We apply the state-of-the-art many-body dispersion (MBD) method to study the anchoring behavior in lithium-sulfur (Li–S) batteries, which is closely related to the notorious “shuttle effect”. Based on the experimental results of metal sulfides (FeS and SnS₂), we find that the MBD method gives a more accurate prediction of anchoring mechanism compared with other van der Waals (vdW) inclusive methods. We systematically investigate the anchoring mechanism of two prototypal anchoring materials—\(\text{Ti}_2\text{CF}_2\) and doped-graphene systems. The many-body effect is found to play an important role on the reduction of anchoring behaviors, especially when the systems have large polarization and the vdW interactions predominate the anchoring behavior. Our work deepens the fundamental understanding of the anchoring mechanism, and provides a more accurate criterion for screening anchoring materials for suppressing the shuttle effect.

**RESULTS**

Performance of FeS and SnS₂ for trapping Li₂S₆

Zhou et al. [28] have experimentally investigated the anchoring behavior of metal sulfides for trapping Li₂S₆ by comparative tests (different metal sulfides with equivalent total surface area were added into originally yellow-colored 1,2-dimethoxyethane/1,3-dioxolane (DME/DOL) solution with Li₂S₆). According to the discoloration of solution, they found that the metal sulfides have different adsorption capability for Li₂S₆ and several of them completely suppressed the shuttle effect. The competition between anchoring materials and electrolytes for trapping soluble LiPSs has been concerned to evaluate anchoring materials [29,30]. However, in their density functional theory (DFT) calculation the anchoring factor \(\Delta E (\Delta E = E_{\text{AM}} - E_{\text{so}})\) was not considered. Here \(E_{\text{AM}}\) is the binding energies of LiPSs absorbed on anchoring materials, and \(E_{\text{so}}\) denotes the binding energies of LiPSs with electrolyte molecules. The positive \(\Delta E\) indicates that the interaction between polysulphides and anchoring materials is stronger than polysulphides with electrolyte molecules; the negative \(\Delta E\) means that polysulphides tend to dissolve into electrolyte rather than absorb on anchoring materials.

To compare theoretical prediction from different vdW methods, we apply a criterion \(\Delta E\) to evaluate the performance of FeS and SnS₂ for trapping Li₂S₆ and compare with experimental observation. [28] The optimized configurations of Li₂S₆ absorbed on FeS and SnS₂, and its binding with DME/DOL molecule are shown in Supplementary Fig. 1. Recently, Brandenburg et al. [31] reported that the MBD method performs better than most other approaches,
such as DMC and CCSD(T), for the fundamental system. Meanwhile, it has been demonstrated that it is essential to include the many-body effect in adsorption systems for the evaluation of binding energies.23–25 In this context, here we apply the MBD method to predict the interaction between Li$_2$S$_6$ and FeS/SnS$_2$. From the results of PBE + MBD method in Table 1, ΔE (FeS-DME) and ΔE (SnS$_2$-DME) are negative values (−0.10 eV and −0.07 eV), ΔE (FeS-DOL) and ΔE (SnS$_2$-DOL) are positive values (0.02 eV and 0.05 eV). We predict that a part of Li$_2$S$_6$ species will be anchored on the surface of FeS and SnS$_2$ and the rest of Li$_2$S$_6$ still binds with DME molecules. In other words, the yellow DME/DOL solution with Li$_2$S$_6$ just has an incompletely discoloration when FeS and SnS$_2$ are added as anchoring materials. This conclusion is fully compatible with the experimental observation.

According to the above analysis, the MBD method is more reasonable conclusions of the anchoring materials for suppression of the shuttle effect.26,30,35 Therefore, to attain an in-depth understanding of the many-body effect on adsorption systems, we selected Ti$_2$CF$_2$ and NG as platforms and investigated their intrinsic different anchoring mechanisms. Ti$_2$C-based materials are the lightest Mxenes and atom-multilayered 2D materials, NG is a typical heteroatom-doped anchoring material with one-atomic-layer structure. As for Ti$_2$CF$_2$, we note that the F-termination has different adsorption sites on Ti$_2$C surface36,37 and the HCP site is chosen in our work because of the stronger binding strength of adsorbed species.24,38 Nevertheless, the major component causing the shuttle effect is solvent molecules in electrolyte, which competes with anchoring materials and introduces solution of high-order LiPSs. As such, in the present work, and the same in previous work,29 we used DME and DOL molecules to explain the interaction between LiPSs and electrolyte. We considered that one LiPSs cluster interacts with one or two DME (DOL) molecules (Supplementary Fig. 2). From Supplementary Table 2 we find that the $E_{rb}$ are very similar whatever soluble LiPSs binding with one or two DME (DOL) molecules from the vdW$^\text{surf}$ and MBD methods. For systematically examining the $E_{mb}$ between LiPSs and Ti$_2$CF$_2$/NG, various initial adsorption configurations of Li$_2$S$_n$ ($n = 1, 2, 4, 6, 8$) clusters are considered to find the optimized structures. The most stable structures with the lowest energy are shown in Fig. 1a. Comparing with Li$_2$S$_6$ and Li$_2$S$_8$, Li$_2$S, Li$_2$S$_2$, and Li$_2$S$_4$ prefer to adsorb vertically on Ti$_2$CF$_2$, with two Li atoms binding with NN, Fi, Si, and Li atoms, respectively.

|       | FeS       | SnS$_2$  | DME | DOL | ΔE (FeS-DME) | ΔE (FeS-DOL) | ΔE (SnS$_2$-DME) | ΔE (SnS$_2$-DOL) |
|-------|-----------|----------|-----|-----|--------------|--------------|------------------|------------------|
| PBE   | 0.84      | 0.87     | 0.94| 0.82| −0.10        | 0.02         | −0.07            | 0.05             |
| MBD   | 1.31      | 1.06     | 0.83| 0.77| 0.48         | 0.54         | 0.23             | 0.29             |
| vdw$^\text{surf}$ | 0.88      | 0.79     | 0.94| 0.84| −0.06        | 0.04         | −0.15            | −0.05            |
| PBE + D2 | 1.02 | 0.96 | 0.84 | 0.78 | 0.18 | 0.24 | 0.12 | 0.18 |
| PBE + D3 | 1.37 | 1.27 | 0.94 | 0.91 | 0.43 | 0.46 | 0.33 | 0.36 |
| vdW-DF2 | 1.02 | 0.94 | 0.83 | 0.74 | 0.19 | 0.28 | 0.11 | 0.20 |
| optB86b-vdW | 1.02 | 0.94 | 0.83 | 0.74 | 0.19 | 0.28 | 0.11 | 0.20 |

Figure 2a shows that the PBE + MBD method reduces the $E_{mb}^{b}$ over 20% compared to the PBE + vdw$^\text{surf}$ method at high-order lithiation stages for Ti$_2$CF$_2$ systems. In contrast, the binding energies for the NG systems from the two methods are almost identical (Fig. 2b). To assess the contribution of MBD to the $E_{mb}^{b}$, we determine the ratio of MBD contribution ($R_{mbd}$) as follows,

$$R_{mbd} = (E_{mb} - E_{mbd}^b)/E_{mb}$$

### Table 1. The binding energies (eV) between Li$_2$S$_6$ and anchoring materials (FeS and SnS$_2$) as well as electrolyte molecules (DME and DOL) from several DFT methods, the anchoring factor ΔE are also listed.

| Li$_2$S$_6$ | PBE + MBD | PBE + vdw$^\text{surf}$ | PBE + D2 | PBE + D3 | vdW-DF2 | optB86b-vdW |
|------------|-----------|-------------------------|----------|----------|---------|-------------|
| FeS        | 0.84      | 1.31                    | 0.88     | 1.02     | 1.37    | 1.02        |
| SnS$_2$    | 0.87      | 1.06                    | 0.79     | 0.96     | 1.27    | 0.94        |
| DME        | 0.94      | 0.83                    | 0.94     | 0.84     | 0.94    | 0.83        |
| DOL        | 0.82      | 0.77                    | 0.84     | 0.78     | 0.91    | 0.74        |
| ΔE (FeS-DME) | −0.10   | 0.48                    | −0.06    | 0.18     | 0.43    | 0.19        |
| ΔE (FeS-DOL) | 0.02    | 0.54                    | 0.04     | 0.24     | 0.46    | 0.28        |
| ΔE (SnS$_2$-DME) | −0.07 | 0.23                    | −0.15    | 0.12     | 0.33    | 0.11        |
| ΔE (SnS$_2$-DOL) | 0.05 | 0.29                    | −0.05    | 0.18     | 0.36    | 0.20        |
The magnitudes of the many-body effect and vdW interaction in Ti$_2$CF$_2$ and NG systems

| Ti$_2$CF$_2$ | PBE + vdW$^{surf}$ | PBE + MBD | $R_{MBD}$ | $R_{vdW}$ | $\Delta E_{MBD}$ | NG | PBE + vdW$^{surf}$ | PBE + MBD | $R_{MBD}$ | $R_{vdW}$ | $\Delta E_{MBD}$ |
|------------|---------------------|------------|---------|---------|----------------|----|---------------------|------------|---------|---------|----------------|
| Li$_2$S    | 2.36                | 2.02       | 16.8    | 53.5    | -               |    | 2.76                | 2.80       | 1.4     | 17.9    | -               |
| Li$_2$S$_2$| 2.14                | 1.86       | 15.1    | 59.1    | -               |    | 2.85                | 2.81       | 1.4     | 23.1    | -               |
| Li$_2$S$_4$| 1.61                | 1.24       | 29.8    | 99.2    | 0.34            |    | 2.33                | 2.33       | 0.0     | 34.8    | 1.43            |
| Li$_2$S$_6$| 1.28                | 0.96       | 33.3    | 110.4   | 0.02            |    | 2.37                | 2.34       | 1.3     | 41.9    | 1.40            |
| Li$_2$S$_8$| 1.51                | 1.20       | 25.8    | 105.0   | 0.24            |    | 2.63                | 2.65       | 0.8     | 44.9    | 1.69            |

Summary of the binding energies, ratio for the many-body effect and vdW interaction in Ti$_2$CF$_2$ and NG systems

$R_{MBD}$ (%) and $R_{vdW}$ (%) is the ratio for the many-body effect and vdW interaction of binding energies. $\Delta E_{MBD}$ = $E_{AM} - E_{PBE}$ is the anchoring factor of high-order LiPSs from the PBE + MBD method.

$E_{PBE}^{vdW}$ and $E_{MBD}^{vdW}$ denote the binding energies of Ti$_2$CF$_2$ (NG) from the PBE + vdW$^{surf}$ and PBE + MBD methods, respectively. The magnitudes of $R_{MBD}$ for LiPSs absorbed on Ti$_2$CF$_2$ and NG are shown in Fig. 2c, d. From Table 2, when Ti$_2$CF$_2$ are selected as anchoring materials, we find that $R_{MBD}$ varies from 16.8% to 33.3% with the delithiation of LiPSs. The many-body effect affects Li$_2$S$_n$-Ti$_2$CF$_2$ system largely, which has weakened the binding strength by 33.3% and may lead to the dissolution of Li$_2$S$_6$ due to the small $\Delta E$ (0.02 eV). While for the NG system, we find that the $R_{MBD}$ (range from 0 to 1.4%) is slight and the many-body effect could be ignored.

To attain an in-depth understanding why the MBD method reduces the binding strength of LiPSs with anchoring materials, we divide the $E_{AM}$ into two aspects: the vdW part corresponds to the physical interaction, and the PBE part (termed as $E_{PBE}^{vdW}$) corresponds to the chemical interaction using pairwise-based method vdW$^{surf}$, because the MBD effect mainly contributes to the part of physical interaction. To clarify how these two aspects affect the anchoring behavior, we define the ratio of the vdW interaction ($R_{vdW}$) as follows,

$$R_{vdW} = \frac{(E_{PBE}^{vdW})}{(E_{PBE}^{vdW} - E_{MBD}^{vdW})}$$

In Eq. (2), $E_{PBE}^{vdW}$ from the pairwise PBE + vdW$^{surf}$ method. The ratio of vdW contribution to $E_{PBE}^{vdW}$ for Ti$_2$CF$_2$ systems is shown in Fig. 2c, the vdW interaction shows different weights towards different lithiation stages. During the delithiation from Li$_2$S to Li$_2$S$_8$, the Li-F bond length increases from 1.86 to 2.01 Å, suggesting that the chemical interaction is gradually weakened. The bond length is 1.86 and 1.88 Å for Li$_2$S and Li$_2$S$_2$ absorbed on Ti$_2$CF$_2$ (within the distances of covalent bonds), and the $R_{vdW}$ is 53% and 59%, respectively. This suggests that both chemical interaction and vdW interactions play important roles in these two adsorption systems. However, the physical interaction dominates the $E_{AM}$ of high-order Li$_2$S$_n$ species (n = 4, 6, 8) absorbed on Ti$_2$CF$_2$ (the $R_{vdW}$ nearly 100%). In contrast, although the $R_{vdW}$ for the NG systems increases with the increasing size of LiPSs, the $R_{vdW}$ of NG systems (ranges from 18% to 45%) is smaller than those of Ti$_2$CF$_2$ systems especially for high-order LiPSs, so the chemical interaction (the bond length of Li-N ranges from 1.86 Å to 1.90 Å) dominates the whole process of lithiation (Fig. 2d).

Static polarizability of adsorption systems and charge transfer Comparing with pairwise vdW-correction methods, the MBD method computes the correlation energy of long-range electrostatic screening through the coupled harmonic oscillator model Hamiltonian, and considers dipolar vdW interactions to all orders in perturbation theory. The reduction of $E_{AM}$ from the PBE + MBD method must come from the collective inclusion of the long-range electrostatic screening. Polarizability is central to the description of the long-range electron correlation, which indicates the willingness of a material to respond under the influence of a perturbation of the electric field. It is known that five atomic layers of Ti$_2$CF$_2$ are stacked along the c-axis direction, middle Ti atoms experience the dynamic electric field created by the upper and lower atoms, which gives rise to polarization effects. To provide a quantitative description of the polarizability, we define the changes in static polarizability of the adsorption systems $\Delta \alpha$ by

$$\Delta \alpha = \Delta \alpha_{total} - \Delta \alpha_{AM} - \Delta \alpha_{LiPS}$$

where $\Delta \alpha_{total}$, $\Delta \alpha_{AM}$ and $\Delta \alpha_{LiPS}$ represent the screened static polarizabilities of the adsorption systems, the anchoring materials and the free-standing LiPSs, respectively. Considering the similar polarizabilities along x and y coordinates, we present the $\Delta \alpha$ along x and z directions, termed as $\Delta \alpha_x$ and $\Delta \alpha_z$, which are parallel and perpendicular to the surface of 2D anchoring materials, respectively. The calculated $\Delta \alpha_x$ and $\Delta \alpha_z$ are listed in Table 3. We find that for Ti$_2$CF$_2$ systems, contrary to the magnitude of $\Delta \alpha_x$ that varies slightly, the magnitudes of $\Delta \alpha_z$ are very different from the delithiation of LiPSs. We find that $\Delta \alpha_z$ are positive for Ti$_2$CF$_2$ systems, which means that the adsorption of LiPSs increases the $\Delta \alpha_z$ of the systems. However, the values of $\Delta \alpha_z$ in N-doped graphene adsorption systems are negative, indicating that the $\Delta \alpha_z$ are decreased after LiPSs adsorbed on N-doped graphene.

We notice that the magnitudes of $\Delta \alpha_z$ of Li$_2$S$_6$ and Li$_2$S$_8$ absorbed on Ti$_2$CF$_2$ decrease to 10 bohr$^3$. The decreasing values of $\Delta \alpha_z$ suggest the weakening of the polarization along...
much larger than that of Li$_2$S$_6$ and Li$_2$S$_8$, consistent with the electrons directly to the redox reaction of the anchored LiPSs. To

Meanwhile, from the density of states (DOS) of NG and Ti$_2$CF$_2$ optimized adsorption structures. Figure 2a shows that the Li$_2$S, transform to in NG adsorption configuration, along with a charge transfer of 0.75 $\text{e}$ and Li$_2$S$_8$ and adjacent F atoms in Ti$_2$CF$_2$ adsorption configurations. Figure 3 displays the charge transfers of S/Li atoms and adjacent N atoms in NG adsorption configurations.

perpendicular direction. The characteristics of anisotropic polarizability can be simply estimated by atomic polarizability matrix, which exhibits both spatial distributions and orientations of the polarizability in LiPSs cluster. For Li$_2$S$_6$ adsorbed on Ti$_2$CF$_2$ in Supplementary Fig. 5, the polarizability matrices show different anisotropic characteristics and the xy-orientational polarizability is much larger than that of Li$_2$S$_6$ and Li$_2$S$_8$, consistent with the optimized adsorption structures. Figure 2a shows that the Li$_2$S, Li$_2$S$_2$, and Li$_2$S$_6$ species "stand" on the surface with two Li atoms parallel to the surface of Ti$_2$CF$_2$, along with a charge transfer of 0.73–1.08 e. For Li$_2$S$_6$ and Li$_2$S$_8$, however, the configurations transform to "lying-in-plane" configuration, with only one Li atom binding with Ti$_2$CF$_2$, and a decreased charge transfer (0.42 e for Li$_2$S$_6$ and 0.58 e for Li$_2$S$_8$).

In light of the charge distribution analysis$^{41}$ shown in Fig. 3, we find that all F atoms in the F-terminated surface have a negative charge of 0.75 e. As for NG, N atoms obtain a large charge of 1.2 e, but other C atoms are nearly electroneutral. Since the vdW forces arise from the electrostatic interactions between the constantly fluctuating electron clouds, the spontaneous polarization in Ti$_2$CF$_2$ make the polarizability sensitive to electron exchange. The above analysis shows that reduction of electron transfer is probably the major reason that causes the sharply reduction of the $\Delta\alpha_{\parallel}$. Meanwhile, from the density of states (DOS) of NG and Ti$_2$CF$_2$ (Supplementary Fig. 6) we find that they maintained its metallic properties after adsorption of Li$_2$S$_6$, implying that they can supply electrons directly to the redox reaction of the anchored LiPSs. To further understand the many-body effect in MXene systems, we calculated the anchoring behavior of Ti$_2$CF$_2$ (Supplementary Table 4), which was also applied as an anchoring material in Li-S batteries.$^{42}$ Compared with five atomic-layer Ti$_2$CF$_2$, we find that the polarizability perpendicular to plane ($\Delta\alpha_{\perp}$) and the ratio of MBD contribution ($R_{\text{MBD}}$) are both enhanced with the increasing thickness of anchoring materials.

From the above analysis, we find that Ti$_2$CF$_2$ systems has large polarization (22.2–41.3 bohr$^3$) and adsorption of LiPSs is dominated by the vdW interactions, which generates stronger many-body effect (large $R_{\text{MBD}}$). We also investigate other 2D materials such as TiS$_2$, Ti$_2$CO$_2$, and Ti$_3$C$_2$F$_2$ and the binding energies from two methods (PBE + vdW$^{\text{surf}}$ and PBE + MBD) are listed in Supplementary Table 5. We find that the many-body effect also exists in these systems. Therefore, for this type of anchoring materials with large $R_{\text{MBD}}$, pairwise-vdW methods tend to overestimate the anchoring performance ($\Delta E$) even get an inverse conclusion of anchoring materials. Conversely, chemical bonding plays an important role during the whole process of lithiation in NG systems, and NG has a small polarization (4.3–12 bohr$^3$). As such, $R_{\text{MBD}}$ is very small and pairwise-vdW and MBD method have the same prediction about $\Delta E$.

In Li-S batteries, the adsorption of LiPSs on loading materials or solvent molecules is a process of competition, thus positive $\Delta E$ is the prerequisite for the anchoring materials.$^{5}$ It is clearly seen that NG has a large $\Delta E$, which agrees with the experimental results that NG can effectively anchor lithium polysulfides. However, the limited number of adsorption sites discourages high energy density of sulfur cathodes. In addition, the $\Delta E$ of Li$_2$S$_6$ is as small as 0.02 eV, which demonstrates that Ti$_2$CF$_2$ would not effectively trap Li$_2$S$_6$ species, and the desorption and dissolution of Li$_2$S$_6$ species has a high probability to take place during lithiation.

**DISCUSSION**

We find the many-body dispersion interaction has a substantial impact on anchoring mechanism through binding energies of adsorption systems, especially for Ti$_2$CF$_2$ with strong polarization. According to the anchoring factor $\Delta E$ from the PBE + MBD method, we theoretically predict that Li$_2$S$_6$ partly dissolves into electrolytes solution and the DME/DOL solution with Li$_2$S$_6$ discolors incompletely when FeS and SnS$_2$ as anchoring materials, which agree well with the experiment. We demonstrated that the MBD approach can accurate predict the anisotropic polarizability and the anchoring behavior in the Li-S batteries. By systematically investigating the many-body effect on Ti$_2$CF$_2$ and NG systems, we found that the PBE + MBD method reduces the $E_{\text{AM}}$ over 20%, as compared to the PBE + vdW$^{\text{surf}}$ method at high-order lithiation stages for Ti$_2$CF$_2$ systems. While for NG systems, the energy difference from two methods is slight. Our work deepens the understanding of the anchoring mechanism, and provides a more accurate criterion for screening anchoring materials to control shuttle effect and to design more reliable cathode in Li-S batteries.

**METHODS**

**Computational details**

Our density functional theory (DFT) calculations were performed using the Fritz-Haber-Institute ab initio molecular simulations (FHI-aims) package$^{45}$ and the Vienna Ab initio Simulation Package (VASP) code.$^{46,47}$ The geometric optimization and the calculations of the charge transfer were performed within the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof (PBE) as implemented in VASP. For geometric optimizations, all atomic positions were relaxed until the maximal forces per atom were less than 0.03 eV Å$^{-1}$ and energy difference was smaller than $10^{-5}$ eV. The plane-wave cutoff energy was set to 450 eV. A 3 × 3 supercell of monolayer FeS (SnS$_2$), a 5 × 5 supercell of Ti$_2$CF$_2$ with 5 × 5 × 1

| Table 3. The total static polarizability ($\Delta\alpha$), and the $\Delta\alpha$ along $x$ ($\Delta\alpha_x$) and $z$ ($\Delta\alpha_z$) directions of Ti$_2$CF$_2$ adsorption configurations. |
|---|---|---|---|---|---|
| Ti$_2$CF$_2$ | Li$_2$S | Li$_2$S$_2$ | Li$_2$S$_4$ | Li$_2$S$_6$ | Li$_2$S$_8$ |
| $\Delta\alpha_{\parallel}$ (bohr$^3$) | 33.7 | 41.3 | 37.2 | 22.7 | 22.2 |
| $\Delta\alpha_x$ (bohr$^3$) | 52.1 | 51.2 | 54.2 | 51.4 | 48.3 |
| $\Delta\alpha_z$ (bohr$^3$) | 32.7 | 52.8 | 48.9 | 10.5 | 9.6 |
| $Q$ (e) | 0.73 | 0.85 | 1.08 | 0.42 | 0.58 |
| NG | Li$_2$S | Li$_2$S$_2$ | Li$_2$S$_4$ | Li$_2$S$_6$ | Li$_2$S$_8$ |
| $\Delta\alpha_{\parallel}$ (bohr$^3$) | 4.3 | 5.7 | 12.0 | 11.9 | 11.0 |
| $\Delta\alpha_x$ (bohr$^3$) | $-7.4$ | $-9.2$ | $-20.3$ | $-12.1$ | $-14.7$ |
| $Q$ (e) | 0.67 | 0.75 | 0.55 | 0.36 | 0.38 |

Summary of the static polarizability and charge transfer in Ti$_2$CF$_2$ and NG systems

The charge transfer ($Q$) between LiPSs and Ti$_2$CF$_2$(NG) are also shown in the table.

Fig. 3 Charge distribution analysis of LiPSs adsorbed on Ti$_2$CF$_2$ and NG. a–c The charge transfers (e) of S and Li atoms in Li$_2$S$_2$, Li$_2$S$_4$, and Li$_2$S$_6$ and Li$_2$S$_8$ and adjacent F atoms in Ti$_2$CF$_2$ adsorption configurations. d–f The charge transfers between S/Li atoms and adjacent N atoms in NG adsorption configurations.
Van der Waals inclusive methods

For the description of the van der Waals (vdW) interactions we applied two methods in DFT calculations. The PBE + vdw\textsuperscript{def} method\textsuperscript{50} were employed to account for the pairwise van der Waals (vdW) interactions. The PBE + vdw\textsuperscript{surf} total energy includes the dispersion energy by considering a sum of $-C_{6}R_{6}^{6}$ terms, where $R_{6}$ is the distance between atoms $a$ and $b$, the $C_{6}$ coefficients and vdW radii (vdW parameters) are determined by the collective screening of the substrate electrons, which are captured by mean of the vdw\textsuperscript{surf} method. We employed the PBE + MBD method to describe the many-body dispersion (MBD) effect. The MBD method computes the correlation energy of long-range electrostatic screening through the coupled harmonic oscillator model Hamiltonian, and considers dipolar vdW interactions to all orders (many-body effect) in perturbation theory beyond the vdw\textsuperscript{surf} method.

DATA AVAILABILITY

The data supporting the findings of this study are available from the corresponding author on reasonable request.

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AUTHOR CONTRIBUTIONS

S.L. and W.L. directed and designed the whole research. M.F. did all calculations and wrote the manuscript. All authors discussed the results and provided inputs to the manuscript.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

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