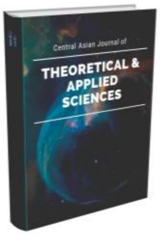

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Article

A Computational Study of the Effect of Adsorbed Nickel on the Hydrogen Storage Capacity in the Solid State on the Surface of Molybdenum Disulfide

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Abstract: Hydrogen is a promising renewable energy carrier, but its safe storage remains a major challenge, particularly in achieving acceptable volumetric density. Recent research has explored solid compound storage methods. This study investigates the adsorption of nine hydrogen (H_2) molecules on a nickel-adsorbed molybdenum disulfide (MoS_2) supercell (3×3×1) using Density Functional Theory (DFT) and the CASTEP program. Geometry optimization was used to describe the system's exchange-correlation energy. Results showed that the hydrogen molecules, with binding energies between 0.28 eV and 0.73 eV, were adsorbed on the surface with a total adsorption energy of 3.4 eV. These binding energies suggest that hydrogen can be released through simple heating, indicating potential for practical storage applications.

Keywords: Monolayer MoS2, Department of Energy (DOE) Targets, Density function theory (DFT), Adsorption, Approximation (GGA-PBE), CASTEP Program

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1. Introduction

One of the most important global concerns for sustainable economic and social growth is energy and the environment. The search for clean and renewable alternatives to fossil fuels, which now account for the majority of greenhouse gas emissions, is hoped to help alleviate some of the problems associated with these two themes. Finding a fossil fuel substitute that offers energy with the same efficiency but with greater sustainability and environmental friendliness was a global trend. Both the scientific community and the International Atomic Energy Agency (IAEA) have acknowledged the importance of hydrogen in this process, which started a few decades ago. Hydrogen (H2O) combustion is seen as a byproduct of [1].

Coal, natural gas, and oil can all be used to make hydrogen (sometimes known as blue hydrogen). in a procedure where carbon dioxide is completely controlled and not released into the atmosphere. There are two ways to manufacture hydrogen from fossil fuels: pyrolysis of hydrocarbons or hydrocarbon reforming technologies (steam reforming is the most often used method). Green hydrogen, or the electrolysis of water, is another method of producing hydrogen from renewable resources. Clean electrical energy is used to start an electrochemical reaction that splits water molecules into hydrogen and oxygen gases. Subsequently, hydrogen molecules are extracted for use as an energy source in piston engines, gas turbines, and hydrogen fuel cells. [2].

Water electrolysis is a straightforward method that can be used to produce very efficient and reasonably priced green energy [3]. Compared to other fuel sources like methane and petrol, hydrogen has been shown to have a very excellent gravimetric energy density, or energy density by weight, making it suitable for use as fuel. However, because it is one of the lightest elements, it has a relatively low volumetric energy density, necessitating large storage containers. Under normal circumstances, hydrogen is a very common element in the universe and can be found in nature as a gas at 20 degrees Celsius and 1 ATM. It is a recognised colourless, tasteless, and odourless gas that is non-toxic. But regrettably, it suffers from [5, 6].

And this presents a significant conflict between the economics of hydrogen and the security of its storage. Additionally, it can be kept in a variety of ways, including physically as liquid or compressed gas. However, techniques based on chemical absorption can be used to store hydrogen. For this aim, a variety of materials have recently been investigated, including complex hydrides, interstitial hydrides, porous materials, and liquid organic materials [7]. The volume that hydrogen takes up under typical temperature and pressure circumstances must be decreased in order to increase its volumetric density and make it a competitive energy carrier. This can be accomplished physically by compressing small amounts of hydrogen gas or chemically liquefying hydrogen using extremely[7] Regretfully, from an engineering and financial standpoint, neither of the two approaches is the best option [1].

Physical adsorption is another extremely promising method that uses an adsorbent surface to attract hydrogen molecules in order to decrease the interaction between hydrogen molecules in the gas phase. Although material-based hydrogen storage has a very low gravimetric capacity, it has a high volumetric energy density. In order to boost gravimetric capability, scientists are working to identify the ideal adsorbent surface. Interestingly, because of their high aspect ratio and low density, two-dimensional materials are thought to be perfect for physisorption-based hydrogen storage [8, 9]. However, the majority of two-dimensional materials are inert in their initial state, and hydrogen storage is essentially a surface reaction [10, 11]. Transition metal-based materials have been frequently employed to increase active adsorption sites and, consequently, to improve H2 molecule absorption [12].

Transition-metal dichalcogenides (TMDs), for instance, have emerged as novel two-dimensional materials with promising mechanical and electrical properties as well as a strong spin-orbit coupling (SOC), elevating their category to the status of top contenders in a wide range of electronic applications [13, 14]. Pioneering studies to examine their unique characteristics and the principles of their interfacial interactions have been produced by the successful synthesis of heterogeneous structures of two-dimensional materials. Apart from their two-dimensional form, these novel heterogeneous artificial structures provide unique characteristics and potential uses, such as memory cells, biosensors, batteries, and flexible optoelectronic devices [15, 16].

Numerous two-dimensional heterogeneous structures have been successfully created experimentally because of their layered structure and the weak Van der Waals (vdW) interaction of the interlayer. TMDs are a very sophisticated class of layered materials that show their use in hydrogen research. For this specific situation, TMD devices (Transition-Metal dichalcogenide) have already shown themselves to be a formidable rival [17, 18]. Large-scale hydrogen molecule absorption on MoS2 has been demonstrated to be a realistic undertaking with appropriate absorption energy and acceptable stability [9]. MoS2 nanotubes (NT) have been found by Wang and his colleagues to be effective at drawing methane and hydrogen molecules to their inner and outer surfaces. They stated that, depending on the nanotube's diameter, the hydrogen storage capacity varies from 0.7% to 0.9% by weight [19]. In the current work, the mixture is also suggested for energy storage.

2. Materials and Methods

Accounts

In this study, first-principle calculations were used through Density Functional Theory (DFT) with the CASTEP program (Cambridge Series Total Energy Package). The calculations were performed on a large supercell (3x3x1) of pure molybdenum disulfide (MoS2) adsorbed with a nickel (Ni) atom. The calculations were conducted through geometry optimization, where the exchange-correlation energy between the electrons of the hydrogen molecule (H2) and the surface of molybdenum disulfide (MoS2) was described using DFT with the Generalized Gradient Approximation (GGA) and the Pardew-Burke-Ernzerhof exchange-correlation functional. (PBE) [20. 21].

3. Results and Discussion

1.3 Nickel atom adsorption on molybdenum disulfide surface: Nickel Adsorption on Molybdenum Disulfide (MoS2) Sheet

The calculations were conducted to determine the preferred adsorption sites of nickel (Ni) atoms on the surface of molybdenum disulfide by applying periodic boundary conditions to the large unit cell. (3x3x1). There are four potential sites for the adsorption of a nickel (Ni) atom on the surface of molybdenum disulfide (MoS2), which are:

a) Above the sulfur atom site (S).
b) Above the molybdenum atom site (Mo).
c) Above the center of the hexagonal ring of molybdenum disulfide.
d) Above the bond that connects sulfur (S) with molybdenum (Mo).

After conducting the geometry optimization process to determine the preferred site for nickel (Ni) adsorption among the four sites, it was found that the best site for nickel adsorption is above the molybdenum (Mo) atom, as shown in the figure. (1B). And when the nickel (Ni) atom is positioned above the sulfur (S) atom and above the bond that connects sulfur (S) with molybdenum (Mo), as well as above the center of the hexagonal ring of molybdenum disulfide, in all likelihood, the nickel (Ni) atom shifted directly during the positioning above the molybdenum atom. (Mo). This is consistent with previous studies conducted by the scientist Shulin Yang and others [22].

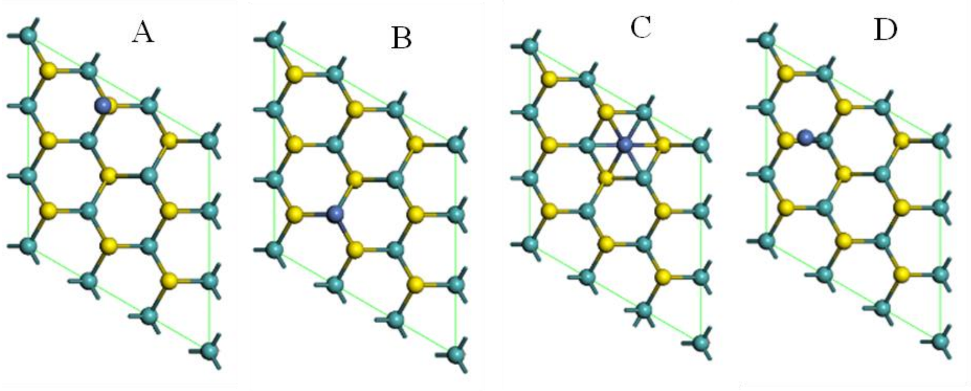

Figure 1. Shows the optimal region for nickel stability on the molybdenum disulfide (MoS2) molecule.

And then we performed the calculation of the binding energy resulting from the adsorption of a nickel (Ni) atom on the surface of molybdenum disulfide (MoS2) using the following mathematical relationship [23]:

$$\mathbf{E_b} = -[\boldsymbol{E}_{\textbf{Molybdenum Disulfide+metal}} - (\boldsymbol{E}_{\textbf{Molybdenum Disulfide}} + \boldsymbol{nE}_{\boldsymbol{metal}})]/\boldsymbol{n}$$

(1)

$\boldsymbol{E}_{\textbf{Molybdenum Disulfide}}$ **:** The total energy of the system (with n number of nickel (Ni) atoms adsorbed on the surface of molybdenum disulfide (MoS2)).

$\boldsymbol{E}_{\boldsymbol{metal}}$ **:** The total energy of a nickel atom (Ni).

I found that the total binding energy we obtained is (3.44 eV) through the above equation and on the same unit cell. (3x3x1).

Adsorption of hydrogen (H2) on the surface of molybdenum disulfide (MoS2) doped with nickel atoms (Ni).

The geometry optimization calculations for the adsorption of a nickel atom (Ni) on the surface of molybdenum disulfide were conducted by applying periodic boundary conditions on a large unit cell (3x3x1). For the adsorption of hydrogen molecules (H2) on the nickel-adsorbed molybdenum disulfide surface, one hydrogen molecule was added and optimized each time, and the binding energy was calculated according to the previously mentioned equation (6).

Table 1. Shows the distance and binding energy values calculated for the adsorption of hydrogen (H2) molecules on the surface of molybdenum disulfide (MoS2) doped with a nickel atom. (Ni).

$\mathbf{d}_{\text{Ni-S}}$ ^{0}**A**	$\mathbf{d}_{\text{Ni-Mo}}$ ^{0}**A**	$\mathbf{d}_{\text{H2-Mo}}$ ^{0}**A**	$\mathbf{d}_{\text{H2-S}}$ ^{0}**A**	$\mathbf{d}_{\text{H2-Ni}}$ ^{0}**A**	$\mathbf{E}_{\text{bH2}}$ **(eV)**	$\mathbf{E}_{\text{baver}}$ **(eV)**	**Number of adsorbed H2**
2.171	4.152	5.223	3.057	1.639	0.733603	0.733603	**1**
2.174	4.158	5.468	3.281	1.638	0.40928	0.5714415	**2**
2.172	4.153	5.116	3.042	1.639	0.301225	0.4813776	**3**
2.169	4.150	5.078	3.071	1.638	0.244836	0.422236	**4**
2.171	4.152	5.286	3.092	1.639	0.213816	0.380552	**5**
2.170	4.153	5.084	3.114	1.643	0.19066	0.3489033	**6**
2.170	4.152	5.083	3.062	1.639	0.175	0.32406	**7**
2.175	4.158	5.177	3.290	1.641	0.163464	0.3039855	**8**
2.173	4.157	5.469	3.283	1.642	0.154044	0.28732533	**9**

Where it represents:

1. EbH2: The binding energy of hydrogen (H2) molecules on the surface of molybdenum disulfide (MoS2) adsorbed with a nickel atom (Ni).
2. Ebaver: The binding energy rate of hydrogen (H2) molecules adsorbed on the surface of molybdenum disulfide (MoS2) doped with nickel atoms. (Ni).
3. dH2-Ni: The distance between the nickel atom (Ni) and the hydrogen molecule (H2) adsorbed on the surface of molybdenum disulfide (MoS2) adsorbed with the nickel atom (Ni).
4. dH2-S: The distance between the sulfur atom (S) and the hydrogen molecule (H2) adsorbed on the surface of molybdenum disulfide (MoS2) adsorbed with a nickel atom (Ni).

5. dH2-Mo: The distance between the molybdenum (Mo) atom and the hydrogen (H2) molecule adsorbed on the surface of molybdenum disulfide (MoS2) adsorbed with a nickel atom (Ni).
6. dNi-Mo: The distance between the nickel (Ni) atom and the molybdenum (Mo) atom on the surface of the molybdenum disulfide (MoS2) adsorbed with a nickel atom (Ni).
7. dNi-S: The distance between the nickel (Ni) atom and the sulfur (S) atom on the surface of the molybdenum disulfide (MoS2) adsorbed with the nickel atom (Ni)

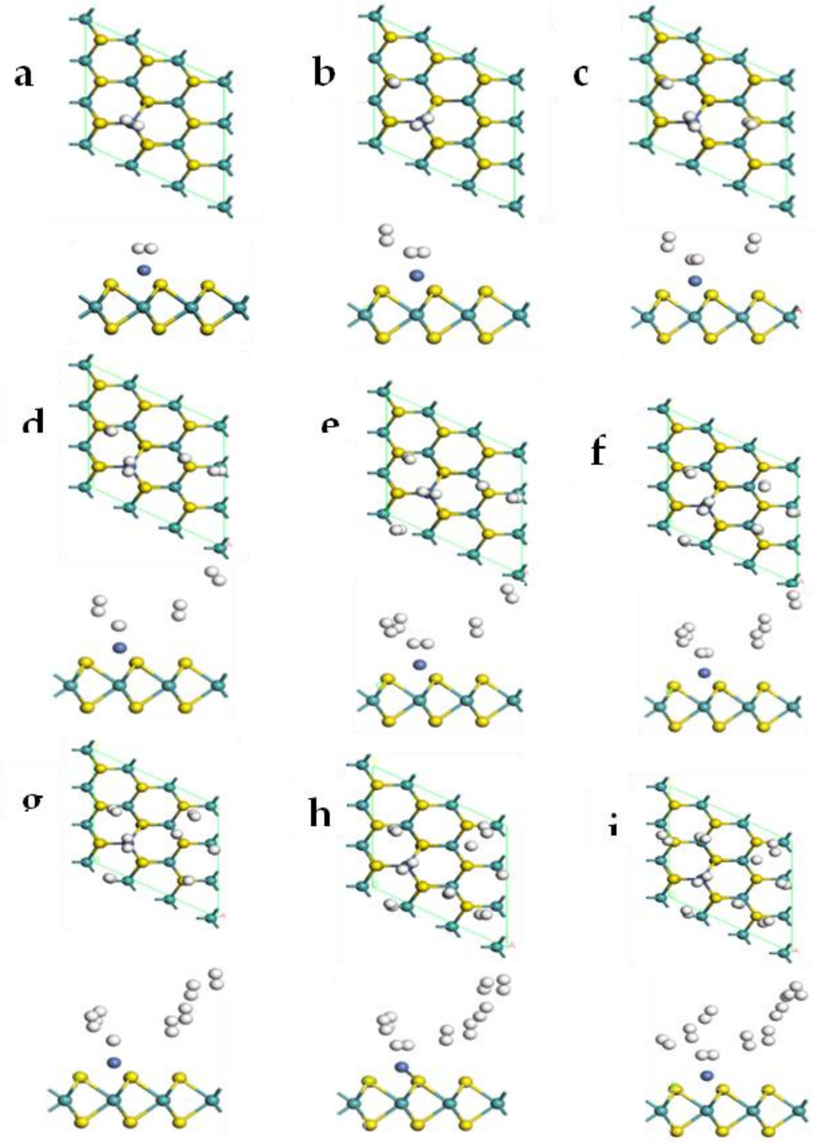

Figure 2. Illustrates the adsorption of the hydrogen molecule H2, colored in white, on the surface of molybdenum disulfide (MoS2), where the yellow color represents sulfur and the blue color represents molybdenum adsorbed with a nickel (Ni) atom, also colored in blue

The hydrogen molecule (H2) and the nickel atom (Ni) is (1639 0A). When a second hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) stabilized above the sulfur atom (S) at a distance of (1.638 0A) as shown in figure (2b). When a third hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2).

It also settled above the sulfur atom at a distance of (1.639 Å) as shown in figure (2c). When a fourth hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) settled above the molybdenum atom at a distance of (1.638 Å) as shown in figure (2d). When a fifth hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) settled above the sulfur atom at a distance of (1.639 Å) as shown in figure (2e). When a sixth hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) settled above the central region near the molybdenum atom at a distance of (1.643 0A)

As shown in Figure (2-1f), when a seventh hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) stabilized above the bond between the molybdenum atom and the sulfur atom at a distance of (1.639 0A) as shown in Figure (2g). When an eighth hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) stabilized above the molybdenum atom at a distance of (1.641 0A) as shown in Figure (2h).

When a ninth hydrogen molecule (H2) was added and the geometric configuration was performed, it was found that the hydrogen molecule (H2) stabilized above the sulfur atom at a distance of (1.642 0A) as shown in Figure (2i) [22]. The values we obtained, as shown in Table (1), illustrate the relationship between the number of hydrogen (H2) molecules and the binding energy rate, where the relationship is inverse. As the number of hydrogen (H2) molecules adsorbed on the surface of molybdenum disulfide (MoS2) increases, the binding energy decreases. Figure (3) illustrates this relationship

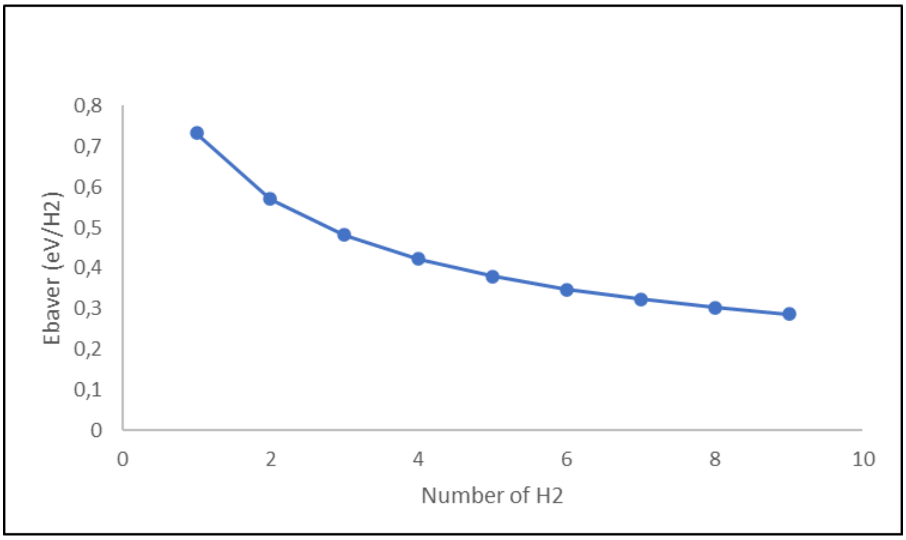

Figure 3. Is a diagram of the inverse relationship between the binding energy rate (Ebaver) and the number of hydrogen molecules. (H2)

The adsorbed hydrogen molecule (H_2) has a binding energy rate that should be between (0.2-0.8 eV) (ranging between physical and chemical adsorption) [24]. Through the study we conducted, we obtained binding energy values within the desired range (0.2-0.8 eV), which is consistent with previous studies [23]. The required percentage for hydrogen storage on the surface of nickel-adsorbed molybdenum disulfide was calculated using the equation below [25].

$$H_2\ (wt\%) = \left[\frac{M_{H_2}}{M_{H_2} + M_{MoS_2} + M_{Ni}}\right] \times 100\% \qquad (2)$$

Since:
M_(MoS_2): Represents the mass of hydrogen (H2) adsorbed on the surface of molybdenum disulfide. (MoS2). M_(MoS_2) represents the molybdenum disulfide mass. (MoS2).

M_Ni is the mass of the nickel atom (which is the adsorbed atom). The storage ratios that were found were for nine hydrogen (H2) molecules on the surface of a nickel-adsorbed molybdenum disulfide cell, which was (2.4 wt.%) and it is lower than the percentage set by the Department of Energy (DOE), which is equal to (6.5 wt.%) This is because molybdenum (MO) as a two-dimensional structure contains more atoms than traditional hexagonal structures like graphene and boron. (B).

4. Conclusion

In this study, first-principles calculations were performed using Density Functional Theory (DFT) with the CASTEP program. The calculations were conducted on a large unit cell (3x3x1) of molybdenum disulfide (MoS2) adsorbed with a nickel atom, using the Generalized Gradient Approximation (GGA) for the large unit cell (1x3x3). The exchange-correlation energy between the electrons of the hydrogen molecule was described, and it was concluded that the addition of nine hydrogen molecules to the surface of the nickel-adsorbed molybdenum disulfide, which settled above the molybdenum, resulted in a total adsorption energy equal to (3.4 eV). Where hydrogen molecules have taken different positions on the surface of molybdenum disulfide with a binding energy ranging from (0.28 eV-0.73 eV), which is within the physical range and can be released by a simple heating process.

REFERENCES

[1] W. Alfalasi, Y. P. Feng, and N. J. Tit, "Enhancement of hydrogen storage using functionalized $MoSe_2$/Graphene monolayer and bilayer systems: DFT study," Int. J. Hydrogen Energy, vol. 50, pp. 1189-1203, 2024.

[2] P. Nikolaidis and A. Poullikkas, "A comparative overview of hydrogen production processes," Renewable Sustainable Energy Rev., vol. 67, pp. 597-611, 2017.

[3] A. Arsad, M. H. Ani, R. Rahman, Z. Salam, and S. Mekhilef, "Hydrogen energy storage integrated hybrid renewable energy systems: A review analysis for future research directions," Renewable Sustainable Energy Rev., vol. 47, no. 39, pp. 17285-17312, 2022.

[4] J. O. Abe, A. Popoola, E. Ajenifuja, and O. M. Popoola, "Hydrogen energy, economy and storage: Review and recommendation," Int. J. Hydrogen Energy, vol. 44, no. 29, pp. 15072-15086, 2019.

[5] Y. S. Najjar, "Hydrogen safety: The road toward green technology," Int. J. Hydrogen Energy, vol. 38, no. 25, pp. 10716-10728, 2013.

[6] R. W. Schefer, W. G. Houf, and T. J. Williams, "Investigation of small-scale unintended releases of hydrogen: Buoyancy effects," Int. J. Hydrogen Energy, vol. 33, no. 17, pp. 4702-4712, 2008.

[7] A. Kovač, M. Paranos, and D. Marciuš, "Hydrogen in energy transition: A review," Int. J. Hydrogen Energy, vol. 46, no. 16, pp. 10016-10035, 2021.

[8] S. Kaskun, Y. Akinay, and M. Kayfeci, "Improved hydrogen adsorption of ZnO doped multi-walled carbon nanotubes," Int. J. Hydrogen Energy, vol. 45, no. 60, pp. 34949-34955, 2020.

[9] H. Liu, Y. Shen, L. Zhao, Y. Wei, and X. Qiu, "Y-decorated MoS_2 monolayer for promising hydrogen storage: A DFT study," Int. J. Hydrogen Energy, vol. 47, no. 24, pp. 12096-12106, 2022.

[10] P. Panigrahi, A. Kumar, A. Karton, R. Ahuja, and T. Hussain, "Remarkable improvement in hydrogen storage capacities of two-dimensional carbon nitride (g-C_3N_4) nanosheets under selected transition metal doping," Int. J. Hydrogen Energy, vol. 45, no. 4, pp. 3035-3045, 2020.

[11] S. Shevlin and Z. Guo, "Transition-metal-doping-enhanced hydrogen storage in boron nitride systems," Appl. Phys. Lett., vol. 89, no. 15, 2006.

[12] G. Qin, Q. Cui, B. Yun, L. Sun, A. Du, and Q. Sun, "High capacity and reversible hydrogen storage on two-dimensional C_2N monolayer membrane," Int. J. Hydrogen Energy, vol. 43, no. 21, pp. 9895-9901, 2018.

[13] C. Gong, X. Zhang, L. Zhou, W. Zhao, and L. Gu, "Electronic and optoelectronic applications based on 2D novel anisotropic transition metal dichalcogenides," Adv. Funct. Mater., vol. 4, no. 12, p. 1700231, 2017.

[14] P. De Miranda, E. Carreira, U. Icardi, and G. Nunes, "Brazilian hybrid electric-hydrogen fuel cell bus: Improved on-board energy management system," Int. J. Hydrogen Energy, vol. 42, no. 19, pp. 13949-13959, 2017.

[15] G. W. Shim, S. Jung, D. H. Choe, S. H. Lee, and Y. H. Lee, "Large-area single-layer $MoSe_2$ and its van der Waals heterostructures," 2D Mater., vol. 8, no. 7, pp. 6655-6662, 2014.

[16] J. Gong, S. Li, Y. Zhu, Z. Li, and H. Lu, "Surface engineering of Ni wires and rapid growth strategy of Ni-MOF synergistically contribute to high-performance fiber-shaped aqueous battery," Adv. Energy Mater., vol. 18, no. 42, p. 2204346, 2022.

[17] B. Qu, C. Li, C. Zhu, S. Wang, X. Zhang, and Y. Chen, "Growth of $MoSe_2$ nanosheets with small size and expanded spaces of (002) plane on the surfaces of porous N-doped carbon nanotubes for hydrogen production," Nanoscale, vol. 8, no. 38, pp. 16886-16893, 2016.

[18] D. K. Sharma, S. Kumar, and S. Auluck, "Electronic structure, defect properties, and hydrogen storage capacity of 2H-WS_2: A first-principles study," Int. J. Hydrogen Energy, vol. 43, no. 52, pp. 23126-23134, 2018.

[19] X. Wang, B. Li, D. R. Bell, W. Li, and R. Zhou, "Hydrogen and methane storage and release by MoS_2 nanotubes for energy storage," J. Mater. Chem. A, vol. 5, no. 44, pp. 23020-23027, 2017.

[20] I. Z. Hassan, H. A. Kadhem, and A. H. S. Mohammed, "DFT study of hexagonal boron nitride electronic properties using different types of exchange correlation functionals," Indian J. Pure Appl. Phys., vol. 61, no. 10, pp. 840-845, 2023.

[21] R. Ahmed and I. Hassan, "Study of the electronic properties of pure nanostructured hexagonal zinc oxide by DFT method," Al-Kitab J. Pure Sci., vol. 7, no. 2, pp. 78-88, 2023.

[22] S. Yang, L. Dong, Q. Zhang, Z. Zhang, and C. Zheng, "A DFT study on the outstanding hydrogen storage performance of the Ti-decorated MoS_2 monolayer," Surf. Interfaces, vol. 26, p. 101329, 2021.

[23] A. Sharma, M. Husain, A. Srivastava, and S. Khan, "DFT study of Ca-adsorbed MoS_2 monolayer for hydrogen storage application," Adv. Mater. Proc., vol. 3, no. 1, pp. 25-30, 2018.

[24] D. C. Young, Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, 9th ed., New York: John Wiley & Sons, 2001.

[25] I. Z. A. Hassan and S. M. Nayif, "Computational study of the effect of adsorbed lithium on solid-state hydrogen storage capacity of pristine and boron-doped graphene," Kirkuk J. Sci., vol. 15, no. 4, pp. 45-52, 2020.