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Multiscale Modelling of Two-dimensional Materials for Solar Water Splitting and Hydrogen Storage

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Introduction:

The increasing energy demands due to technology and population growth, along with the depletion of traditional non-renewable energy sources, pose a significant hurdle for finding alternative fuels, especially for vehicles [1]. Hydrogen fuel shows great promise as an alternative due to its abundant availability, eco-friendliness, and high energy density compared to other fuels [2,3]. It produces only clean water and heat as by-products. However, the practical use of hydrogen fuel faces two main challenges: efficient and cost-effective production, and compact storage [4,5]. This thesis proposes addressing these challenges by designing advanced two-dimensional (2D) nanomaterials and using them to produce hydrogen through water splitting, as well as exploring efficient methods for hydrogen storage [4,5].

Water splitting:

Recently, water splitting has become a promising method for producing hydrogen gas [6,7]. It involves two half reactions: the hydrogen evolution reaction (HER) at the cathode, where water is reduced to generate H_2, and the oxygen evolution reaction (OER) at the anode, where water is oxidized to produce O_2 [8]. Currently, noble metals like Pt are efficient catalysts for HER but limited by high cost and availability [9]. Thus, researchers are exploring earth-abundant materials as alternative catalysts to overcome these limitations [10]. Recently, single-atom catalysts (SACs) have emerged as an ideal for clean and renewable energy technology [11]. They offer benefits like single active sites, strong metal-support interactions, and impressive catalytic activity for HER [12]. Additionally, 2D materials show promise as supports for SACs in HER. Pristine graphene doesn't interact well with hydrogen, so it's not suitable for HER activity [13]. Hossain et al.

conducted density functional theory (DFT) simulations and experiments to study SACs of transition metals (TMs) on N-doped graphene. They found that Rh, Cr, Co, V, and Fe showed good HER activity, with Co-SAC having the lowest Gibbs free energy (ΔG) (-0.20 to 0.30 eV) and potential, making it a highly efficient HER catalyst [14]. Dušan et al. employed DFT study to discover effective SACs featuring TMs inserted into the monovacancies of h-BN and graphene. Monovacancies prevented aggregation, and 27 SACs were examined, identifying several candidates with HER activity close to Pt surfaces [15]. DFT simulations were performed to study HER activity on graphyne supported SACs. Among the tested TMs (Cu, Fe, Zn, Ni, and Co), Ni SACs displayed the excellent HER activity (0.08 eV) [16]. Xue et al. investigated the use of graphdiyne as a support for SACs in HER activity, focusing on Ni and Fe as active metals. DFT calculations indicated that Ni and Fe SACs anchored on graphdiyne exhibited favorable HER activity [17]. Apart from SACs, non-transition metal doping (B, N, C and etc.) and defects engineering are also one of the excellent ways for the improvement in the HER activity of the 2D materials [18,19]. In this context, the HER activity of the graphene monolayer was found to increase with the B, S, and N dopants [20,21]. Similarly, pristine g-C_3N_4 is also not suitable for HER activity, but the dopants S, Na and O enhance the HER activity as compared to its pristine counterpart [22,23]. The study by Wan et al. showed that the porous boron nitride (p-BN) is an insulator with a very wide band gap, similar to h-BN monolayer, and is not suitable for catalytic activity. However, when p-BN is doped with carbon (C), the band gap is tuned, making it suitable as a metal-free photocatalyst for overall water splitting under visible light irradiation [24]. Previously, Yixin and collaborators demonstrated that the presence of different defects can modify the electronic properties of MoS_2 and significantly enhance its HER activity [25].

In the present thesis, we investigated the HER activity of various unexplored materials, including α-SiX (X = N, P, As, Sb, and Bi) [26], holey graphyne [27], and o-B_2N_2 monolayers [28]. It was observed that the pristine forms of α-SiX, holey graphyne, and o-B_2N_2 were not suitable for HER activity without any tuning [26–28]. The HER activity improved when decorated with TMs on α-SiX (X = N, P, As, Sb, Bi) and holey graphyne. The Ni@ α-SiX (X = N, P, As, Sb, Bi) SACs exhibited significantly improved HER activity, with enhancements of 95.00%, 29.24%, 67.97%, 69.71%, and 39.53%, respectively, compared to their pristine counterparts. Notably, the Ni@α-SiN single-atom catalysts showed promising potential as an ideal HER catalyst due to a near-zero ΔG (~0 eV) [26]. For holey graphyne, we predicted that Co, Fe, and Cr anchored on holey graphyne exhibited high HER activity, with ΔG values as low as -0.21, -0.14, and -0.05 eV, respectively. These values are comparable to those of the best-known HER catalyst, Pt metal [27]. To enhance the HER activity of the o-B_2N_2 monolayer, we implemented several strategies such as introducing vacancy defects and doping the C atom into the structure. The incorporation of a BN vacancy defect and C doping at B and N sites in the monolayer resulted in a substantial improvement in the HER activity, with enhancements of 77.34%, 86.71%, and 83.59%, respectively, compared to the pristine monolayer [28].

Hydrogen storage:

Designing advanced materials for high-capacity, recyclable hydrogen storage devices present a significant challenge due to limitations with current hydrogen storage technologies [29,30]. Conventional methods such as high-pressure tanks and liquid storage have drawbacks, including large size and weight of the tank, as well as high energy costs associated with liquefaction [31]. Solid-state storage holds promise as a more efficient and desirable alternative, provided the storage medium can effectively absorb a substantial amount of hydrogen and release

it easily without altering its structure [31]. The US Department of Energy (DoE) has established guidelines for efficient hydrogen storage devices. According to these guidelines, a system should be capable of storing a minimum of 6.5 wt.% of hydrogen by weight, while the binding energy of hydrogen (H_2) molecules should fall within the range of 0.2 – 0.8 eV [32]. Various 2D nanomaterials such as graphene, **ψ**-graphene, graphyne, h-BN, and g-C_3N_4 have been extensively investigated as potential hydrogen storage devices, primarily due to their large surface area and lightweight nature [33–38]. However, hydrogen storage on these pristine materials is typically negligible under ambient conditions. Recent studies have highlighted the potential of alkali metals (Li, Na, K and etc.), alkaline earth metals (Be, Mg, Ca and etc.), and transition metals (Ti, Sc, Y, V and etc.) decorated graphene, **ψ**-graphene, graphyne, h-BN, and g-C_3N_4 as promising candidates for ambient hydrogen storage [33–38]. These metals can form strong bonds with the nanostructures and have demonstrated the ability to bind H_2 molecules even at room temperature [33–38]. This discovery opens up new possibilities for efficient hydrogen storage using metal-decorated 2D nanomaterials.

In this thesis, we have also investigated the hydrogen storage capacity of the newly predicted o-B_2N_2 monolayer. It was found that the pristine o-B_2N_2 monolayer is not suitable for hydrogen storage application. To enhance its hydrogen storage capacity, we introduced defects and decorated the monolayer with various metals, including Na, K, Be, Mg, Ca, Sc, Ti, Y, and Zr. Among these approaches, the defected and metal-decorated o-B_2N_2 monolayers with Na, K, Be, Mg, Ca, Sc, Y, and Zr did not demonstrate improvements in hydrogen storage properties. However, the o-B_2N_2 monolayer decorated with Ti showed promising results as a hydrogen storage medium, satisfying all the criteria established by the DOE. Therefore, based on our findings, Ti-

decorated o-B_2N_2 monolayers hold potential as efficient hydrogen storage materials, showcasing their suitability for future applications.

Thesis Outline:

The present thesis is organized as follows.

Chapter I : Introduction

This chapter provides an overview of the interconnected issues surrounding the energy crisis and pollution, highlighting their far-reaching consequences. In the following sections, we explore potential solutions to the energy crisis, focusing on the production of hydrogen through water splitting and its subsequent storage. We also examine the positive and negative aspects of various techniques used in water splitting and hydrogen storage. Furthermore, we investigate the advancements made in 2D nanomaterials for water splitting and hydrogen storage since the synthesis of graphene. We describe the selected materials for our study, including their properties, and explain the motivation behind conducting this research. Additionally, we present a literature survey that encompasses past experimental and theoretical work conducted on these materials.

Chapter II : Methodology

Chapter 2 provides a comprehensive overview of the computational methodology employed in this study. The chapter explores the theoretical foundations of density functional theory (DFT), which serves as the fundamental framework for calculating various properties of 2D materials. Key concepts including the Born-Oppenheimer approximation, Hartree approximation, Hartree-Fock approximation, and density-based methods are discussed in detail. Furthermore, Chapter 2 examines the importance of the Kohn-Sham equation in DFT applications. The chapter also explains the use of plane waves to represent electron wave functions and discusses the density

calculation techniques required for addressing valence and core electrons. Special emphasis is given to the implementation of these methods in the Quantum Espresso simulation code [39].

Chapter III : Single Atom Catalysts Supported on 2D α-SiX (X = N, P, As, Sb, Bi) and Holey Graphyne for HER activity

In this chapter, we present our work on TMs supported by α-SiX (X = N, P, As, Sb, Bi) and holey graphyne (HGY) monolayers as SACs to enhance the HER activity [26,27]. We systematically discuss the structural and electronic properties of both pristine and TMs-anchored monolayers as SACs using DFT simulations. Additionally, we analyze the effects of TMs on the supports by studying the partial density of states (PDOS), electronic band structure, charge transfer, and other relevant factors. To evaluate the suitability of the HER activity, we examine the changes in ΔG of the adsorbed hydrogen systems and compare them with previous reports. Furthermore, we discuss the room temperature stability of the predicted best HER catalyst using ab initio molecular dynamics (AIMD). Figure 1 below illustrates the results of ΔG for our studied systems.

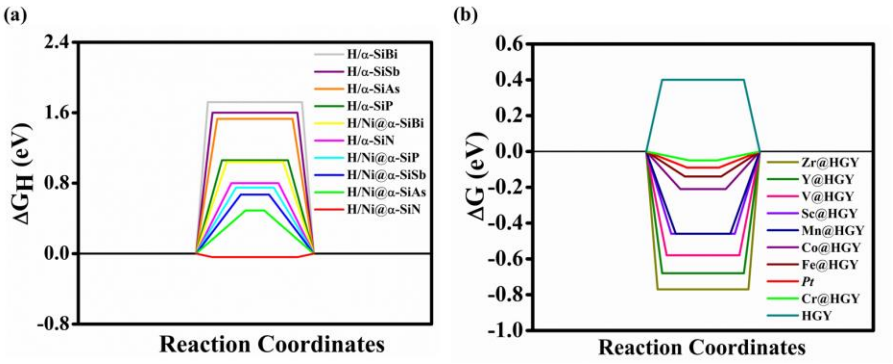

Figure 1: The change in the Gibbs free energy (ΔG) of H adsorbed α-SiX (a), HGY (b) and TMs decorated both monolayers.

Chapter IV: Defects and Doping Engineered 2D o-B_2N_2 for HER Activity

In this chapter, we discuss the structural and electronic properties, HER activity, and stability of the pristine, vacancy, and C-doped o-B_2N_2 monolayer [28]. The chapter includes a comparative analysis of the structural and electronic properties before and after introducing defects and C doping. For the HER analysis, we present the obtained ΔG values of the H-adsorbed pristine, defected, and C-doped monolayers and compare them with previous reports. In this study, we have discovered that C doping renders o-B_2N_2 metallic, making it suitable as an "electrocatalyst," while the BN vacancy-defected o-B_2N_2 monolayer exhibits semiconducting behavior with a band gap of approximately 1 eV, qualifying it as a "photocatalyst" for HER activity.

Chapter V : Hydrogen Storage in Defected and Metals Decorated 2D o-B_2N_2

This chapter focuss on studying the hydrogen storage application of the newly predicted o-B_2N_2 monolayer. We discuss the suitability of defected o-B_2N_2 monolayers, as well as o-B_2N_2 monolayers decorated with metals (Na, K, Be, Mg, Ca, Sc, Ti, Y, and Zr), for hydrogen storage. Our discussion in this chapter involves the calculation of various properties such as average adsorption energy, desorption temperature, hydrogen gravimetric density, and other electronic parameters using dispersion-corrected DFT simulations. We also validate the room temperature stability of the best case through AIMD simulations.

Chapter VI : Summary and Future Prospects

The last chapter concludes and summarizes the most important findings and potential applications of this thesis work. Additionally, it explores future research directions and the scope of 2D materials in the field of water splitting and hydrogen storage, incorporating an improved strategy and testimonials.

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List of publications related to thesis:

1. **Darshil Chodvadiya**, Prafulla K. Jha, and Brahmananda Chakraborty. "Theoretical inspection of Ni/α-SiX (X= N, P, As, Sb, Bi) Single-Atom catalyst: Ultra-high performance for hydrogen evolution reaction." ***International Journal of Hydrogen Energy (2022)*:** 47(99), 41733-41747.
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2. Bhautik R. Dhori, **Darshil Chodvadiya** and Prafulla K. Jha. "Evidence of topological phase transition with excellent catalytic activity in AgCaAs Heusler alloy: A first-principles investigation." *(Status: Submitted to The Journal of Physical Chemistry C).*
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