Electro-lubrication in Janus transition metal dichalcogenide bilayers

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Received: 30 July 2021 / Revised: 27 September 2021 / Accepted: 14 October 2021

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Abstract: Lubrication induced by a vertical electric field or bias voltage is typically not applicable to two-dimensional (2D) van der Waals (vdW) crystals. By performing extensive first-principles calculations, we reveal that the interlayer friction and shear resistance of Janus transition metal dichalcogenide (TMD) MoXY ($X/Y = \text{S, Se, or Te, and } X \neq Y$) bilayers under a constant normal force mode can be reduced by applying vertical electric fields. The maximum interlayer sliding energy barriers between AA and AB stacking of bilayers MoSTe , MoSeTe , and MoSSe decrease as the positive electric field increases because of the more significant counteracting effect from the electric field energy and the more significant enhancement in interlayer charge transfer in AA stacking. Meanwhile, the presence of negative electric fields decreases the interlayer friction of bilayer MoSTe , because the electronegativity difference between Te and S atoms reduces the interfacial atom charge differences between AA and AB stacking. These results reveal an electro-lubrication mechanism for the heterogeneous interfaces of 2D Janus TMDs.

Keywords: Janus transition metal dichalcogenide (TMD); electro-lubrication; electric field tuning; first-principles calculations

1 Introduction

To increase the capability and service life of engineering equipments, lubrication for reducing friction and energy dissipation in mechanical devices and components is crucial. Many effective methods, such as designing interfacial or contacting structures, decreasing surface roughness and mechanical loading, and adding solid or liquid lubricant additives, have been developed to control and reduce friction and wear. Previous studies have shown that applying external electric fields can modify the molecular structure and charge transfer at solid–solid interfaces, thereby decreasing the interfacial friction and resistance [1, 2]. Moreover, the distribution or orientation of ions at solid–liquid interfaces can be controlled and changed via electric fields to achieve the desired lubricating

effect [3–7]. Electric-field-mediated lubrication is an attractive and promising route for improving tribological performance.

Two-dimensional (2D) van der Waals (vdW) crystals, including graphene, hexagonal boron nitride (h-BN), and transition metal dichalcogenides (TMDs), exhibit ultra-low friction and superlubricity behaviors, depending on the stacking commensurability [8–13], interface interaction and structure [14–18], mechanical stiffness [18–21], substrate effect, and adhesion [22, 23]. Nevertheless, the friction of 2D vdW crystals in the presence of bias voltages or vertical electric fields is enhanced, and ultra-low friction states cannot be maintained as electric fields result in surface state changes and interlayer charge exchange [24–28]. Lubrication induced by the bias voltage is not typically applicable to 2D vdW crystals. Recently, Janus TMD

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monolayers were successfully synthesized via chemical vapor deposition and thermal selenization methods [29, 30]. The Janus configuration of TMD MXY ($M = \text{Mo or W}$, $X/Y = \text{S, Se, or Te}$, and $X \neq Y$) monolayers breaks the out-of-plane structural symmetry, and results in a vertical dipole moment. Theoretical studies [31–34] further reveal that in addition to their excellent in-plane piezoelectricity, Janus MXY monolayers and multilayers exhibit significant out-of-plane piezoelectric polarization. In multilayer Janus TMDs, their interfacial atoms indicate different electronegativities; hence, the response of their interlayer interactions to the electric field will differ from that of multilayer graphene, h-BN, and TMDs. However, the effect of the vertical electric field on the interlayer friction properties of Janus TMDs has rarely been considered and remains elusive.

In this study, the interlayer friction behaviors of Janus TMD MoXY ($X/Y = \text{S, Se, or Te}$, and $X \neq Y$) bilayers under vertical electric fields and a constant normal force mode were extensively investigated using first-principles calculations. For bilayer MoSTe, the maximum interlayer sliding energy barrier between AA and AB stacking decreases as the positive or negative electric field increases, indicating a reduction in the interlayer friction. The maximum interlayer sliding energy barriers of bilayers MoSeTe and MoSSe decrease under a positive electric field but increase under a negative electric field. The fewer charge changes between AA and AB stacking under positive electric fields and the different electronegativities of interfacial atoms result in a more significant counteracting effect from the electric field energy to the maximum interlayer sliding energy barrier, thereby reducing the interlayer friction of Janus TMD bilayers. These results can provide insights into the lubricating mechanism and performance of Janus TMD bilayers in the presence of vertical electric fields.

2 Model and methods

Figure 1 shows the models of 2H MoSTe, MoSeTe, and MoSSe bilayers with initial AB stacking in rhombus unit cells, where each MoSTe, MoSeTe, and MoSSe monolayers contain one Mo and two different chalcogen atoms. A vacuum region exceeding 25 Å perpendicular to the plane was applied. For comparison, a 2H MoS₂ bilayer with an initial AB

stacking was considered in our study. All computations were performed within the framework of density functional theory (DFT), as implemented in the Fritz Haber Institute *ab initio* material simulations (FHI-aims) code with “tight” computational settings [35], in which the Perdew–Burke–Ernzerhof (PBE) [36] exchange–correlation functional was employed. The effect of vdW interactions was considered using a many-body dispersion (MBD) vdW model [37, 38]. A k -point grid measuring $15 \times 15 \times 1$ was used throughout the study. First, the entire system was relaxed using the PBE + MBD method until the force on each atom was less than 0.01 eV/Å. The optimized lattice constants of MoSTe, MoSeTe, MoSSe, and MoS₂ unit cells were 3.329, 3.398, 3.215, and 3.147 Å, respectively. To simulate interlayer sliding, the entire a_1 – a_2 planes of the unit cells were equally partitioned into 81 positions (Fig. S1 in the Electronic Supplementary Material (ESM)), where the nearest positions were separated by 0.37, 0.378, 0.357, and 0.35 Å for MoSTe, MoSeTe, MoSSe, and MoS₂, respectively. The top monolayer was shifted both transversely with respect to the bottom monolayer and relative to the positions partitioned; subsequently, the chalcogen atoms at the top and bottom surfaces were fixed. Next, an electric field [35] was applied in the direction perpendicular to the a_1 – a_2 plane. The interlayer distances d of the TMD bilayers were modified by changing the z -direction coordinates of the atoms in the top layers. Next, those systems were relaxed again using the PBE + MBD method, and the normal forces at different d and shifted positions were calculated by summing the z -direction forces of all atoms in one monolayer. By adjusting the d between the two monolayers, the normal forces at the 81 shifted positions were maintained at approximately the same value. Hence, an interlayer sliding simulation under a constant normal force mode was realized for the considered TMD bilayers. For the case of a zero normal force, the total z -direction forces of all atoms in one monolayer at different shifted positions were less than 0.01 eV/Å (Fig. S2 in the ESM). In other cases, the deviations between the desired and calculated normal forces at different shifted positions were less than 1% (Fig. S3 in the ESM). Based on the maximum and minimum normal forces in the errors, the corresponding deviations in the energies and d were obtained and regarded as errors in the energies and d , respectively.

Fig. 1 Atomic structures of bilayers: (a) MoSTe, (b) MoSeTe, and (c) MoSSe with AB stacking, and corresponding maximum sliding energy barriers $\Delta E_{\max}$ and shear strengths $\tau_{\max}$ (right pictures) with vertical electric field under normal pressures of 0, 1, 2, and 3 GPa, respectively. The purple, yellow, red, and cyan balls represent Mo, S, Te, and Se atoms, respectively. The blue arrow in (a) represents positive direction of vertical electric field, and the black arrow in (a) indicates interlayer sliding of top monolayer with respect to bottom monolayer.

After relaxation, the total energies of the bilayers at different shifted positions were calculated using the PBE + MBD method, and the corresponding potential energy surface (PES) for interlayer sliding under a normal pressure P_n ($P_n = F_n/A$, where F_n is the normal force and A is the area of the unit cell) was constructed based on the differences in energy $\Delta E = E - E_{\min}$, where E is the total energy of the system and $E_{\min}$ is the lowest total energy (Figs. S4 and S5 in the ESM).

3 Results and discussion

Based on the PESs obtained, it was discovered that under a constant normal force mode, AA and AB stacking yielded the highest and lowest energies, respectively, in the presence of a vertical electric field for all the MoSTe, MoSeTe, MoSSe, and MoS₂ bilayers. We calculated the maximum sliding energy barrier $\Delta E_{\max}$ using the formula $\Delta E_{\max} = E_{AA} - E_{AB}$, and calculated the maximum interlayer resistance force $F_R^{\max}$ and shear strength $\tau_{\max}$ [39] using the formulas $F_R^{\max} = \Delta E_{\max} / \Delta r$ and $\tau_{\max} = F_R^{\max} / A$, respectively, where Δr is the displacement along the pathway

from the lowest to the highest energy stacking state. The interlayer friction force of the TMD bilayer was proportional to $\Delta E_{\max}$ [40]. As shown in Fig. 1(a), the $\Delta E_{\max}$ and $\tau_{\max}$ of bilayer MoSTe decreased as the electric field strength increased, regardless of the electric field direction. For bilayers MoSeTe and MoSSe, their $\Delta E_{\max}$ and $\tau_{\max}$ decreased under a positive electric field but increased under a negative electric field. By contrast, $\Delta E_{\max}$ and $\tau_{\max}$ of bilayer MoS₂ increased under both positive and negative electric fields, as shown in Fig. S6 in the ESM. In contrast to the increase of the interlayer friction in bilayer MoS₂ with a homogeneous interface, the decrease of $\Delta E_{\max}$ and $\tau_{\max}$ in the Janus TMD bilayers with heterogeneous interfaces indicates that the vertical electric field can reduce the interlayer friction, and serves as electro-lubrication in the Janus TMD bilayers. Meanwhile, the interlayer friction of the Janus TMD bilayers is associated closely with interlayer adhesion or binding interactions. We calculated the interlayer binding energy difference ΔE_b between AA and AB stacking. As shown in Fig. S7(a) in the ESM, the variation trends of ΔE_b with the electric field were similar to that of $\Delta E_{\max}$ for the three Janus TMD bilayers, further demonstrating the reduction in the interlayer sliding resistance under vertical electric fields.

In our DFT calculations, the total energy is calculated as $E_{\text{total}}[n] = E_K[n] + E_{\text{ES}}[n] + E_{\text{XC}}[n] + E_{\text{vdW}}$, where $n(r)$ is the electron density, E_K is the kinetic energy of electrons, E_{ES} is the electrostatic energy, E_{XC} is the exchange-correlation energy, and E_{vdW} is the vdW energy. If an external homogeneous electric field $E = (e_x, e_y, e_z)$ with strength e_γ aligned along the different Cartesian axes, γ is applied to an isolated system, and then an additional electric field energy

$E_{\text{EF}}[n] = -\sum_\gamma \int e_\gamma r_\gamma n(r) dr$ contributes to the total energy [41]. To understand the effect of the electric field on the interlayer interactions of Janus TMD bilayers, the electric field energy E_{EF} of the systems at different shifted positions were calculated. Here, the system energy excluding the electric field energy is defined by $E_S = E_{\text{total}} - E_{\text{EF}}$. The differences in E_{EF} and E_S between AA and AB stacking were calculated using $\Delta E_{\text{EF}} = E_{\text{EF}}^{\text{AA}} - E_{\text{EF}}^{\text{AB}}$ and $\Delta E_S = E_S^{\text{AA}} - E_S^{\text{AB}}$, respectively. Subsequently, $\Delta E_{\max}$, ΔE_{EF} , and ΔE_S are correlated as $\Delta E_{\max} = \Delta E_{\text{EF}} + \Delta E_S$. As shown in Fig. 2, ΔE_{EF} was

Fig. 2 Differences in electric field energy ΔE_{EF} and system energy without electric field energy ΔE_{S} between AA and AB stacking with electric field for bilayers MoSTe, MoSeTe, and MoSSe under normal pressures of (a) 0 GPa and (b) 2 GPa. Error bars are included to account for errors in normal forces.

positive under negative electric fields and negative under positive electric fields for bilayers MoSTe, MoSeTe, and MoSSe. ΔE_{EF} decreased as the positive electric field increased, but increased as the negative electric field increased. By contrast, ΔE_{S} increased in a positive electric field but decreased in a negative electric field. Under positive electric fields, the counteracting effect between ΔE_{EF} and ΔE_{S} as well as the more significant contribution of ΔE_{EF} to ΔE_{max} resulted in a reduction in ΔE_{max} . For bilayer MoSTe under negative electric fields, the decrease in ΔE_{max} with the electric field was attributed to the higher decrease in ΔE_{S} compared with the increase in ΔE_{EF} . In contrast to the Janus TMD bilayers, the ΔE_{EF} of bilayer MoS₂ increased, whereas its ΔE_{S} decreased under both positive and negative electric fields, as shown in Fig. S8 in the ESM. The effect of positive electric fields on the interlayer friction of the Janus TMD bilayers differed completely from that of bilayer MoS₂.

To better elucidate the roles of electron kinetic energy, exchange-correlation, vdW, and electrostatic interactions in the interlayer friction, we separately calculated the energy differences in exchange-correlation energy ΔE_{XC} , electron kinetic energy ΔE_{K} , electrostatic energy ΔE_{ES} , and vdW energy ΔE_{vdW} between AA and AB stacking using the following formulas: $\Delta E_{\text{XC}} = E_{\text{XC}}^{\text{AA}} - E_{\text{XC}}^{\text{AB}}$, $\Delta E_{\text{K}} = E_{\text{K}}^{\text{AA}} - E_{\text{K}}^{\text{AB}}$, $\Delta E_{\text{ES}} = E_{\text{ES}}^{\text{AA}} - E_{\text{ES}}^{\text{AB}}$, and $\Delta E_{\text{vdW}} = E_{\text{vdW}}^{\text{AA}} - E_{\text{vdW}}^{\text{AB}}$, respectively. Addi-

tionally, we derived $\Delta E_{\text{S}} = \Delta E_{\text{XC}} + \Delta E_{\text{K}} + \Delta E_{\text{ES}} + \Delta E_{\text{vdW}}$. As shown in Fig. 3 and Figs. S9 and S10 in the ESM, ΔE_{ES} for bilayers MoSTe, MoSeTe, and MoSSe increased under positive electric fields and decreased under negative electric fields. Meanwhile, ΔE_{K} decreased under positive electric fields and increased under negative electric fields. Compared with the changes in ΔE_{ES} and ΔE_{K} , the variations in ΔE_{vdW} and ΔE_{XC} were relatively small. It was evident that ΔE_{ES} and ΔE_{K} provide important but opposite contributions to ΔE_{S} . A lower electron kinetic energy barrier implies that the electrons propagate closer to the nuclei when the bilayer slides to AA stacking. The vertical electric fields impose a slight effect on the vdW and exchange-correlation energy barriers. Therefore, the variations in ΔE_{S} shown in Fig. 2 are primarily due to the changes in the electrostatic energy barriers ΔE_{ES} and the electron kinetic energy barriers ΔE_{K} .

Owing to the heterogeneous interfaces of Janus TMD bilayers and the different electronegativities of interfacial atoms, charge changes in interfacial atoms under electric fields must be analyzed to understand the electro-lubrication of Janus TMD bilayers. Figure 4 shows the differences in the charge deviations of interfacial atoms $\Delta C^{\text{AA}} - \Delta C^{\text{AB}}$ between AA and AB stacking in the presence of electric fields, where ΔC^{AA} and ΔC^{AB} are the charge deviations of interfacial atoms [42] at AA and AB stacking with respect to their single-atom states, respectively. For bilayer MoSTe, the $\Delta C_{\text{Te}}^{\text{AA}} - \Delta C_{\text{Te}}^{\text{AB}}$ of interfacial Te atoms decreased under both positive and negative electric fields.

Fig. 3 Differences in (a) vdW energy, ΔE_{vdW} , (b) exchange-correlation energy, ΔE_{XC} , (c) electrostatic energy, ΔE_{ES} , and (d) kinetic energy, ΔE_{K} , between AA and AB stacking with electric field for bilayer MoSTe under normal pressures of 0 and 2 GPa. Error bars are provided to account for errors in normal forces.

Fig. 4 Differences in charge deviations of interfacial atoms between AA and AB stacking with electric field for bilayers (a, b) MoSTe and (c, d) MoSeTe under normal pressures of 0 and 2 GPa.

Similarly, the absolute values of $\Delta C_s^{AA} - \Delta C_s^{AB}$ of interfacial S atoms decreased under both the positive and negative electric fields. The decrease in the absolute values of $\Delta C^{AA} - \Delta C^{AB}$ in the presence of electric fields indicates that the charge differences in the interfacial atoms between AA and AB stacking decrease, inducing a smaller energy change when the bilayer slides from AB to AA stacking. However, the absolute values of $\Delta C_{Te}^{AA} - \Delta C_{Te}^{AB}$ and $\Delta C_{Se}^{AA} - \Delta C_{Se}^{AB}$ of interfacial Te and Se atoms for bilayer MoSeTe decreased under positive electric fields but increased under negative electric fields, and bilayer MoSSe exhibited similar trends (Fig. 4(b) and Fig. S12 in the ESM). The variations in $\Delta C^{AA} - \Delta C^{AB}$ of the interfacial atoms of the Janus TMD bilayers between AA and AB stacking were consistent with the interlayer sliding energy barriers ΔE_{max} shown in Fig. 1.

Furthermore, the charge density differences $\Delta\rho$ in the presence and absence of electric fields for AB and AA stacking were calculated as follows: $\Delta\rho = \rho_{bilayer}^{elec} - \rho_{bilayer}^{noelec}$, where $\rho_{bilayer}^{elec}$ is the charge density of the bilayer under an electric field and $\rho_{bilayer}^{noelec}$ is the charge density without an electric field. Among the S, Se, and Te atoms, the electronegativity of the S atom was the highest, whereas that of the Te atom was the weakest. At the interface of the bilayer MoSTe, charge transfer from Te to S atoms occurred for both AA and AB stacking. The applied positive electric field facilitated and enhanced the charge transfer from Te to S atoms, as shown in Fig. 5(a). Under positive electric fields, enhancement in charge transfer from Te to Se

Fig. 5 2D projections of charge density differences $\Delta\rho$ (in unit of $e/\text{\AA}^3$) in the presence and absence of electric fields of bilayers: (a) MoSTe, (b) MoSeTe, and (c) MoSSe for AB stacking (top) and AA stacking (bottom) under normal pressure of 0 GPa. Ball denotation is the same as that in Fig. 1.

atoms and Se to S atoms was indicated in bilayers MoSeTe and MoSSe, as shown in Figs. 5(b) and 5(c). This facilitating effect of charge transfer induced by positive electric fields was more significant for AA stacking, which resulted in a relative decrease in the total energy of AA stacking with respect to that of AB stacking. The more prominent charge transfer of AA stacking was consistent with the decrease in the absolute value of $\Delta C^{AA} - \Delta C^{AB}$ of the interfacial atoms, as shown in Fig. 3. However, the negative electric fields induced charge transfer from Se to Te atoms and S to Se atoms, which was opposite to the charge transfer caused by the electronegativity of the interfacial atoms. The interlayer charge transfer and exchange of bilayers MoSeTe and MoSSe under negative electric fields were more prominent for AA stacking; this resulted in a relative increase in the total energy of AA stacking with respect to that of AB stacking. For bilayer MoSTe, no interlayer charge transfer and exchange occurred under a negative electric field because of the significant electronegativity difference between Te and S atoms, as shown in Fig. 5(a), which reduced the interlayer resistance when the bilayer slid from AB to AA stacking. Under a normal pressure of 2 GPa, similar charge density differences in the presence and absence of electric fields at AB and AA stacking were observed, as shown in Fig. S13 in the ESM. Moreover, we investigated the interlayer friction of Janus TMD WXY ($X/Y = S, Se, \text{ or } Te, \text{ and } X \neq Y$) bilayers under vertical electric fields using the same method.

Similar to Janus TMD MoXY bilayers, the maximum sliding energy barriers of the WXY bilayers decreased as the positive electric field increased, as shown in Fig. S14 in the ESM, and the negative electric field reduced the interlayer friction of the WSTe bilayer.

4 Conclusions

In summary, by performing comprehensive DFT calculations, we demonstrate that the interlayer friction and shear resistance in Janus TMD bilayers under a constant normal force mode can be reduced by applying vertical electric fields. Under positive electric fields, bilayers MoSTe, MoSeTe, and MoSSe exhibited interlayer friction reduction because of the more prominent counteracting effect from the electric field energy and the more significant enhancement in interlayer charge transfer for AA stacking induced by electric fields. The interlayer friction of bilayer MoSTe was reduced by negative electric fields because the significant electronegativity difference between Te and S atoms decreased the charge differences in the interfacial atoms between AA and AB stacking. These results revealed an electro-lubrication mechanism for the heterogeneous interfaces of 2D Janus TMDs and can provide insights into the friction behaviors of 2D Janus TMDs under external electric fields.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Nos. 11972186, 11890674, and 51921003), the Fundamental Research Funds for the Central Universities (No. NE2019001) of China, and the Project Funded by the Priority Academic Program Development of Jiangsu Higher Education Institutions.

Electronic Supplementary Material Supplementary material is available in the online version of this article at <https://doi.org/10.1007/s40544-021-0562-9>.

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