interfaces, and effective lubrication under extreme service conditions remains a major challenge [3]. Layered solid lubricants, such as graphene, molybdenum disulfide, and hexagonal boron nitride, are widely used for interfacial lubrication under extreme conditions including heavy load, high and low temperatures, and strong radiation, owing to their ultralow interlayer shear strength and high load-carrying capacity, and they exhibit excellent lubricating performance [4,5]. Moreover, their intrinsic micro-/nanoscale dimensions make them highly promising for lubrication in micro- and nano-electromechanical systems [6,7]. The superior macroscopic lubrication performance of layered solid lubricants originates from their near- or true-superlubric frictional behavior at the microscopic scale [8].

An interlayer friction coefficient at the level of 10^{-3} is commonly regarded as the hallmark of superlubricity [9–11]. Continuous sliding

between incommensurate interfaces is a key route to achieve ultralow friction. In twisted homostructures, for example bilayer graphene, MoS₂, and h-BN, the formation of Moiré superlattices effectively suppresses the modulation of the interfacial potential landscape, thereby enabling ultralow friction behavior at the atomic scale [12]. Although twisted homostructures provide an important pathway to ultralow friction, maintaining a specific twist angle is difficult in practical applications, which limits their macroscopic realization. In contrast, heterostructures are intrinsically incommensurate due to lattice mismatch, and their weak interlayer van der Waals interactions allow ultralow friction to be more readily achieved [13]. Recently reported heterostructures with ultralow friction potential include graphene/ZrS₂ [14], graphene/tellurene [15] and graphene/GaSe [16]. Furthermore, surface functionalization can further reduce interlayer friction. First-principles simulations indicate that fluorine termination of the graphene/h-BN interface can substantially reduce the interlayer sliding barrier, leading to enhanced friction performance [17]. Consistent conclusions have also been reported experimentally: plasma-fluorinated multilayer graphene exhibits a significantly reduced friction coefficient and improved durability [18]. The combination of heterostructure construction and surface functionalization thus represents an important strategy for

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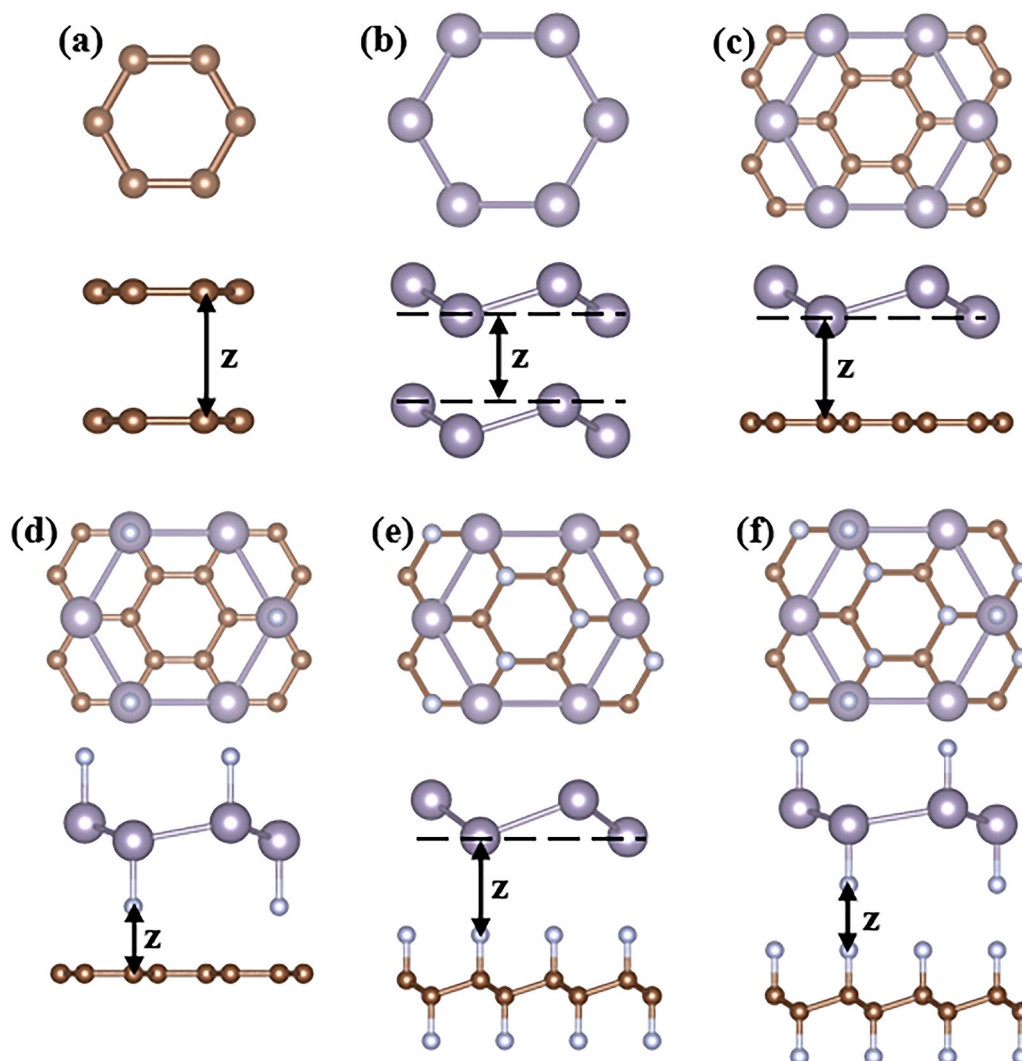


Fig. 1. Top-view and side-view geometries of the six bilayer configurations: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF; and (f) StaF/GrF. Here, z referred to the spacing between the two layers, which was defined as the minimum averaged vertical separation between the bottommost atomic plane of the upper sheet and the topmost atomic plane of the lower sheet.

achieving ultralow friction at solid interfaces.

The development of novel layered solid lubricants with ultralow friction potential has therefore attracted sustained interest. Following graphene, other elements including silicon, germanium, and tin, were also found to form atomically thin sheets [19–21]. Unlike the perfectly planar honeycomb lattice of graphene, silicene, germanene, and stanene exhibit a buckled structure due to their longer bond lengths [22]. Extensive studies have been devoted to the physical properties of silicene and germanene [23–25], and their extremely low sliding barriers on graphene substrates have been confirmed in nanoscale friction investigations [26]. Stanene, a more recently reported member of this family, exhibits remarkable electrical and optical characteristics. Both pristine and chemically functionalized stanene (e.g., fluorinated [27] and hydrogenated [28]) were predicted to be topological insulators. Stanene-based heterostructures on substrates such as graphene [29–31], h-BN [32] and MoS₂ [33] exhibit large-gap quantum spin Hall states at room temperature. Strain [34,35], electric fields [36], and defects [37] have also been shown to enhance spin–orbit coupling and enlarge the band gap. Such unconventional quantum behaviors highlight the great promise of stanene for nanoelectronic and spintronic technologies. In addition, its spin-induced photocurrent [38] and the optical properties of functionalized stanene (Sta-X, X = C, Si, Ge, F) [27, 39] suggest potential in optoelectronic devices. Heterostructures of

stanene with graphene [30], ZnO [40], and fluorinated stanene [27] have also been proposed for photovoltaic and sensing applications. Despite these advances, the tribological behavior of stanene at the nanoscale remains largely unexplored.

The frictional behavior of fluorinated stanene/graphene heterostructures was systematically investigated using density functional theory. The potential energy surfaces (PES) of six representative configurations were obtained, and their sliding energy barriers were compared to preliminarily evaluate their frictional performance. The microscopic mechanisms responsible for the differences in tribological behavior were elucidated through analysis of interlayer charge distribution and charge transfer during sliding. In addition, the influence of applied normal loading on the frictional behavior of the six structures was systematically analyzed. The results demonstrate that the dual strategy of heterostructure construction and surface fluorination is highly effective in achieving ultralow friction. These findings have broadened the range of known ultralow friction systems and offered theoretical insight for developing next-generation solid lubrication materials.

2. Models and methods

First, the atomic structures of four monolayers, namely stanene,

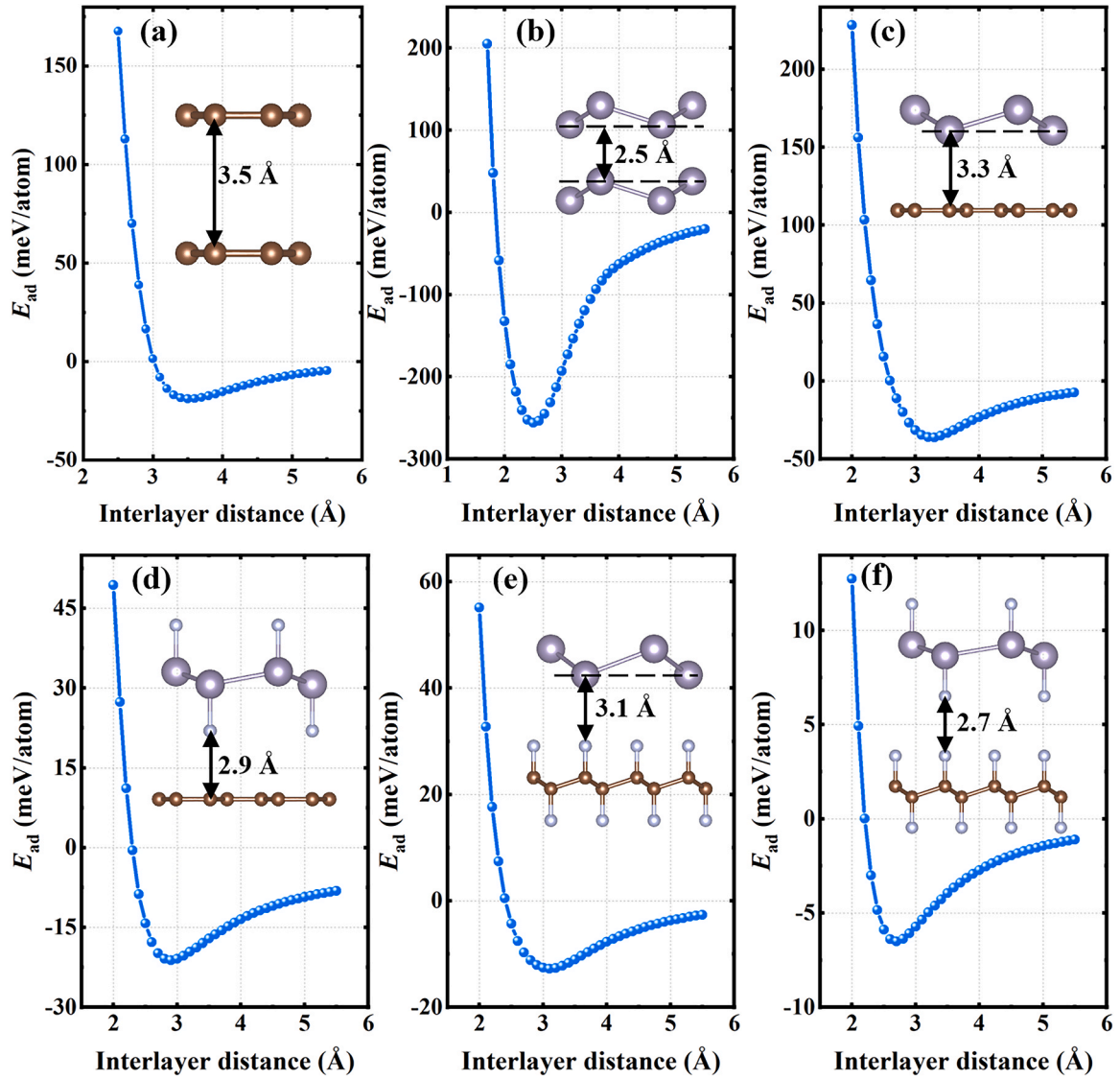


Fig. 2. Interlayer adhesion energy with interlayer distance for the six bilayer structures: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF; and (f) StaF/GrF.

graphene, fluorinated stanene, and fluorinated graphene, were fully optimized. The optimized lattice constants were determined to be 4.67 Å, 2.46 Å, 5.00 Å, and 2.61 Å, consistent with earlier theoretical studies [27,41]. Six bilayer models were then constructed, including graphene/graphene (Gr/Gr), stanene/stanene (Sta/Sta), stanene/graphene (Sta/Gr), fluorinated stanene/graphene (StaF/Gr), stanene/fluorinated graphene (Sta/GrF), and fluorinated stanene/fluorinated graphene (StaF/GrF), as illustrated in Fig. 1. Supercells were built to ensure that the lattice mismatch of all heterostructures was less than 5%. The corresponding in-plane lattice dimensions of the six bilayers were 4.27×2.46 Å, 8.09×4.67 Å, 8.54×4.93 Å, 8.66×5.00 Å, 8.99×5.19 Å, and 8.99×5.19 Å. To avoid artificial coupling between periodic images, a vacuum region exceeding 20 Å was introduced normal to the layers. All first-principles simulations were carried out with the Vienna ab initio Simulation Package (VASP) [42]. Core–valence interactions were described by the projector augmented-wave (PAW) approach [43], while exchange–correlation effects were treated within the generalized gradient approximation using the PBE functional [44]. Long-range dispersion forces were included via the DFT+D2 scheme [45]. The Brillouin-zone k-point mesh was set to $9 \times 17 \times 1$ for the Gr/Gr system and $5 \times 9 \times 1$ for the other five bilayers. A plane-wave cutoff of 500 eV was applied, and the convergence thresholds for electronic

self-consistency and ionic relaxation were set to 10^{-5} eV and $0.02 \text{ eV } \text{\AA}^{-1}$, respectively, ensuring reliable computational accuracy. We compared the AFM experimental results of monolayer graphene, monolayer fluorinated graphene, and the interlayer tribological properties of the graphene/graphene structure with part of the DFT simulation results from this study. This comparison provided support for the rationality of the simulation results. The comparison between the simulation results and the AFM experimental results was placed in the [Supplementary Material](#).

The PES is a key quantity for characterizing atomic-scale friction. To obtain the PES of the six bilayer structures, the upper layer was laterally translated over the lower one on a two-dimensional 13×7 mesh, corresponding to 13 sampling points in the x direction and 7 in the y direction. At each grid point, the in-plane (x and y) coordinates of all atoms were fixed, while full relaxation was allowed along the z direction [46,47]. The interfacial adhesion energy E_{ad} at each position was evaluated using the following relation:

$$E_{\text{ad}}(x, y, z) = \frac{E_{\text{total}} - E_{\text{layer1}} - E_{\text{layer2}}}{N} \quad (1)$$

Where x and y denote the relative lateral shifts of the upper sheet with respect to the lower one, whereas z denotes their vertical separation. E_{ad} refers to the adhesion energy of the bilayer, E_{total} to the total energy of

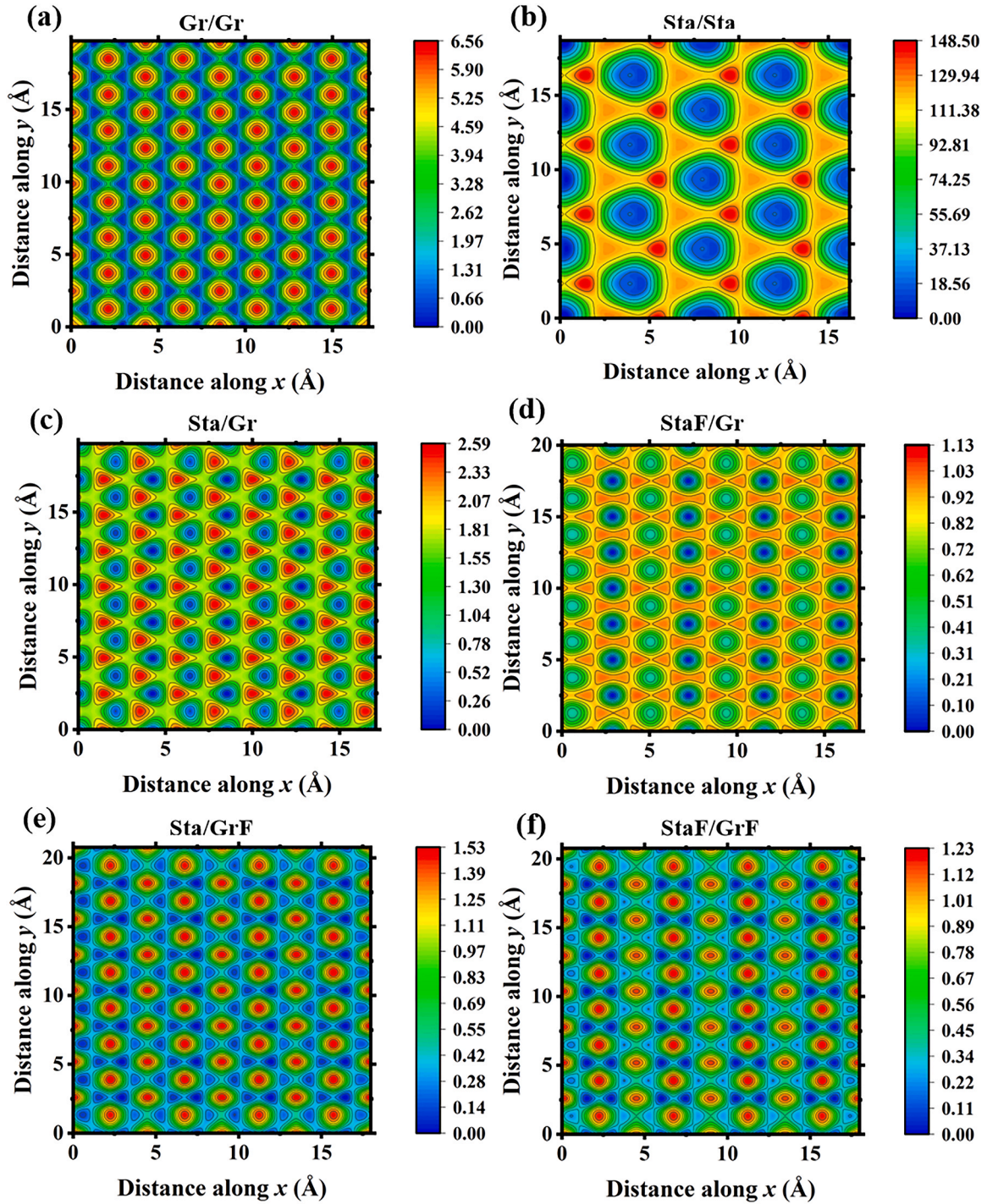


Fig. 3. Potential energy surfaces of the six bilayer structures: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF; and (f) StaF/GrF.

the combined structure, and E_{layer1} and E_{layer2} to the energies of the isolated top and bottom sheets, respectively, with N being the total atom count.

When no normal force was applied, z corresponded to the equilibrium spacing between the two layers, and the sliding energy barrier during relative motion was obtained from the following formula:

$$\Delta E = E_{\text{adMax}} - E_{\text{adMin}} \quad (2)$$

where ΔE denotes the sliding energy barrier, E_{adMax} is the maximum interlayer adhesion energy during sliding, and E_{adMin} is the minimum interlayer adhesion energy along the sliding path.

The differential charge density during relative sliding was obtained by subtracting the charge densities of the two isolated layers from that of the combined bilayer, as given by

$$\rho_{\text{diff}} = \rho_{\text{tot}} - \rho_1 - \rho_2 \quad (3)$$

where ρ_{diff} denotes the differential charge density, ρ_{tot} represents the overall charge distribution of the bilayer, and ρ_1 and ρ_2 correspond to the charge densities of the separated upper and lower layers.

In this work, a constant normal force was imposed by tuning the vertical separation between the two layers [48,49]. For lateral motion along the x direction, the interfacial normal force could be evaluated

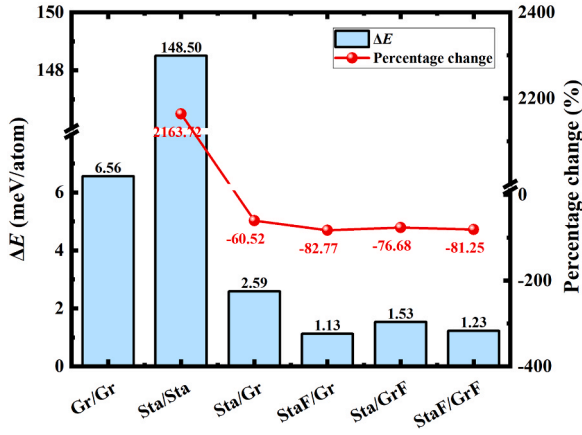


Fig. 4. Sliding energy barriers of the six bilayer structures under zero external normal force.

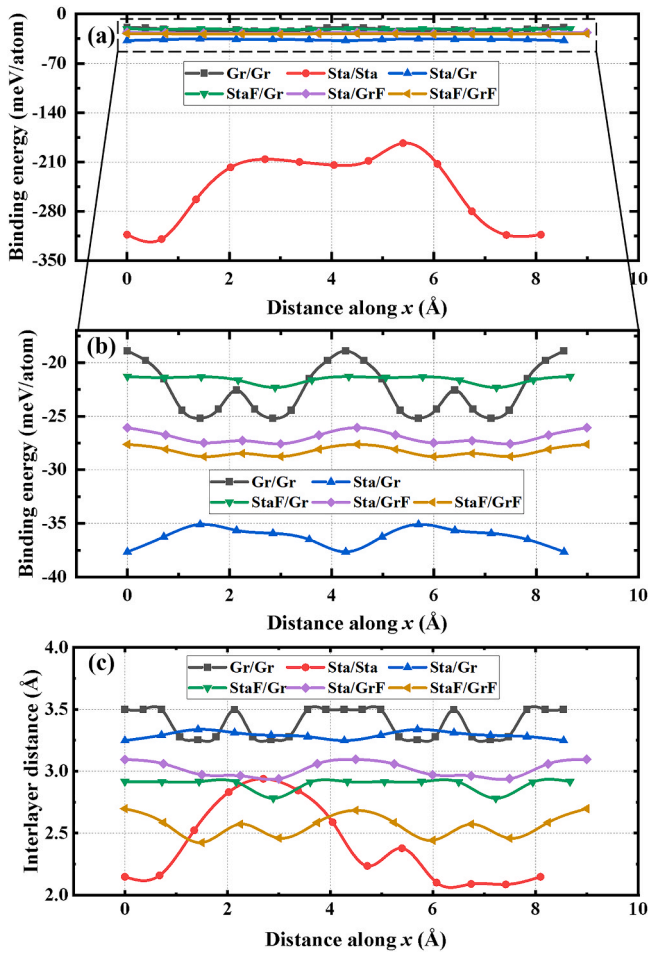


Fig. 5. Variations of interlayer distance and binding energy with lateral displacement: (a) Binding energy along the sliding path; (b) Enlarged view of the binding energy variations and (c) Interlayer distance along the sliding path.

from

$$F_n(x, z) = -\frac{\partial E_{ad}(x, z)}{\partial z} \quad (4)$$

Where F_n is the normal load, E_{ad} is the interlayer adhesion energy, z denotes the layer spacing, and x is the relative sliding coordinate.

Compared with the system energy calculated for the potential energy

surface, the work done by the normal load was further considered. The total energy of the system at nonequilibrium separations during sliding was expressed as [48]:

$$V(x, F_n) = E_{ad}(x, z(x, F_n)) + F_n \times z(x, F_n) - V_0(F_n) \quad (5)$$

where V represents the system energy under a given normal force F_n , E_{ad} is the adhesion energy, and V_0 is the minimum energy along the sliding path under the same loading condition.

The sliding barrier under an external load was then evaluated by [48]:

$$\Delta V_{max}(F_n) = V_{max}(F_n) - V_{min}(F_n) \quad (6)$$

where V_{max} and V_{min} are the highest and lowest values of V along the sliding trajectory.

Finally, the lateral friction force during relative motion was obtained from the following relation [14,50,51]:

$$F_f = \frac{\Delta V_{max}(F_n)}{\Delta x} \quad (7)$$

where Δx is the sliding distance between the V_{max} and V_{min} .

Therefore, the friction coefficient during the sliding process was given by [14,50,51]:

$$\mu = \frac{F_f}{F_n} = \frac{\Delta V_{max}(F_n)}{F_n \Delta x} \quad (8)$$

To further elucidate the fundamental physical mechanism underlying the load-induced collapse and inversion of the potential energy surface, the interlayer adhesion energy (E_{ad}) was decomposed into the interlayer Coulomb interaction energy (E_C) and van der Waals interaction energy (E_{vdW}), as expressed in Eq. (9).

$$E_{ad} = E_C + E_{vdW} \quad (9)$$

where E_{ad} denotes the interlayer adhesion energy, E_C represents the Coulomb interaction energy, and E_{vdW} represents the van der Waals interaction energy.

To quantify the relative contributions of van der Waals and Coulomb interactions, a coefficient K was defined as shown in Eq. (10). A value of K greater than 1 indicated that the interlayer interaction was dominated by van der Waals force, whereas K less than 1 indicated that the interaction was dominated by Coulomb force.

$$K = \left| \frac{E_{vdW}}{E_C} \right| \quad (10)$$

The total energy of system (V) could also be decomposed into the contribution from Coulomb interaction energy (V_C) and from van der Waals interaction energy (V_{vdW}), as given in Eq. (11).

$$V(x, F_n) = V_C(x, F_n) + V_{vdW}(x, F_n) \quad (11)$$

3. Results and discussion

3.1. Potential energy surface (PES) and sliding energy barrier

First, the relationship between the interlayer adhesion energy and the interlayer distance was calculated for the six bilayer structures, as shown in Fig. 2. The spacing normal to the interface scanned from 5.5 Å down to 2.0 Å with an increment of 0.1 Å, and the interlayer adhesion energy E_{ad} was recorded at each step. As the layers approach each other, the adhesion energy first decreased and then increased, and the minimum of each curve identifies the equilibrium separation. The equilibrium interlayer distances of the homostructures Gr/Gr and Sta/Sta were 3.5 Å and 2.5 Å, respectively, while those of the heterostructures Sta/Gr, StaF/Gr, Sta/GrF, and StaF/GrF were 3.3 Å, 2.9 Å, 3.1 Å, and 2.7 Å, respectively.

This equilibrium position results from the competition between

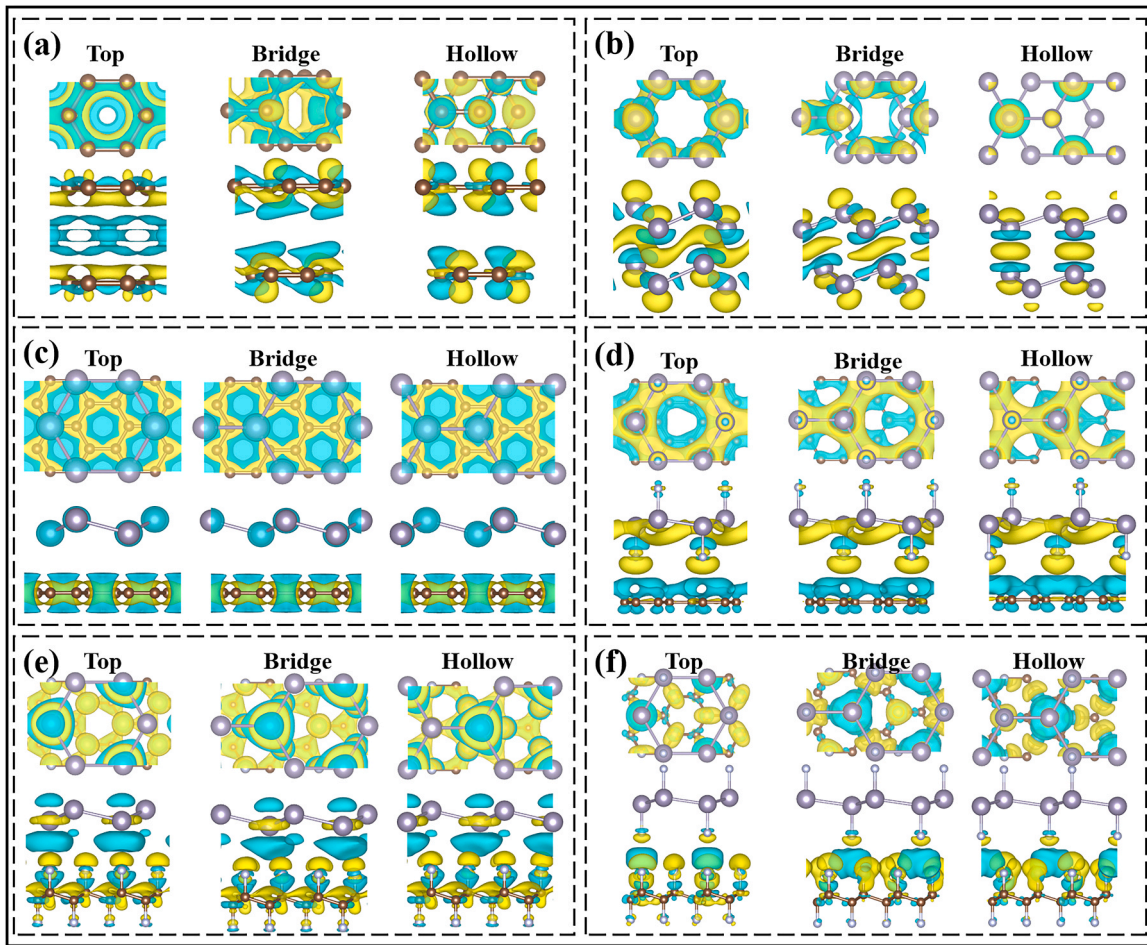


Fig. 6. Differential charge density maps at three representative positions during sliding for the six bilayer structures: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF and (f) StaF/GrF. The top row showed top views of the bilayer system during sliding, and the bottom row showed the corresponding differential charge density profiles. For each model, the configurations from left to right were the top, bridge, and hollow stacking sites. Regions of electron accumulation were colored in yellow, whereas electron depletion was shown in blue.

short-range Pauli exclusion and long-range dispersion interactions, the latter being comparatively weak. Notably, the adhesion curve of Sta/Sta lies far above those of the remaining five systems, implying that, besides Pauli repulsion and van der Waals attraction, interlayer chemical bonding played a non-negligible role in stabilizing this configuration. Since the interlayer binding strength was strongly correlated with potential energy corrugation [52], the Sta/Sta homostructure was expected to exhibit a much higher sliding energy barrier compared to the other five bilayers. To verify this hypothesis, the potential energy surfaces of all six structures were further calculated.

At the equilibrium interlayer distance, variations in the adhesion energy E_{ad} with lateral displacement are the origin of friction. The top layer was displaced to each grid point of the model, and the structures were optimized at each position to obtain the corresponding energies. The resulting potential energy surfaces at equilibrium were shown in Fig. 3. Due to the inherent lattice periodicity, the PES exhibited periodic features with a length scale corresponding to the lattice constants. For the Gr/Gr bilayer, the calculated barrier was 6.56 meV/atom, which was consistent with the literature value of 6.47 meV/atom [49]. As shown in Fig. 4, comparison of the sliding barriers for the six bilayers revealed that the Sta/Sta homostructure exhibited the highest barrier of 148.50 meV/atom. In contrast, the Sta/Gr heterostructure had a much smoother PES compared to the two homostructures. Surface fluorination further reduced the interlayer sliding barrier, with StaF/Gr—where only the stanene layer was fluorinated—showing the lowest barrier. Using the maximum sliding barrier of the graphene bilayer as a reference, the

Sta/Sta barrier increased by 2163.72%, while the Sta/Gr heterostructure decreased by 60.52%. The fluorinated heterostructures StaF/Gr, Sta/GrF, and StaF/GrF reduced the sliding barriers by 82.77%, 76.68%, and 81.25%, respectively.

Fig. 5 presented the evolutions of the interlayer spacing and adhesion energy along the maximum-energy sliding pathway. For Gr/Gr, Sta/Gr, StaF/Gr, Sta/GrF, and StaF/GrF, the change in layer separation mirrors the variation in adhesion energy, and the smallest spacing coincided with the energy minimum. In contrast, Sta/Sta exhibited a distinct behavior due to its buckled structure. In Sta/Sta, the central atom in the upper sheet sat above the hexagonal hollow of the lower sheet and was lifted upward, giving the largest separation, whereas the sublayer atoms of the upper sheet were located closer to the hollow sites of the lower sheet and thus experienced stronger attraction, resulting in the shortest distance. The maximum interlayer distance variations for the homostructures Gr/Gr and Sta/Sta were 0.25 Å and 0.85 Å, respectively, while the heterostructure Sta/Gr showed a much smaller maximum variation of 0.09 Å, indicating that heterostructures underwent smaller configurational changes during zero-load sliding. For the fluorinated systems StaF/Gr, Sta/GrF, and StaF/GrF, the corresponding variations were 0.14 Å, 0.16 Å, and 0.28 Å, all larger than that of the pristine heterostructure.

3.2. Interlayer charge distribution and transfer during sliding

During the relative sliding of the bilayer structures, changes in

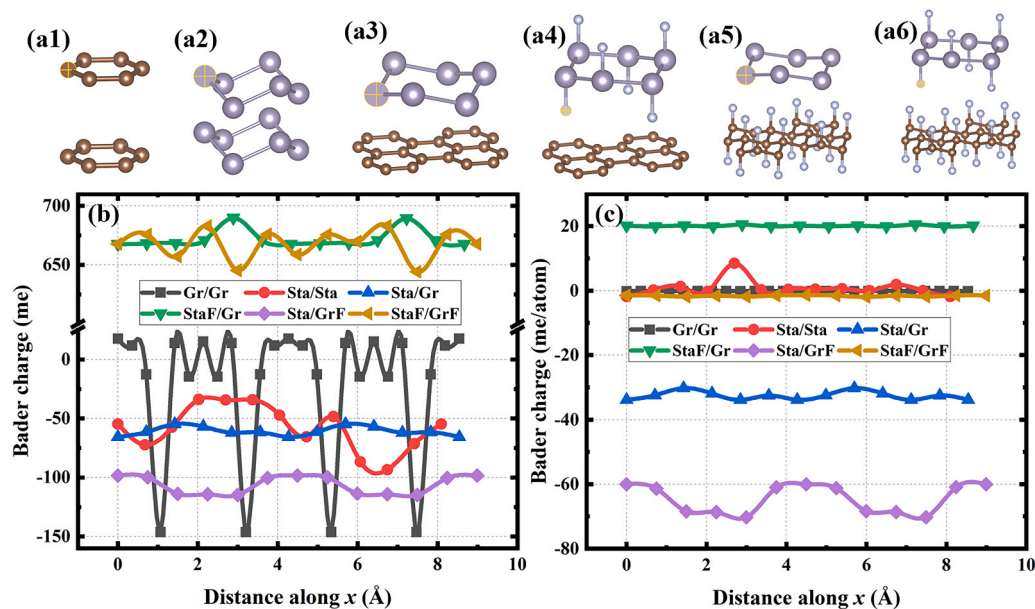


Fig. 7. Bader charge analysis: (a1)-(a6) Six bilayer sliding models, with one atom in the top layer highlighted for each structure; (b) Charge transfer analysis of the individual highlighted atom and (c) Charge transfer analysis of all atoms in the top layer.

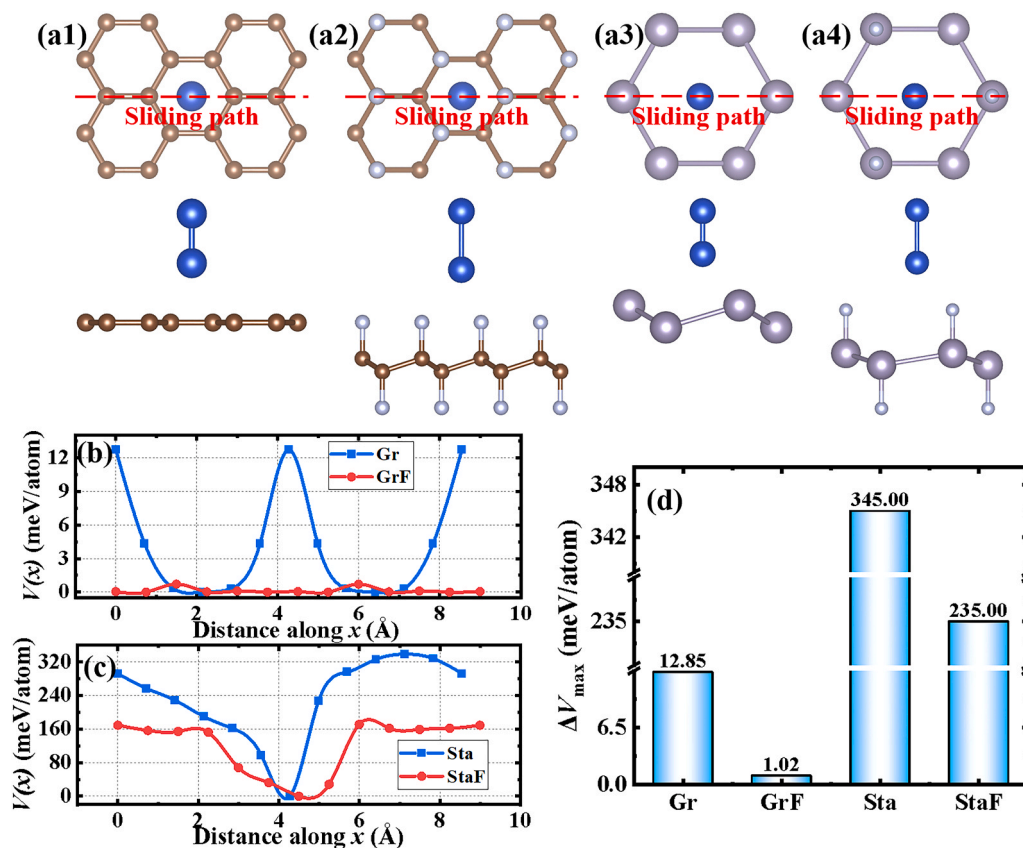


Fig. 8. DFT-based AFM simulations: (a1) Tip-Gr, (a2) Tip-GrF, (a3) Tip-Sta, (a4) Tip-StaF; (b) PES variation of Gr and GrF along the scanning path; (c) PES variation of Sta and StaF along the scanning path; (d) Maximum PES corrugation of the four monolayer structures.

configuration led to variations in both interlayer interactions and charge distribution. The distribution of charge density was closely related to the interlayer sliding energy barrier [52–55]. Differential charge density analysis provides an intuitive visualization of how charge is distributed within a region. To explain the significant differences in friction among

the bilayer structures, the redistribution and transfer of interlayer charge during sliding were examined. Both graphene and stanene exhibited a regular hexagonal in-plane atomic arrangement. Three typical stacking sites—top, bridge, and hollow—were selected as representative configurations along the sliding path to observe

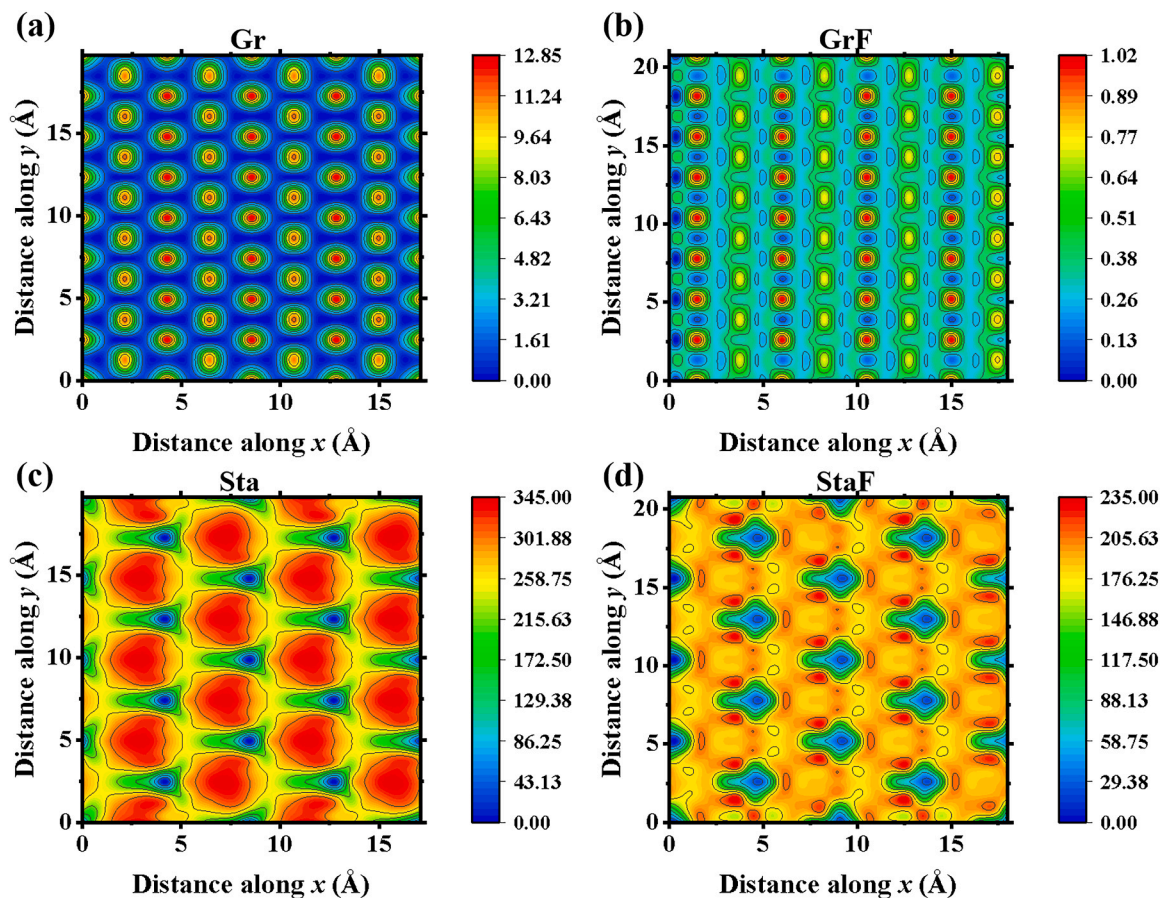


Fig. 9. Complete PES of four monolayer structures measured by a dimer probe: (a) Gr; (b) GrF; (c) Sta; (d) StaF.

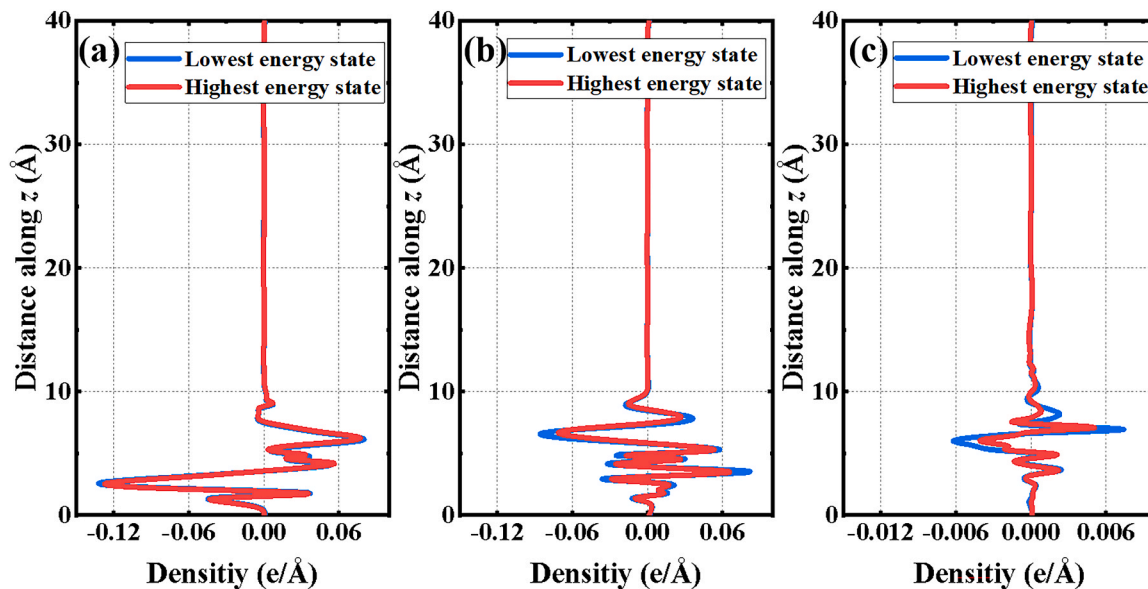


Fig. 10. Plane-averaged differential charge density at the highest and lowest energy states: (a) StaF/Gr; (b) Sta/GrF; (c) StaF/GrF.

interlayer charge redistribution. The differential charge density distributions at these three representative positions for all six bilayer structures during sliding were displayed in Fig. 6.

As shown in Figs. 6(a) and 6(b), both Gr/Gr and Sta/Sta exhibited pronounced interfacial charge rearrangement along the sliding path, consistent with their relatively large energy barriers in Fig. 5(a) and 5

(b). The differential charge density map of Sta/Sta indicated strong interactions between the top and bottom stanene layers: electrons from individual Sn atoms were depleted and accumulated in the interlayer region. This significant redistribution of interlayer charge during sliding was one of the main pathways for energy dissipation, providing an explanation for the substantially higher sliding barrier of the Sta/Sta

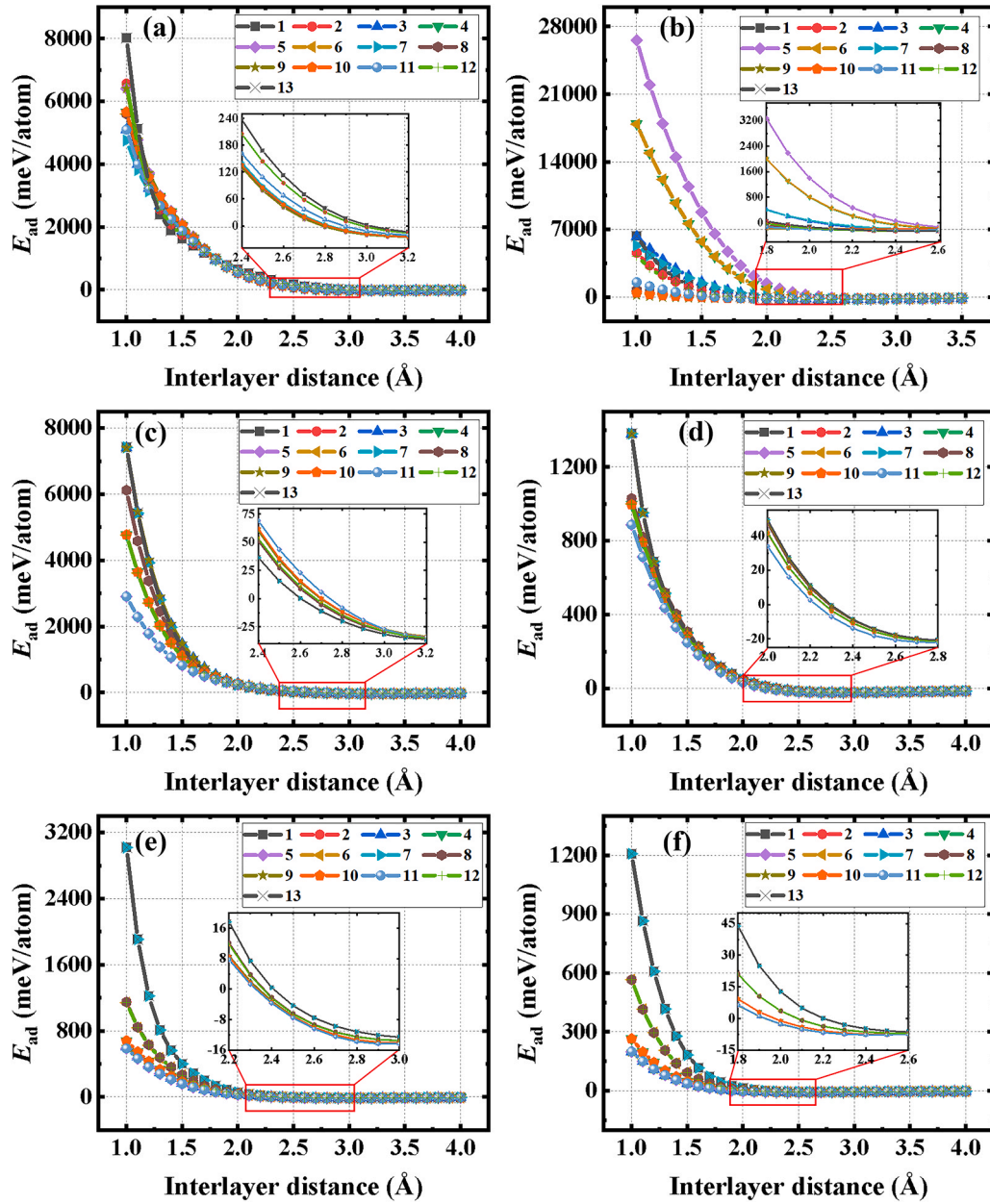


Fig. 11. Interlayer adhesion energy as a function of fixed interlayer distance at 13 sliding positions for the six bilayer structures: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF and (f) StaF/GrF.

structure. In contrast, the Gr/Gr homostructure showed relatively weak interlayer charge transfer, with much less redistribution during sliding, resulting in a smoother potential energy surface. For the Sta/Gr heterostructure, almost no interlayer charge redistribution occurred during sliding, which corresponded to its significantly lower sliding barrier compared to the homostructures. Furthermore, for the three fluorinated heterostructures, the redistribution of interlayer charge during sliding was minimal, consistent with their relatively small sliding barriers.

To quantitatively describe interlayer charge transfer during sliding, Bader charge analysis was performed for both the entire top layer and individual highlighted atoms within the layer. As shown in Fig. 7(b), the Bader analysis of a single F atom provided a microscopic electronic-level explanation for the further reduction of the interlayer sliding barrier upon fluorine incorporation. Electrons accumulated strongly around the interfacial F atom and maintained this localized accumulation throughout the sliding process. Fig. 7(c) showed that Sn atoms in the upper sheet of the Sta/Gr structure tended to lose electrons. In the

fluorinated StaF/Gr structure, where the top layer was fluorinated, the top-layer atoms overall gained electrons due to the effect of F atoms. For Sta/GrF, where only the bottom layer was fluorinated, the top-layer Sn atoms lost significantly more electrons. In StaF/GrF, where both layers were fluorinated, the top-layer atoms overall lost electrons, reflecting the larger population of fluorine atoms in the lower sheet. Fluorine effectively modulated the interlayer charge distribution and, by stabilizing accumulated electrons, significantly suppressed interlayer charge redistribution during sliding, thereby reducing the interlayer sliding barrier.

3.3. Mechanism of the effect of fluorination on tribological properties

At the microscopic level, the origin of friction arose from the corrugation of the potential energy surface (PES). Generally, a larger PES corrugation corresponded to poorer tribological performance. In addition, charge transfer and redistribution during interlayer sliding

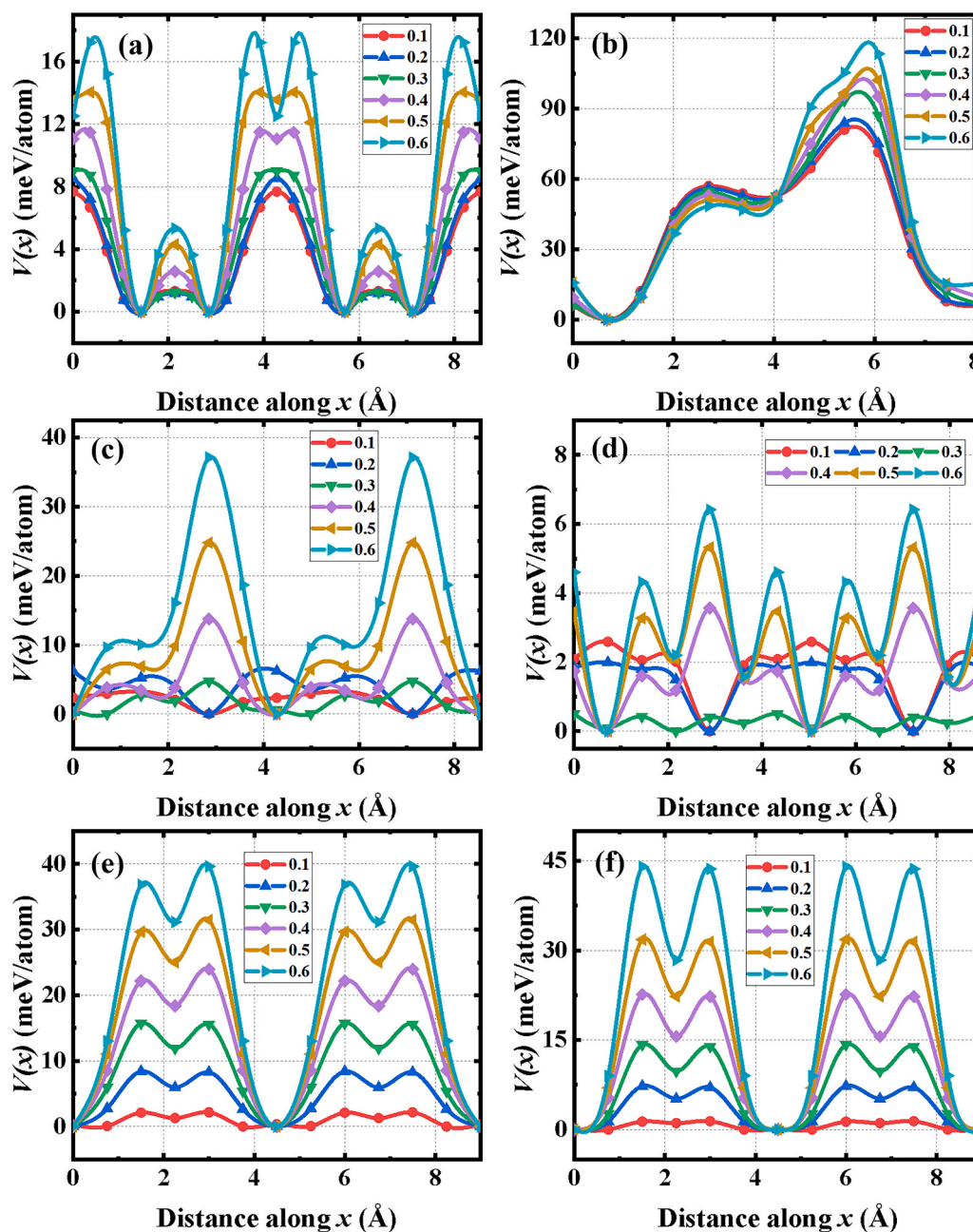


Fig. 12. Variations of system energy along the sliding path under different normal loads for the six bilayer structures: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF and (f) StaF/GrF.

also affected the interfacial frictional properties of bilayer structures. In bilayer systems, interlayer interactions made it difficult to directly evaluate the effect of surface fluorination on the PES of a single layer. To systematically reveal the mechanism of fluorination, we further carried out density functional theory (DFT) simulations based on atomic force microscopy (AFM) to investigate the influence of surface fluorination on the PES of monolayer materials. Meanwhile, the plane-averaged charge density was used to quantify charge redistribution in bilayer structures.

As shown in Fig. 8(a1)–8(a4), the AFM probe used in the simulations was a rigid Cu–Cu dimer, and the substrates were four types of monolayer structures: Gr, GrF, Sta, and StaF. The sliding path of the probe was indicated in the figures. The Cu dimer probe has been successfully used in studies of pressure-induced superlubricity in graphene [56], and has been further applied to investigate the tribological properties of emerging two-dimensional layered materials such as GPAene [57]. After

fluorination, the corrugation of the PES along the sliding path was significantly reduced for all monolayer structures, as shown in Figs. 8(b) and 8(c). For example, the maximum PES corrugation of monolayer GrF decreased from 12.85 meV/atom (Gr) to 1.02 meV/atom, while that of StaF decreased from 345.00 meV/atom (Sta) to 235.00 meV/atom, as shown in Fig. 8(d). Reducing the wrinkle effect of two-dimensional structures was beneficial for improving the tribological performance of materials [58]. The wrinkle effect of the Gr monolayer structure was not significant before and after fluorination. However, the wrinkle effect of the Sta monolayer structure was significant, and the wrinkle effect of StaF was alleviated to a certain extent after fluorination, which facilitated the sliding of diatomic probes on the surface. The complete PES of the four monolayer structures measured by the dimer probe was presented in Fig. 9.

It was evident that surface fluorination was more effective in

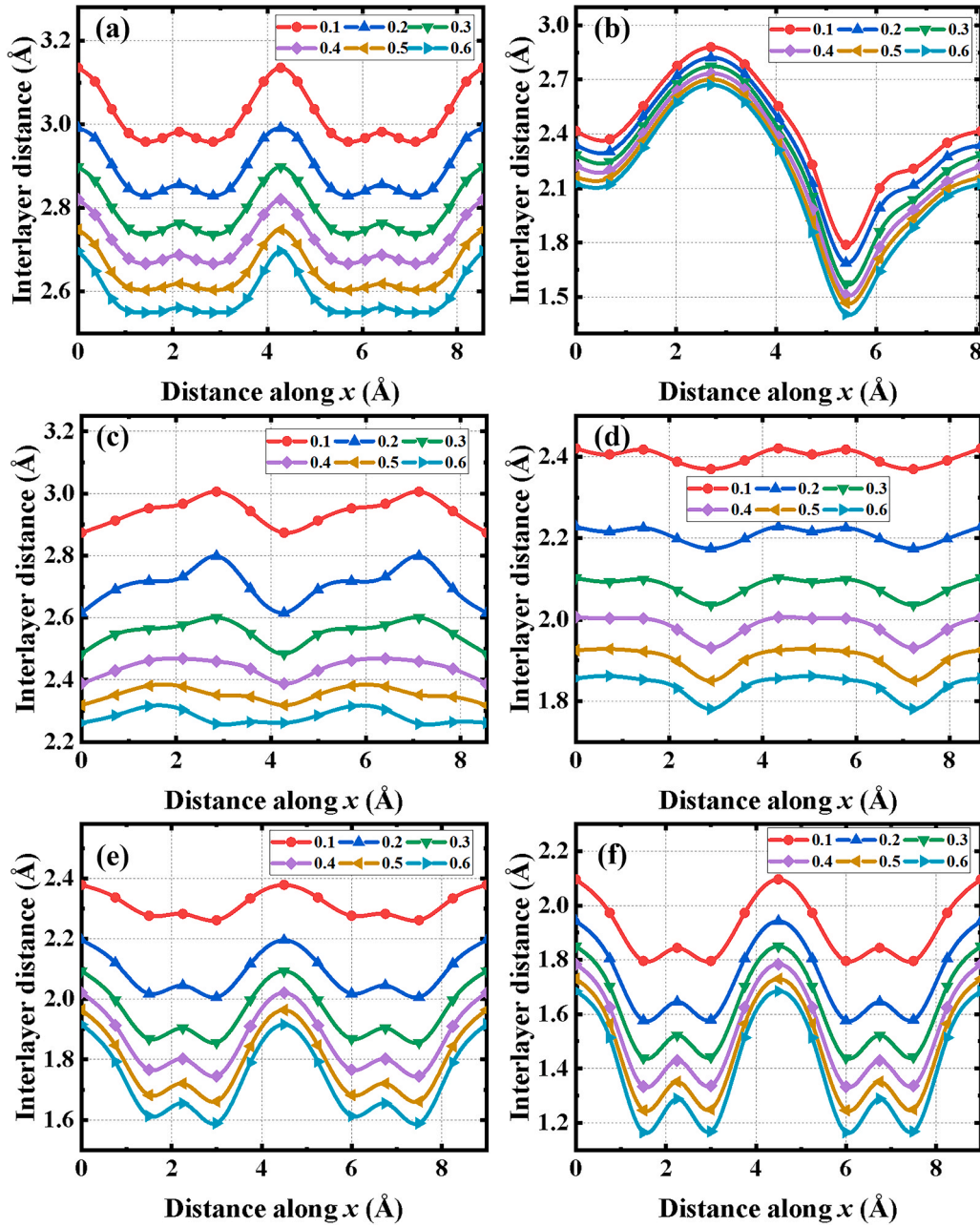


Fig. 13. Variations of interlayer distance along the sliding path under different normal loads for the six bilayer structures: (a) Gr/Gr; (b) Sta/Sta; (c) Sta/Gr; (d) StaF/Gr; (e) Sta/GrF and (f) StaF/GrF.

reducing the PES corrugation of monolayer graphene. However, in the three bilayer structures (StaF/Gr, Sta/GrF, and StaF/GrF), the interlayer sliding energy barrier was the lowest for StaF/Gr (1.13 meV/atom), the highest for Sta/GrF (1.53 meV/atom), and intermediate for StaF/GrF (1.23 meV/atom). This indicated that although surface fluorination played an important role in smoothing the PES, changes in the PES were not the dominant factor governing the tribological performance of fluorinated Sta/Gr bilayer structures. To further analyze this phenomenon, we calculated the plane-averaged differential charge density at the highest and lowest energy states during interlayer sliding for the three bilayer systems, as shown in Fig. 10. The results showed that the degree of interlayer charge redistribution in Sta/GrF was greater than that in StaF/Gr during sliding, which explained the superior tribological performance of the StaF/Gr structure. Although the fully fluorinated bilayer StaF/GrF exhibited flatter PES in each individual monolayer, the charge redistribution during interlayer sliding was more pronounced, which

weakened its tribological performance. From the above analysis, surface fluorination served to smooth the PES of monolayer structures. However, its more significant role lay in influencing the charge redistribution during interlayer sliding in bilayer systems, thereby affecting the overall tribological properties. Charge redistribution was an important energy dissipation path during friction, which significantly affected tribological performance [59].

3.4. Effect of load on tribological properties and its mechanism

To assess the practical applicability of the six bilayer structures, the effect of normal load on their tribological performance was investigated. Fig. 11 showed the relationship between the interlayer adhesion energy and fixed interlayer distance, $E_{ad}(x,z)$, at 13 positions along the maximum energy path for all six structures. The calculation of $E_{ad}(x,z)$ was central to the method of applying a constant normal load by

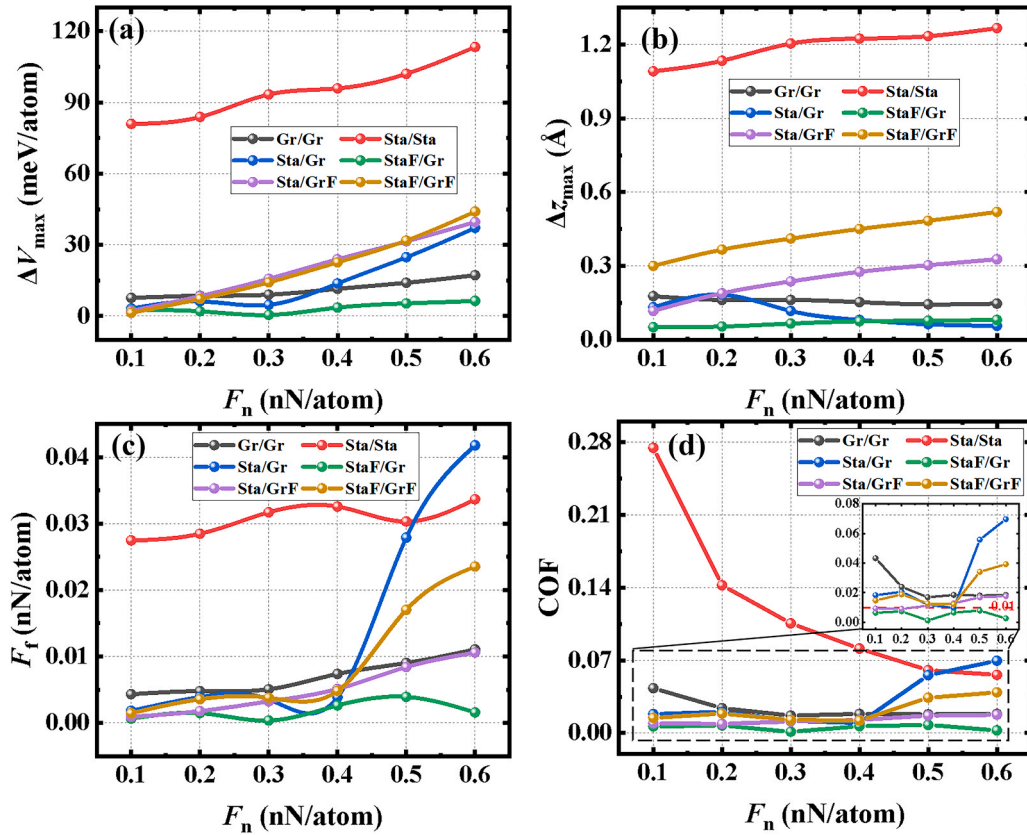


Fig. 14. Tribological properties of the six bilayer structures: (a) Maximum potential energy variation; (b) Maximum interlayer distance fluctuation; (c) Friction force and (d) Friction coefficient.

adjusting the interlayer distance.

Constant normal loads ranging from 0.1 to 0.6 nN/atom were applied, and the variations of system energy and interlayer distance during sliding were shown in Figs. 12 and 13, respectively. The mechanical work associated with an external normal force raised the total energy of the interface and led to pronounced modifications of the potential energy surface as the load was progressively increased. As shown in Fig. 12(a), the PES of the Gr/Gr homostructure exhibited a tendency toward collapse and inversion when the normal load reached 0.4 nN/atom, resembling phenomena observed in studies where stress-induced PES collapse led to ultralow friction [60,61]. In contrast, the PES of Sta/Sta, Sta/GrF, and StaF/GrF (Figs. 12(b), 12(e), and 12(f)) showed little change in response to applied normal loads. For the Sta/Gr heterostructure (Fig. 12(c)), the PES inverted when the load reached 0.3 nN/atom, and the fluctuations increased significantly at 0.4 nN/atom. The StaF/Gr heterostructure (Fig. 12(d)) exhibited a nearly flat PES at a critical load of approximately 0.3 nN/atom; further increased in load cause inversion and larger fluctuations, but the overall amplitude remained relatively small. These results indicated that the sensitivity of the PES to normal load differs among the structures. The observed load-dependent PES variations in Gr/Gr, Sta/Gr, and StaF/Gr suggested the feasibility of tuning their tribological properties through applied normal loads.

Fig. 13 showed the interlayer distance variations of the six structures under different normal loads and the trends of interlayer distance changes during sliding. The application of normal load compressed the interlayer spacing, and the rate of reduction gradually decreased as the load increased; however, the overall trend of interlayer distance variation along the sliding path remained largely unchanged. For Gr/Gr, Sta/Sta, Sta/GrF, and StaF/GrF, the changes in interlayer distance during sliding closely followed the variations in system energy. In Sta/Gr and StaF/Gr, the interlayer distance and system energy exhibited similar

trends when the applied load was below 0.2 nN/atom, but at higher loads, PES collapse and inversion led to significant deviations between the two quantities.

Figs. 14(a) and 14(b) showed the sliding energy barriers and the maximum interlayer distance variations, respectively, for the six structures under different normal loads. Overall, the sliding barriers increased with increasing normal load. Notably, for the Sta/Gr structure, the sliding barrier rose sharply when the normal load reached 0.3 nN/atom, while the maximum interlayer distance variation decreased significantly. In contrast, for the other five structures, the maximum interlayer distance variation generally increased as the normal load increased.

Figs. 14(c) and 14(d) showed the friction force and friction coefficient of the six bilayer structures under different normal loads. For Gr/Gr, Sta/Sta, and Sta/GrF, the friction force generally increased with increasing normal load, in agreement with Amontons' law [62]. In contrast, Sta/Gr, StaF/Gr, and StaF/GrF exhibited nonlinear and anomalous fluctuations in friction force as the normal load increased. Under normal loads below 0.4 nN/atom, the Sta/Sta structure showed significantly higher friction force and friction coefficient, while Gr/Gr exhibited lower values compared to Sta/Sta but remained higher than those of the heterostructures, reflecting the correlation with their respective sliding barriers. Once the load surpassed 0.4 nN/atom, load-induced reshaping of the potential energy surface led to a sharp rise in both the friction force and coefficient for Sta/Gr, while StaF/Gr preserved low and nearly constant values. Under loads below 0.2 nN/atom, both StaF/Gr and Sta/GrF achieved ultralow friction; however, at higher loads, only StaF/Gr maintained a friction coefficient below 0.01, demonstrating stable ultralow friction behavior.

To elucidate the intrinsic relationship between potential energy surface (PES) evolution and tribological behavior, we further analyzed the critical load effect. For both Sta/Gr and StaF/Gr, the PES underwent

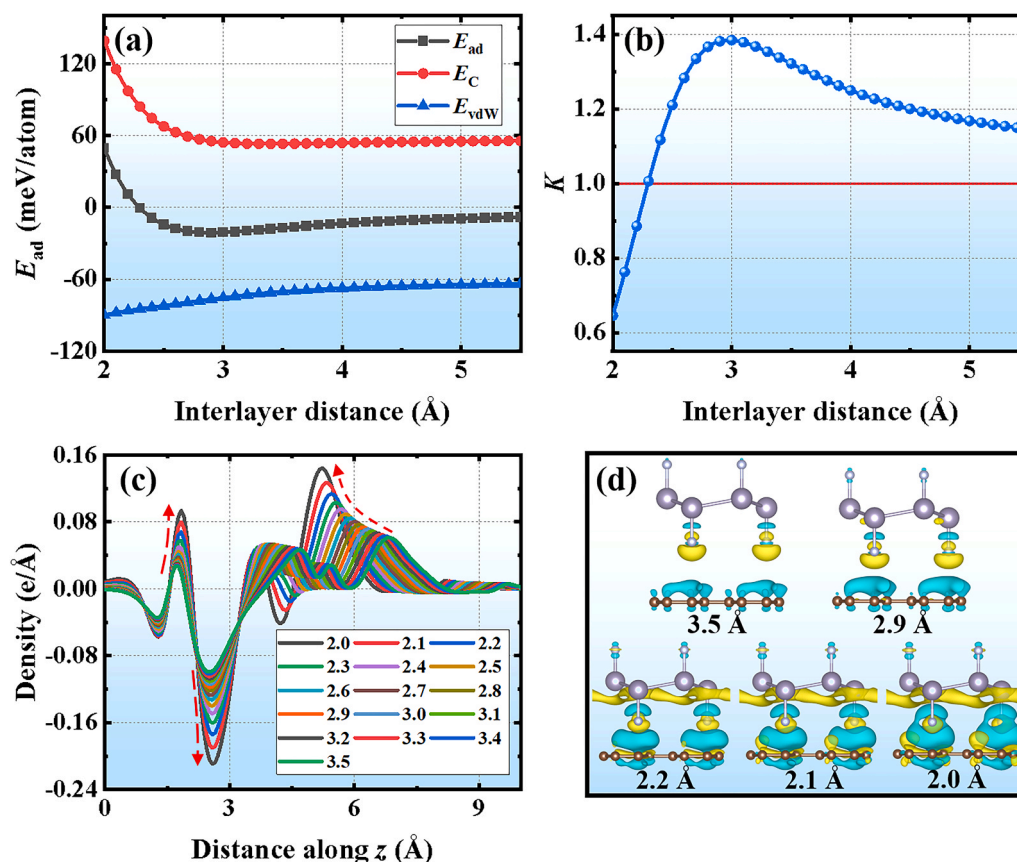


Fig. 15. Loading process of StaF/Gr structure at the Top site: (a) Three types of interlayer interaction energies; (b) Variation of K with interlayer distance; (c) Plane-averaged differential charge density curves; (d) Differential charge density distribution (yellow indicated electron accumulation and blue indicated electron depletion, with a range of $\pm 3.374 \text{ me}/\text{\AA}^3$).

collapse and inversion at a critical load, resulting in extremely low sliding barriers and, consequently, ultralow friction. Specifically, for Sta/Gr, the critical load was 0.3 nN/atom , corresponding to a sliding barrier of 4.73 meV/atom , a friction force of $3.87 \times 10^{-3} \text{ nN}$, and a friction coefficient of 0.0121 . For StaF/Gr, the same critical load of 0.3 nN/atom yielded a much lower sliding barrier of 0.50 meV/atom , a friction force of $3.72 \times 10^{-4} \text{ nN}$, and a friction coefficient of 0.0012 . To further uncover the underlying physical mechanism of load-induced PES collapse and inversion, the StaF/Gr structure was taken as a representative system. As shown in Fig. 15(a), the evolution of adhesion energy (E_{ad}), Coulomb interaction energy (E_C), and van der Waals energy (E_{vdW}) during the loading process provided deeper insight into this phenomenon.

For the Top site of StaF/Gr structure, the value of K reached the maximum of 1.38 at an equilibrium interlayer spacing of approximately $2.9 \text{ \AA}$, where the interlayer interaction was dominated by van der Waals force. As the load was further increased, the interlayer distance decreased and the value of K dropped rapidly. When the interlayer distance became smaller than $2.3 \text{ \AA}$, the interlayer interaction began to be dominated by Coulomb interaction, as shown in Fig. 15(b). The plane-averaged differential charge density curves and differential charge density distributions corresponding to different interlayer distances were presented in Figs. 15(c) and 15(d), respectively. As the interlayer distance decreased, the interlayer charge density gradually increased. The interlayer distance corresponding to the collapse and inversion of the potential energy surface was $2.1 \text{ \AA}$ (0.3 nN/atom). It was evident that a prerequisite for the collapse and inversion of the potential energy surface was that the interlayer interaction entered a regime dominated by Coulomb interaction. To further verify this viewpoint, we analyzed the contributions of van der Waals interaction and

Coulomb interaction during interlayer sliding under different loads.

When the normal load was 0.1 nN/atom , the interlayer interaction was dominated by van der Waals force, as shown in Fig. 16(a). As the load increased to around the critical load of 0.3 nN/atom , the collapse and inversion of the potential energy surface, as well as the competitive evolution between van der Waals and Coulomb interactions, could be observed from Fig. 16(b)–(d). As the load increased from 0.25 nN/atom to 0.35 nN/atom , the contribution of Coulomb interaction gradually increased, while that of van der Waals interaction correspondingly decreased. Their mutual cancellation led to a flattening of the potential energy surface at the critical load, resulting in a significant reduction in the interlayer sliding barrier. Once the load exceeded the critical value, the interlayer interaction became dominated by Coulomb interaction, and the sliding barrier increased again after the inversion of potential energy surface. The underlying physical mechanism of load-induced collapse and inversion of the potential energy surface originated from the competition between interlayer van der Waals interaction and Coulomb interaction.

4. Conclusions

This work demonstrated that constructing heterostructures combined with fluorination provided an effective route to achieve ultralow friction in stanene/graphene systems. Among the six considered configurations, heterostructures showed markedly reduced sliding barriers compared with homostructures, and fluorination further strengthened this advantage, with StaF/Gr exhibiting the best performance, reaching the minimum friction coefficient of 0.0012 and maintaining stability over a broad load range. From the mechanistic perspective, the friction reduction originated from two key factors: fluorination led to a smoother

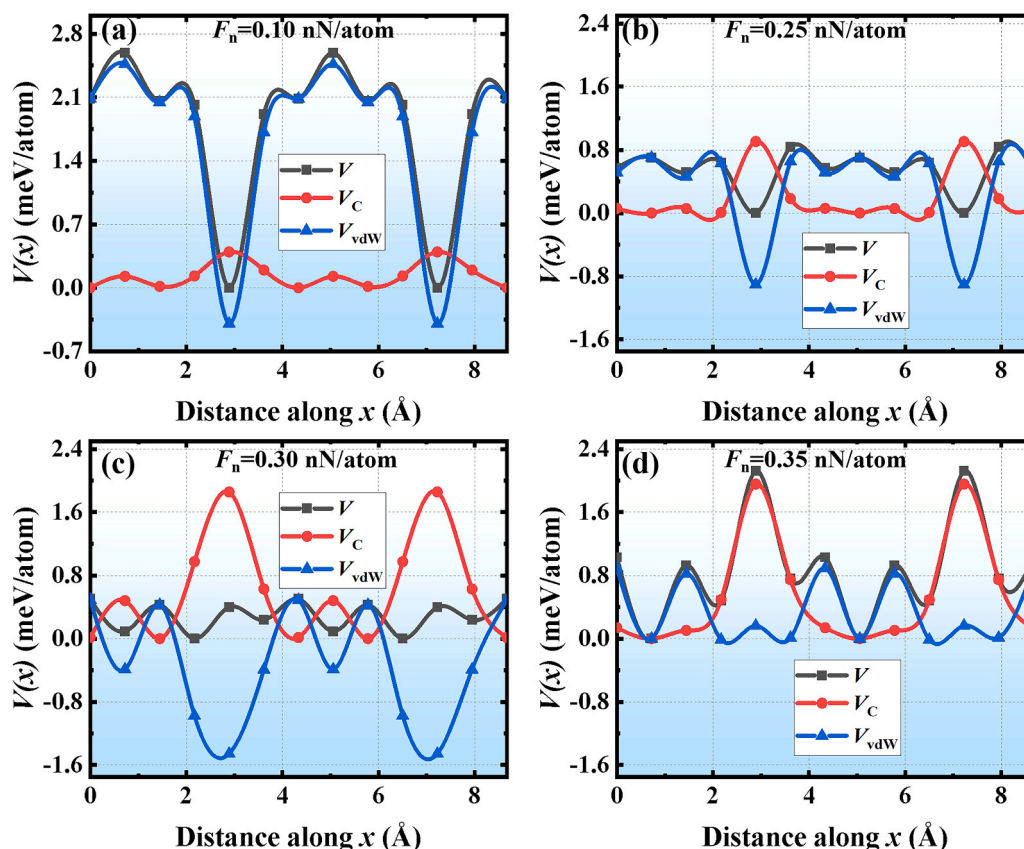


Fig. 16. System energy V , Coulomb interaction V_C and van der Waals interaction V_{vdW} under different loads: (a) $F_n = 0.10$ nN/atom; (b) $F_n = 0.25$ nN/atom; (c) $F_n = 0.30$ nN/atom; (d) $F_n = 0.35$ nN/atom.

potential energy surface and suppressed interfacial charge redistribution, while the load-dependent friction behavior was governed by the competition between interlayer van der Waals and Coulomb interactions, which drove the collapse and reversal of potential energy surface under increasing load. These results clarified the physical origin of ultralow friction in this system and provided a feasible design strategy for next-generation solid lubricants and low-dissipation devices. Nevertheless, the current fabrication techniques for stanene and especially fluorinated stanene remained immature, and further experimental advances were needed to translate these findings into practical applications.

CRediT authorship contribution statement

Gen Chen: Writing – original draft, Software, Methodology, Data curation, Conceptualization. **Rui Li:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **Qingsong Xu:** Methodology, Data curation. **Lei Gao:** Writing – review & editing, Resources, Methodology. **Qing Peng:** Writing – review & editing, Resources.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used DeepSeek in order to correct English grammar. After using this tool/service, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.triboint.2026.112225](https://doi.org/10.1016/j.triboint.2026.112225).

Data Availability

Data will be made available on request.

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