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Role of Van der Waals correction on the catalytic performance of 1T-TiS_2 electrocatalyst

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Abstract

In this paper, the role of Van der Waals (vdW) correction on the catalytic performance of 1T- TiS_2 material was investigated within the framework of density functional theory (DFT) and dispersion-corrected density functional theory (DFT-D3). The exchange-correlation functional was approximated using generalized gradient approximation (GGA) as parameterized by Perdew-Burke-Ernzerhof (PBE). Based on our results, the calculated lattice parameters were a =3.33 Å and a =3.32 Å upon calculations without and with inclusion of vdW correction, respectively, which indicated a slight reduction of ∼ 0.3% when vdW correction was included. In both cases, the value of a was in good agreement with previous experimental and theoretical data. However, the distances between the adsorbed hydrogen (H) and the surface of the catalyst were affected by the vdW correction. Our findings also showed that the vdW correction has an impact on the catalytic performance of 1T-TiS_2. The Gibbs free energy change for hydrogen adsorption ($\Delta G_H{}^*$) calculated for the most stable adsorption location was ∼ - 0.55 eV and ∼ - 0.53 eV without and with vdW correction, respectively. This revealed that the one calculated with the inclusion of vdW correction is closer to the optimal value. Therefore, this emphasized the need of including a vdW correction in any DFT study that involves catalytic properties of this material and its related members for more accurate and reliable results.

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Keywords: Van der Waals correction, Catalytic performance, Density functional theory, Adsorbed hydrogen

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1. Introduction

Van der Waals (vdW) interactions were first discovered in 1873 [1]. However, vdW interactions are of paramount importance in the characterization of layered materials, like transition metal dichalcogenides (TMDs). TMDs are chemical compounds that have a general formula MX_2, where M = transition metals such as titanium (Ti), molybdenum (Mo), tungsten (W), and vanadium (V), and X = chalcogens, either sulfur (S), selenium (Se), or tellurium (Te). This class of materials has gained much attention around the globe due to their unique and fascinating properties that include, but are not limited to, high surface areas, good chemical stability, and tunable band gaps [2, 3]. The layered structure of these materials is similar to that of graphite, with each single layer composed

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of stacked X−M−X sheets and the sequential stacking of layers forming the material. Each layer is weakly coupled by the van der Waals force, whereas the metal−chalcogen bond is covalent in nature [4]. In addition, according to the nature of the metal and chalcogen atoms, the stacking of the various X−M−X layers and the metal coordination in each layer may vary, giving rise to different polymorphs. Thus, TMDs can exhibit three main polymorphs: 1T, 2H, and 3R. The number signifies how many individual (non-repeating) layers are in a unit cell, and the letter denotes symmetry (T-trigonal, H-hexagonal, R-rhombohedral) [5].

Similar to other TMDs, 1T-TiS_2 is composed of layers that are held together by the weak vdW forces. However, density functional theory (DFT) has been used as a powerful approach in describing the fundamental properties of materials, but studies on the surface reactivity, adsorption energies, and defect formation energies of 1T-TiS_2 based on DFT can be impacted by substantial wrong estimation due to the absence of vdW corrections [6]. This is because the widely used approximation schemes for the exchange-correlation (XC) functional in DFT, such as the local density approximation (LDA) [7] and the generalized gradient approximation (GGA) [8], do not accurately account for the vdW interactions. Even though the vdW interactions, like all nonrelativistic electronic effects, are contained in the (unknown) exact DFT XC, several kinds of approaches to approximately include vdW interaction in DFT calculations are now in use. The two main types of possible approaches are (i) adding semi-empirical vdW interactions, like the dispersion-corrected DFT, with different versions: DFT-D, DFT-D2, and DFT-D3 [9–11] and (ii) using a nonlocal exchange-correlation functional accounting for vdW interactions such as the vdW density functional (vdW-DF) [12] and the scheme proposed by Vydrov and Van Voorhis [13] with the revised version rVV10 [14]. The DFT-D3 method is simpler and computationally inexpensive, and thus, it is widely used [15].

In fact, there are very limited direct studies on 1T-TiS_2 that specifically investigate the effects of including vdW corrections in DFT calculations. However, a report has indicated that the rVV10 DFT functional provides an improved description of interlayer bonding in TiS_2, resulting in a more accurate estimate of the interlayer binding energy. Interestingly, it was revealed that the improvement is not restricted only to TiS_2 but also applicable to other similar layered systems involving S atoms, such as TaS2, HfS_2, and MoS_2. Additionally, a recent study on the physical properties of a related material (MoX_2 (X=S, Se, Te)) evaluated the performance of hybrid vdW-D2, rVV10, and PBE functionals [16]. To the best of our knowledge, there is no study that specifically verifies why it is necessary to include vdW correction in DFT calculations of the catalytic performance of 1T-TiS_2.

Therefore, the main aim of this paper is to investigate the impact of vdW correction on the catalytic property of TiS_2 within the framework of DFT with the inclusion of a vdW correction scheme based on Gremme's method (DFT-D3) of dispersion correction [9].

2. Material and method

2.1. Computational details

In this work, all calculations were performed on a 2x2x1 supercell of a 1T-TiS_2 monolayer using first principle calculations within the framework of DFT, as implemented in the Quantum ESPRESSO simulation package [17]. The DFT-D3 method was adopted to account for the vdW interactions. The generalized gradient approximation (GGA) parameterization of Perdew-Burke- Ernzerhof (PBE) [8] has been employed to approximate the exchange-correlation potential for the 1T-TiS_2 monolayer. The plane wave basis sets with the maximum kinetic energy cutoffs of 550 eV and 544 eV were used for the calculations with and without vdW correction, respectively. The electron-ion core interaction was treated by ultrasoft pseudopotentials for Ti ($4s^2 3d^2$), S ($3s^2 3p^4$), and H ($1s^1$) valence orbitals as all in the pseudopotential files for both cases. The Brillouin zone integration was done using the Monkhorst-Pack scheme [18] with 8x8x1 and 7x7x1 k-point grids for the case with and without inclusion of vdW correction, respectively. To avoid interactions between different periodic images of the monolayer, a vacuum region of 20 Å was added in the c-direction. However, the supercell structure was fully relaxed for all calculations using the Broyden-Fletcher-Goldfarb-Shannon (BFGS) algorithms. VESTA software was used for the construction and visualization of the supercell structure [19].

2.1.1. Mechanisms of Hydrogen Evolution Reaction (HER)

Electrocatalytic water splitting involves breaking down water (H_2O) into oxygen (O_2) and hydrogen (H_2) gases with the use of an electric current and a catalyst. The whole process constitutes two half reactions which take place at different electrodes; the hydrogen evolution reaction (HER) at the cathode and oxygen evolution reaction (OER) at the anode [20]. The HER process is governed by two different mechanisms in electrolyte. These are:

i) Volmer–Tafel (V–T) Mechanism: This mechanism forms the adsorbed hydrogen atom (H^*_{ads}) at the active site of the catalyst, when a transferred electron first combines with a proton and is adsorbed by the catalyst (equation (1)). Then, two H^*_{ads}combine to produce H_2 gas (equation (2)). The hydrogen adsorption site is indicated by the symbol "*" in this description.

$$*+H^{+}+e^{-}\rightarrow H^{*}_{ads}. \tag{1}$$

$$2H^{*}_{ads}\rightarrow H_2+2^{*}. \tag{2}$$

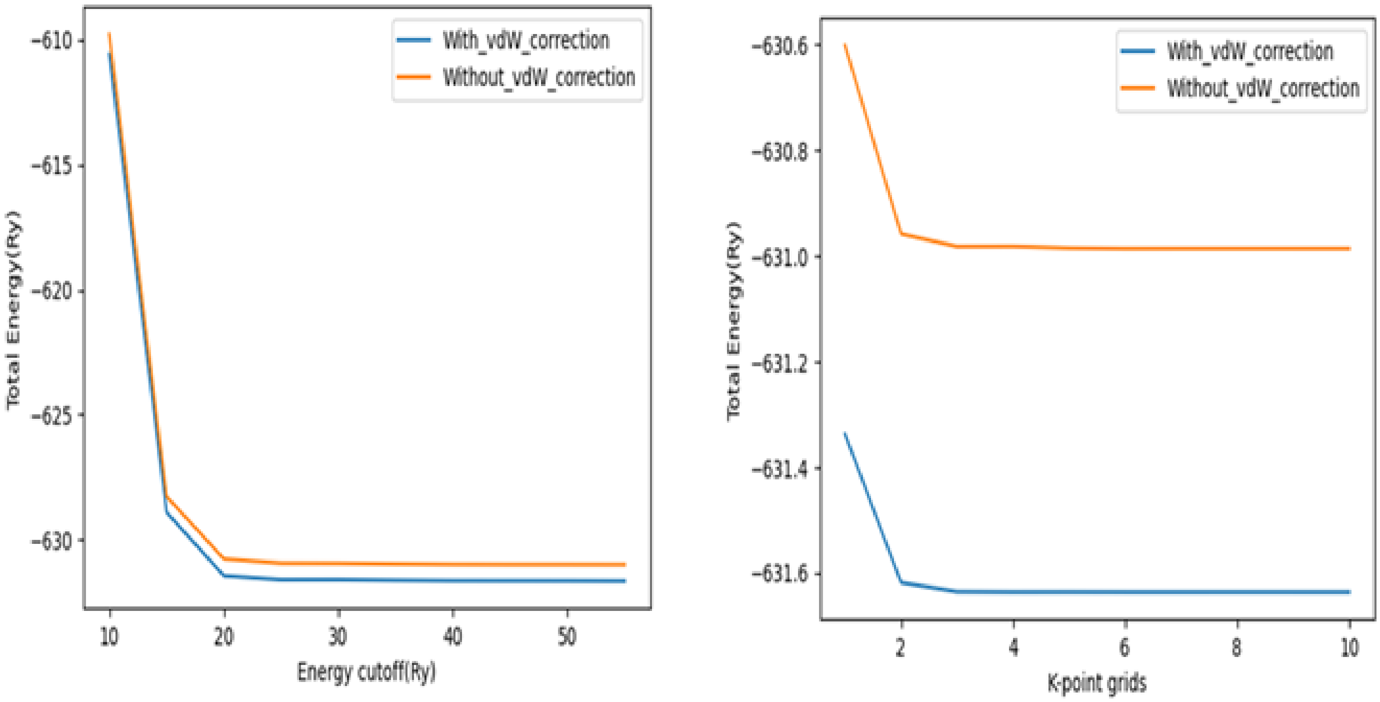

Figure 1. Convergence test calculation results with respect to: (a) kinetic energy cut-off of the system with and without vdW correction (b) k-point sampling of the system with and without vdW correction.

ii) Volmer–Heyrovsky (V–H) Mechanism: In contrast to the V-T process, after the Volmer step, the Heyrovsky step occurs when H^+ in the electrolyte and another transmitted electron from an external circuit combine with the H^*_{ads}, thereby forming H_2 gas as shown in equation (3).

$$*+H^{+}+e^{-}+H^{*}_{ads}\rightarrow H_2+*. \tag{3}$$

It can be seen that hydrogen adsorption is very essential in both V-T and V-H mechanisms, as such Gibbs free energy of hydrogen atom adsorption (ΔG_{H*}) is considered as a crucial descriptor to screen the performance of the acidic HER electrocatalyst [21]. Thus, many previous computational studies have only focused on it [22–24]. Theoretically, ΔG_{H*} and can be computed using the following relations [25, 26].

$$\Delta G_{H^*} = \Delta E_{H^*} + T\Delta S + \Delta ZPE, \tag{4}$$

$$\Delta E_{H^*} = E_{H^*} - E_* - \frac{1}{2}E_{H_2}, \tag{5}$$

where, E_{H^*} and E_* are the DFT total energies of the TiS_2 monolayer with and without absorbed H atoms, respectively, E_{H_2} is the DFT total energy of the free H_2 molecule, T is the room temperature (T=298.15 K), ΔS is the entropy change, and ΔZPE is the zero-point energy change.

3. Results and discussion

3.1. Converged kinetic energy cut-off and K-points grids

In any DFT study, convergence test calculations are very crucial and necessary, because well- converged parameters lead to more accurate and reliable results. We carried out the convergence calculations on the 1T-TiS_2 monolayer with respect to energy cutoff and k-points sampling in both cases (with and without vdW correction), and the results were shown in Figures 1a and 1b below:

It is evident from the figures that the results of the two distinct cases differ. Including the vdW correction in calculations gives the most negative total energies. However, the converged energies cutoffs chosen for the systems with and without vdW correction

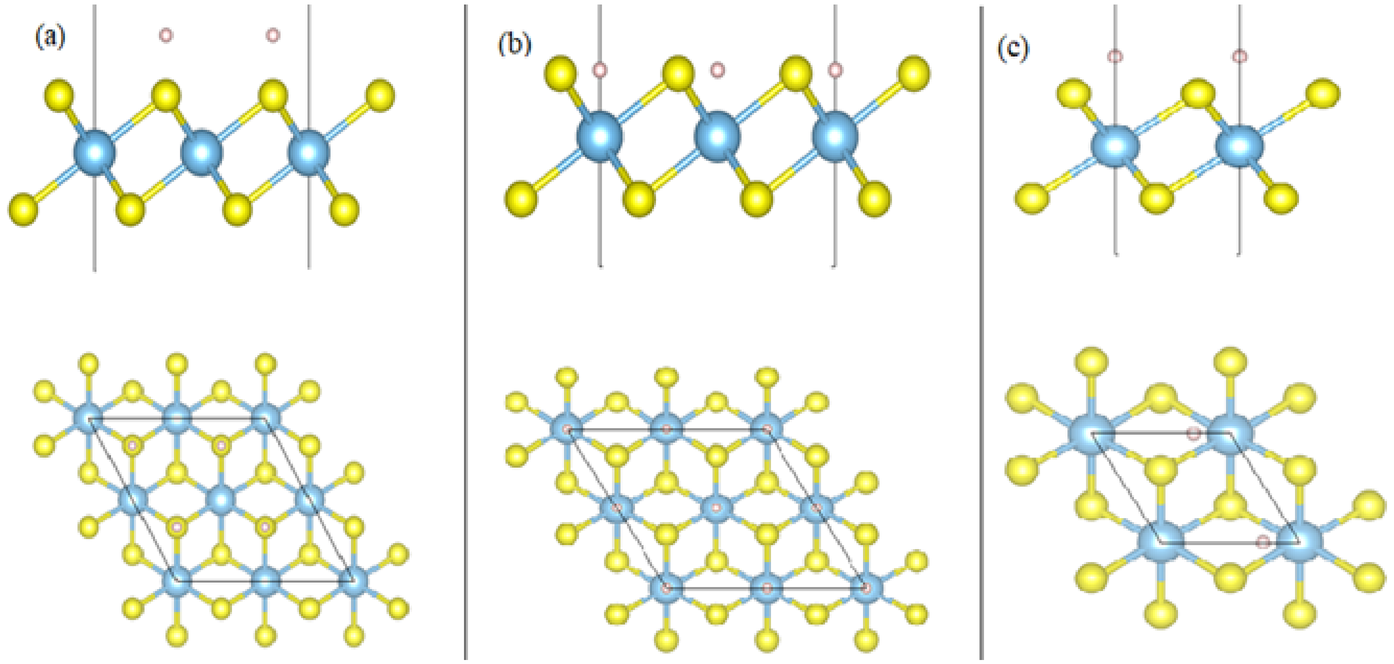

Figure 2. Hydrogen adsorption sites: (a) on top of the S (b) on top of the Ti (c) bridge. The blue, yellow and gold colours represent titanium, sulphur and hydrogen atoms respectively.

are 550 eV and 544 eV, respectively. Additionally, 8x8x1 and 7x7x1 converged k-point grids were selected for the two cases (with and without vdW correction, respectively). The reason these energy cutoff values and k-points were selected is that the total energies stabilize around them.

3.2. *Structural geometry and adsorption site of 1T-TiS$_2$ monolayer*

The 1T-TiS$_2$ exhibits a trigonal crystal structure with space group $P\overline{3}m1$. For calculations without vdW correction, the optimized lattice parameters are a =3.33 Å and c =16.28 Å, whereas for calculations with inclusion of vdW correction, the lattice parameters are a = 3.32 Å and c=16.38 Å. For both cases, the value of a was in good agreement with the previous experimental and DFT results of 3.40 Å [27] and 3.38 Å [28], respectively. The in-plane lattice parameter a calculated for the two cases shows a slight reduction of ~0.3% when vdW correction is incorporated. This small percentage decrease in the lattice parameter a may be due to the fact that the in-plane structure is governed by strong covalent bonds between Ti and S atoms within the layer, making it less sensitive to vdW corrections compared to interlayer interactions. It also suggests that dispersion forces primarily affect interlayer rather than intralayer bonding in monolayers. However, the lattice parameter c shows a slight increase of ~0.6% with vdW correction. This reflects the influence of vdW forces on the relaxation of the monolayer in the presence of a vacuum. Even though, for monolayers, the lattice parameter c is of less importance, and that is why it is not reported by most of the literature.

To determine the most stable and preferred adsorption location for the hydrogen (H) atom on the surface of the 1T-TiS$_2$ monolayer, we considered three different adsorption sites: (i) on top of sulfur (S), (ii) on top of titanium (Ti), and (iii) bridge, as all shown in Figure 2.

However, the adsorption energies for the three different locations were calculated (using equation (5)) in both cases (with and without vdW correction). Meanwhile, the most negative adsorption energy signifies the most energetically preferred site for adsorption. For the calculations without vdW correction, our results showed that two out of the three considered positions are feasible for adsorption: on top of S and bridge locations. They both have negative adsorption energies, as displayed in Table 1. Adsorption on top of the Ti atom is not viable and favorable due to the positive adsorption energy, which translates to weaker interactions between Ti and H. Moreover, it was found that H preferred to be adsorbed on top of S, which agrees well with many previous studies that reported adsorption on top of the chalcogen as the most stable [25, 26, 28].

On the other hand, the values of hydrogen adsorption energy were varied when the vdW correction was applied to the calculations (Table 2). The most stable and favorable adsorption site is on top of the S, as earlier suggested for the first case (without vdW correction). This may be due to the lower distance between the adsorbed H and S (as shown in Tables 1 and 2), which also indicates strong interactions between them. However, it is seen from Tables 1 and 2 that the various distances between H, Ti, and S were decreased after adding the vdW correction except for the case of the bridge position, where the distances increased.

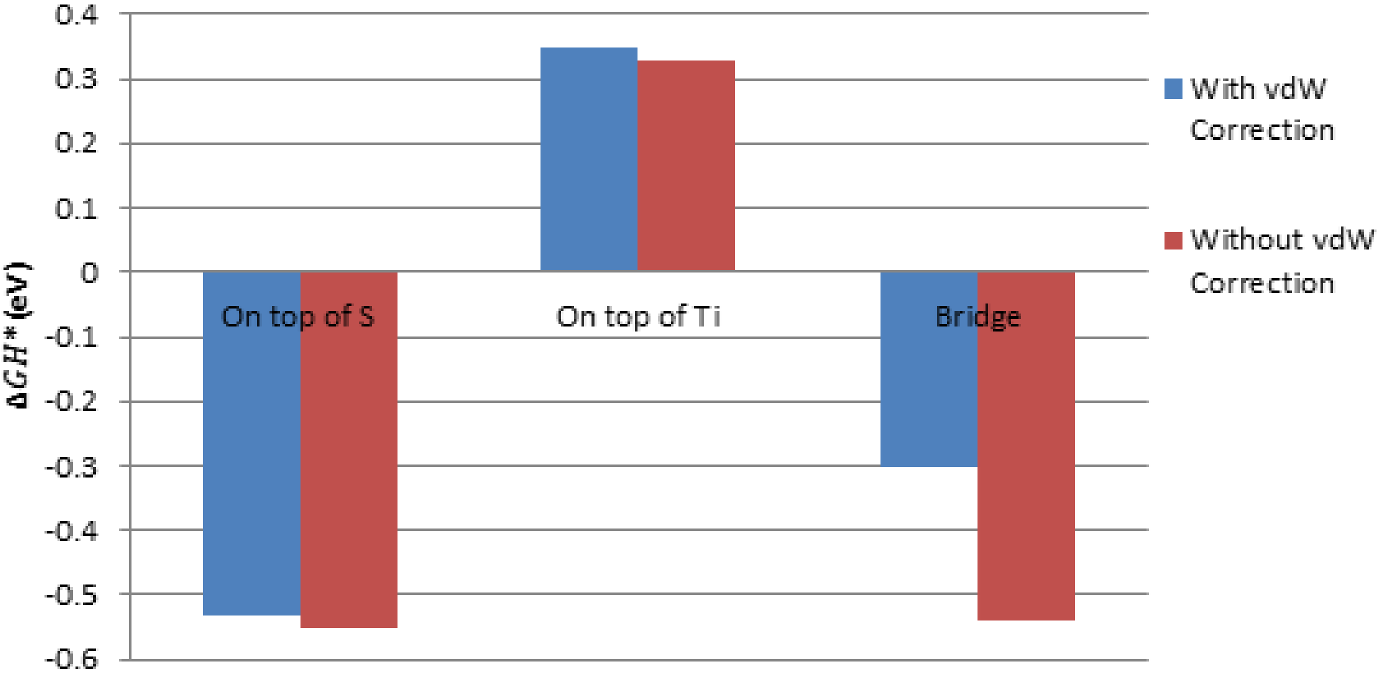

Figure 3. The calculated $\Delta G_H{}^*$ for the three different adsorption sites of the 1T-TiS_2.

Table 1. Calculated adsorption energies and various distances between H, Ti and S for the calculations without vdW correction.

Adsorption Site	ΔE_{H^*} (eV)	**Ti-H (Å)**	**S-H (Å)**
On top of Ti	0.0861	1.9271	-
On top of S	-0.7936	-	1.3595
Bridge	-0.7795	3.4721	1.3609

Table 2. Calculated adsorption energies and various distances between H, Ti and S for the calculations with vdW correction.

Adsorption site	ΔE_{H^*} (eV)	Ti-H (Å)	S-H (Å)
On top of Ti	0.1061	1.9214	-
On top of S	-0.7714	-	1.3587
Bridge	-0.5440	3.4853	1.3765

Table 3. Calculated Gibbs free energies of H adsorption for the three different adsorption sites in both cases (with and without vdW correction).

Adsorption Site	Without vdW Correction ΔG_{H^*} (eV)	With vdW Correction ΔG_{H^*} (eV)
On top of Ti	0.3261	0.3461
On top of S	-0.5536	-0.5314
Bridge	-0.5395	-0.3040

3.3. *Catalytic performance of 1T-TiS_2 monolayer*

The catalytic performance of the 1T-TiS_2 was assessed based on the Gibbs free energy change for hydrogen adsorption ΔG_{H^*} , which was calculated using equation (4). According to the Sabatier principle, the interaction between a catalyst and reactants should be neither too weak nor too strong ($\Delta G_H{}^*$) ≈ 0, i.e., it is the ideal value) [20, 29]. Thus, for a material to have good catalytic performance in the HER process, its ΔG_{H^*} should be very close to zero. The ΔG_{H^*} was calculated for the three different adsorption sites, and the results were shown in Table 3.

However, it can be seen that the ΔG_{H_*} calculated for the most stable adsorption location (on top of S) was approximately -0.55 eV and -0.53 eV without and with vdW correction, respectively. This reveals a difference of -0.02 eV. Based on this, it can be established that calculations with vdW correction give a $\Delta G_H{}^*$ value that is closer to zero. Though, the important adsorption site (whose $\Delta G_H{}^*$

is useful) is the most thermodynamically stable location, we can still discuss further on the $\Delta G_H{}^*$ of other adsorption sites for the purpose of analysis.

For the calculations with inclusion of vdW correction, the values of ΔG_{H*} are closer to the zero as depicted in Figure 3, except for the case of adsorption on top of Ti, which was already considered as nonviable. Additionally, adsorption on top of S and the bridge demonstrated negative values of ΔG_{H*}, which signifies strong hydrogen bonding on a catalyst surface and, therefore, the rate-determining step of Heyrovsky or Tafel, whereas the other adsorption site (on top of Ti) carried a positive value, revealing weak hydrogen-catalyst bonding, which slows down the Volmer step [25, 30].

4. Conclusion

This paper investigated the role of van der Waals (vdW) correction on the catalytic performance of 1T-TiS_2 using density functional theory (DFT) and dispersion-corrected DFT-D3 methods. While the lattice parameter a shows only minor variations, the absence of vdW corrections leads to high values in ΔG_{H*}. In contrast, calculations with vdW correction yield ΔG_{H*} values closer to zero, confirming that hydrogen adsorption and HER activity are better described when vdW correction terms are included. These findings stress that any DFT investigation of layered TMDs must incorporate vdW corrections for accurate and reliable catalytic predictions. Beyond TiS_2, the results suggest that vdW-inclusive computations are crucial for guiding the rational design of next-generation TMD-based electrocatalysts. The study further predicted that 1T-TiS_2 might be an excellent promising candidate for electrocatalytic water splitting. Future work may explore defect engineering and doping strategies under vdW-corrected frameworks to further optimize the catalytic performance of the materials.

Data availability

The data used in this research will be made available by the corresponding author upon request.

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