A review of the development of electrocatalysts to produce green hydrogen using Density Functional Theory

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Renewable energy is currently of great importance to cut the dependence on fossil fuel energy due to environmental concerns, political climate and the unstable global economy. One of the main United Nations Climate Change Conference (COP26 & 27) commitments was/is the energy transition to renewable energy in which green hydrogen is the promising route. Studies are still in progress towards the development of a viable electrocatalyst that will allow the commercial scale production of green hydrogen; this paper presents a review of the development or exploration of electrocatalyst thus far. All catalysts are benchmarked to Pt as a standard catalyst and the main reason for not using Pt is that it is a precious metal, therefore, the process is not economically viable on a commercial scale. For the hydrogen evolution from the water electrolysis process, well-known metal catalysts include Pt-based and Pd-based.

Hydrogen evolution catalysts are well known, and density functional theory (DFT) is the technique mainly used for predicting and explaining the experimental results intrinsically. The fundamental factors that must be taken into consideration when evaluating water electrocatalyst performance include thermodynamic adsorption of intermediate hydrogen on the catalyst active site, kinetic dissociation of water, electrode and electrolyte conductivity, the conductivity of the substrate, electrical contact between electrode and substrate, stability, active surface area and bubble effects.

DFT and experimental work have been used to computationally investigate affordable noble/base metals (Fe, Ni, Mo, etc.) in both different forms using the ($\Delta G°_H \approx 0$) criterion. A transition metal sulphide includes N-$NiCoS_4$, Ni_3S_2, Co_9S_8, WS_2, Ni-FeS_2, MoNiS@NiS/CC, P-MsO_2/Ni_3S_2/N, etc. A transition metal oxide includes NiN_3/MoO_2, Mo_2, CrO_x, C-$Ni_{1-x}O$, etc. A transition-metal dichalcogenide includes P-MoS_2 NSs, Ni-Co/1T-MoS_2, $FePSe_3$/NC, etc; carbon-based materials such as 3D graphene NWs, N,P-doped C NWs, EDA-CNTs, etc.; single-atom catalysts such as Pt SASs/AG, Ru@Co SAs/N–C, 400-SWMT/Pt, etc; as well as transition metal carbides or nitrides (MXenes) such as $Mo_2TiC_2T_x$-Pt_{SA}, $Ni_{0.9}Co_{0.1}$@Nb-Ti_3C_2T, Pt/$Ti_3C_2T_x$-550, etc.

Keywords: Renewable energy, green hydrogen, energy transition, electrocatalyst, hydrogen evolution, DFT

INTRODUCTION

Climate change and the rapid depletion of resources that are utilised as a primary source of energy, such as fossil fuels that are used to power houses, vehicles, industries, etc., are two current concerns facing the world (Energy, 2001). In addition to the issue of the rapid rate of depletion of these current energy sources (such as fossil fuels), the release of greenhouse gases during their transformation into usable energy is also a significant problem for environmental pollution that leads to issues like the rise in global temperature.

Therefore, renewable energy sources—also known as 'clean' or 'green' sources—can minimise or eliminate environmental pollution, have an endless supply, and quickly and organically replace themselves. The demand for renewable energy is rising.

There is growing interest of hydrogen around the world as a promising clean and sustainable energy that can meet the energy demand (Kirubakaran, *et al.,* 2009; Zeng & Zhang, 2010). Hydrogen can be produced by transformation of fossil fuels like natural gases, steam reforming, etc. Unfortunately, these processes still release CO_2 (Acar & Dincer, 2014). The technology that produces hydrogen in an environmentally friendly manner is the water electrolysis process which transforms renewable energy from solar, wind, hydrogen, etc. into high purity hydrogen (Randal, 2011).

Water electrolysis process involves a few technologies for the production of green hydrogen, namely, alkaline water electrolysis, solid oxide water electrolysis and proton exchange membrane water electrolysis (PEMWE) with each technology having its own drawbacks. PEMWE shows greater preferences/advantages over other technologies: such as simplicity, fast response, high current density, high purity of green H2 (Sun, *et al.,* 2018).

Although water electrolysis can produce green hydrogen, the major setback is the use of precious metals as electrodes, like platinum (Pt) for a cathode electrode which is operated in a very acidic condition (Yu, *et al*., 2010; Harriman, 2013). Due to the use of precious metals in PEMWE, this results in soaring capital expenditure for this system to be implemented, with an average cost of $7.1 per kg of H2 which is about five times more than that of producing H_2 using steam methane reforming (James, *et al*., 2013; Bertuccioli, *et al.,* 2014; Santos, *et al*., 2017). Therefore, the research work is intensified across the globe for the development of better catalyst for PEMWE cells in order to drive down the average cost of $7.1 per kg of H2. To addresses this issue of high average cost per kg of green H_2, density functional theory (DFT) is used in development on new materials.

In the political/governance sphere, the Prime Minister of Barbados, Mia Mottely, urged world leaders to have the greatest sense of urgency when it comes to combating climate change by funding the energy transition to renewable (green) energy at the recent UN climate conference UK 2021 (COP26) in Glasgow. In the South African context, President Cyril Ramaphosa acknowledged at the same COP26 that coal-powered fire stations in South Africa are the primary source of carbon emissions and that the plan for low carbon emission processes is urgently needed. The COP26 also reached a consensus that coal-fired systems should be decarbonised by the year 2030. (News24, 2021). Later, Ramaphosa declared that the United Kingdom, United States, European Union, Germany, and France had pledged R131 billion in funding.

LITERATURE

It is feasible to use a variety of techniques to create green hydrogen by water splitting. Although water can be electrolysed, thermalised, photolysed, or combination of both thermalised and photolysed; this research concentrates on the electrolysis process, which is represented by the chemical reaction in Eq. 1. (Kumar & Himabindu, 2019; Brauns & Thomas, 2020)). Due to economic constraints, just 4% of the hydrogen sold on the global market today is produced using water electrolysis (Cipriani, *et al*., 2014). This comprises PEMWE, SO, and microbial electrolysis cells (Kumar & Himabindu, 2019).

$$H_2O \rightarrow H_2 + 0.5\ O_2 \qquad \text{Eq. 1}$$

Electrolysis Thermodynamics

The Gibbs free energy ($\Delta_R G$) for the system may be determined using equation Eq. 2 below. The electrochemical reaction for the splitting of water requires energy from an external source for a cell voltage. As a result, equation Eq. 3 may be used to compute the reversible voltage (E_{rev}) where z is the number of exchanged electrons, which in the water splitting reaction is 1, $\Delta_R S$ is the entropy of the system and F is the Faradays constant, which has a value of 96485.3 C.mol-1.

$\Delta_R G = \Delta_R H - T\Delta_R S$ Eq. 2

$E_{rev} = -\frac{\Delta_R G}{zF}$ Eq. 3

Technique to Develop New Material

DFT derives from quantum theory and uses a specific method to solve the Schrödinger equation to build materials based on their electronic structure. The DFT electronic structure enables accurate computation of the electronic structure to determine the material's physical and chemical properties as well as the adjustment parameters for higher-scale techniques like kinetic Monte Carlo, cluster dynamics, and classical molecular dynamics (Freyss, 2015). The DFT depends on the atomic number of a specific atom rather than any empirical or modifiable factors, and the many-body issue is considered the same as the one-electron problem (Freyss, 2015). According to Freyss (2015), DFT has been used to determine structural and dynamical properties such as lattice structure, charge diversity, magnetisation, and more.

Freyss (2015) described how Kohn and Sham used the Schrödinger equation (Eq. 4) to create one electron Kohn-Sham equation where the wave function (r, R) is the function of radial location (r) for interacting electrons and nuclei at positions (R) rather than the typical cartesian coordinate system (x, y, z); $\psi(x, y, z)$ is the system wave function, H is called the Hamiltonian of the system and E is the total energy of the system Additionally, the Born-Oppenheimer approximation explanation demonstrates that the wave function depends on r because electrons move more quickly than dense nuclei and, as a result, exhibit no reliance on R. The foundation of DFT is the single-electron wave function and single charge density n(r), which is analogous to a system with many interacting electrons (DFT). According to the following two theorems by Hohenberg and (Hohenberg & Korn, 1964; Freyss, 2015), the ground state of an interacting electron system can be fundamentally characterised by the single-particle charge density n(r) as a variable, and the two theorems are as follows:

- All physical quantities of a system, total energy, in particular, are functional of electron density n(r).
- The real/ physical electron density of a system is the one that minimises the total energy of the system.

The total energy of a system can be calculated using a Schrödinger equation and is defined as in Eq. 5. The system's non-interacting electrons' kinetic energy is represented by the first term of the equation (Eq. 5). The second term accounts for Coulombic electron interaction, the third term for Coulombic electron interaction with nuclei, and the final term corrects the first term due to many-body electron interaction. The second, third, and fourth terms of Eq. 5 are used to calculate the system's effective potential, denoted by the symbol V_{eff}, as illustrated in Eq. 6. According to Eq. 8, the single-particle electron wave function is used to derive the electron charge density n(r), each electron wavefunction, and N is the total number of occupied states for all atoms.

$$H\psi(x, y, z) = E\psi(x, y, z) \qquad (Eq.4)$$

$$E[n] = -\frac{1}{2}\sum\int \phi_i^*(r)\nabla^2\phi_i dr + \frac{1}{2}\iint \frac{n(r)n'(r)}{|r-r'|} drdr' + \int V_{ext}(r, R)n(r)dr + E_{xc}[n(r)] \qquad (Eq.5)$$

$$V_{eff} = V_{ext}(r, R) + \int \frac{n'(r)}{|r-r'|}dr' + v_{xc}(r) \qquad (Eq.6)$$

$$and\ v_{xc}(r) = \frac{\partial E_{xc}}{\partial n(r)} \qquad (Eq.7)$$

$$n(r) = \sum_i^N |\phi_i(r)|^2 \qquad (Eq.8)$$

The Kohn-Sham equation, an eigenvalue problem with a formally exact solution that is similar to the Schrödinger equation for a single particle in Eq. 9, is created when the energy functional of a system is minimised in proportion to electron density, and h' is the Plank's constant over 2π (Freyss, 2015). Unfortunately, because $v_{xc}(r)$ is unknown, numerous approximations are utilised, including the local density approximation and many others that are explained in the study by Freyss (2015), and E_{xc} is the energy contribution from exchange correlation. The Bloch theorem also demonstrates how periodicity may be used to simplify the Kohn-Sham equation for crystalline structures, and it states that the Kohn-Sham equation can be expressed as the product of the plane wave function u and the periodicity of a crystal k as shown in Eq. 10. The Bloch theorem must therefore be satisfied when choosing the electron basis set, and the basis set function is the linear combination of the wave function, to solve the Kohn-Sham equation. The electron basis function that is selected distinguishes the DFT approach. Up until the requisite limit is reached for total energy, charge density, or potential, the Kohn-Sham equation is solved iteratively.

$$\left(\frac{-h'^2}{2m}\nabla^2 + V_{eff}\,(\mathrm{r})\right)\phi_i(\mathrm{r}) = \varepsilon_i\phi_i(\mathrm{r}) \qquad (Eq.9)$$

$$\phi_i(\mathrm{k},\mathrm{r}) = u_{i,k}(r)e^{ikr} \qquad (Eq.10)$$

Descriptors used in DFT

As the electrocatalyst system is represented mathematically using the DFT approach, and this section describes the descriptors that are employed.

Formation energy

The formation free energy of a compound containing elements from 1 to n is given as Eq. 11, and thorough calculations are reported by the formation energy physically describing the electrocatalyst (Persson, *et al.*, 2012).

$$\mu^0_{i=1,\dots,n} \equiv \Delta G^0_{i=1,\dots\dots,n} = G^0_{i=1,\dots,n} - \sum_{i=n}^{n}\mu_i^{ref} \qquad (Eq.11)$$

$where\ \mu^o = chemical\ potential$
$\Delta G = formation\ free\ energy$
$G = Gibbs\ free\ energy\ of\ the\ compound\ with\ i\ elements$
$\mu^0_{ref} = chemical\ potential\ of\ element\ i$

The formation energy criterion states that if the formation energy is less than zero, the electrocatalyst is energetically advantageous; if it is more than zero, the electrocatalyst's structure is not stable. (Liao, *et al.*, 2022). The technique has been used to screen, target, create, and build new electrocatalysts, as well as to evaluate their likelihood using DFT predictions and experimental data; as a result, it can be used as a guide (Chen, *et al.*, 2020; Zhao, *et al.*, 2019; Sun, *et al.*, 2019; Liu, *et al.*, 2016).

Adsorption energy

According to the Sabatier principle, adsorption energy is the force that binds the adsorbate to the electrocatalyst's active site (Medford, *et al.*, 2015; Che, 2013). Equation Eq. 12 is used to calculate the adsorption energy (ΔE_{ads}), which is the energy required to bind the adsorbate to the electrocatalyst. Additionally, $E_{cat/adsorbate}$ represents the energy of the complex formed by the adsorbate and electrocatalysts, while E_{cat} represents the energy of the electrocatalyst and $E_{adsorbate}$ is the energy of the adsorbate alone (Cheng, *et al.*, 2019; Sun, *et al.*, 2017). Strong binding forces can result in difficult desorption, conversion, and final products, while weak binding forces can prevent interaction reactions from occurring (Liao, *et al.*, 2022). Accordingly, the adsorption process needs the proper amount of energy. It should be noted that free energy is frequently employed as adsorption energy (ΔG_{ads}) (Zhang, *et al.*, 2019; Zheng, *et al.*, 2015).

$$\Delta E_{ads} = E_{cat/adsorbate} - E_{cat} - E_{adsorbate} \qquad (Eq.12)$$

The electrocatalytic reaction determines the appropriate/optimal range for adsorption energies, according to Liao *et al.,* (2022). In HER, the electrocatalysts that have hydrogen adsorption energies (ΔG_{*H}) closer to zero are the most promising; positive ΔG_{*H} values indicate poor adsorption, whereas negative values indicate poor desorption of H_2 (Wang, *et al.,* 2020; Zhang, *et al.*, 2019).

Scaling relations

Studies such as Abild-Pedersen *et al.*, (2007), Fernandez *et al.,* (2008), and Montemore & Medlin (2014) employed this method to correlate the same adsorbate adsorption energies from distinct systems/reactions. Scaling relation is used to perform correlation between different reaction species. Eq. 13, in which E_A and E_B are the adsorption energies from various species and systems, and m and b are the gradient and slope intercept, respectively, describing the mathematical relationship between species A and B.

$$E_A = \ mE_B - b \qquad (Eq. 13)$$

By correlating only one or two of the most adsorbed adsorbates, the scaling laws can also be applied to multi-step catalytic reactions occurring at the surface, simplifying the complex system (Peterson & Norskov, 2012; Chen, *et al.*, 2019; Montemore & Medlin, 2014; Garlyyev, *et al.*, 2019). The rate-limiting phase is then evidently the adsorption reaction when the species bind weakly on the surface, while the rate-limiting step is desorption when the species bind too strongly (Liao, *et al.*, 2022). This technique is employed for electrocatalyst computation screening (Montemore & Medlin, 2014).

***d*-Band Model**

The strength of adsorbing the adsorbate depends on the d-states of the metal, as demonstrated by the activity of transition-metal-based, which has been fully described by the d-band model theory by Nørskov and Hammer (Nørskov & Bligaard, 2007; Nørskov, *et al.*, 2009). The d-band centre (ϵ_d), which is computed as the local average of the d electron energies (Eq. 14), where x is the energy level and $\rho(x)$ is the density of states for the occupied/corresponding d-orbital, is used to mathematically quantify the impact of the d-band on adsorption interaction.

$$\epsilon_d = \frac{\int_{-\infty}^{\infty} x\rho(x)dx}{\int_{-\infty}^{\infty} \rho(x)dx} \qquad (Eq. 14)$$

In the study by Nørskov *et al.*, (2009), the d-band centre and the difference between the d-band centre and Fermi level ($\epsilon_d - \epsilon_F$) vs. adsorption energy was found to have a linear relationship. It is determined that the electrocatalyst built of transitional metal is most likely to have increased activity of the adsorption if ($\epsilon_d - \epsilon_F$) is close to zero (Xu & Mavrikakis, 2004). Generally speaking, the parameters that control the d-band model are d-band filling and bandwidth (Liao, *et al.*, 2022). If the filling level's bandwidth is fixed, the d-band centre increases and the adsorption interaction is improved when the number of d electrons increases. Otherwise, the number of d electrons cause the d-band filling level to shift upward and the d-band centre to shift downward to the lower energy level (Liao, *et al.*, 2022). The catalytic reaction process on transition metal-based surfaces that are alloys, doped, strain, and heterostructured is described by the d -band model. The orbital hybridisation that leads to an electron transfer in alloy electrocatalysts has a favourable impact on the d-band centre (Xiao, *et al.*, 2014; Stephens, *et al.*, 2012).

e_g Orbital occupations

Despite the d-band model's considerable success, it has one flaw that prevents it from splitting d-orbitals, which is what happens in the majority of situations with transitional metal oxides, where the metal is bonded (coordinated) by six ligands to create an octahedral complex (Wu, *et al.*, 2018). The core metal atom's d orbitals divide into lower-energy (t_{2_g} orbitals = d_{xyxy}, d_{xz}, d_{yz}) and higher-energy antibonding e_g orbitals = $d_{x^2-y^2}$, d_{z^2}) levels (Sun, *et al.*, 2019). The catalytic activity for the adsorption and desorption of intermediates is described by the filling state of the antibonding orbitals (e_g). The DFT estimated e_g filling state defines the electrocatalysts' activity; an approximate e_g value of one denotes the electrocatalysts' optimal activity for oxygen evolution reaction/oxygen reduction reaction (OER/ORR) (Sun, *et al.*, 2018). This e_g has been employed in the electrolysis process to achieve the best catalytic activity on oxide metals with (defect, strain doping, and surface reconstruction) (Sun, *et al.*, 2015; Liao, *et al*., 2022). Yi, *et al*., (2021) explained using DFT calculations of the filling state of the antibonding orbitals (e_g) why Ni and NiO showed an improved HER catalytic performance; this was due to strain on the surface resulting in the shift of the d-band centre.

Tools for DFT theoretical analysis

As DFT attempts to describe the electronic structure of the electrocatalyst as well as the mechanism of the reactions involved, this section explains the most commonly utilised analytical methods.

Bader charge

The Bader charge analysis is one of the charge population analyses that include the Hirshfeld charge, the Mulliken charge, and the Voronoi deformation density, each of which differs from the others due to the algorithm used. It is frequently used to analyse the charge distribution around the atom. An atomic charge can provide information about the electrocatalyst site's charge population and the surrounding bonding environment (Liao, *et al*., 2022). As electrons transfer during the adsorption reaction activates the reactants, it is widely known that improved electrocatalyst performance is due to interface charge transfer. In the study by Wu, *et al*., (2012), it is shown that graphyne high ORR activity is due to interface charge transfer, and this was verified using XPS spectra and computed DFT-based charge analysis.

Difference of charge density

There is a charge transfer occurring during the interaction between the electrocatalyst and intermediates, resulting in a variation in charge density. This establishes the bond strength, which in turn impacts the kinetics of the adsorption and desorption phases of a catalytic reaction. Difference of charge density is frequently employed in the search for novel electrocatalysts.

Electron localisation function

Electron localisation function (ELF) provides a value between 0 and 1 that represents the likelihood of finding the electron at a certain point (Savin, 2005). This number indicates the sort of bond that exists at that place. A value of 0.5 denotes a metallic bond with an electron that behaves like a gas, a value of 0.0 an ionic bond with a delocalised electron, and a value of 1 a pure covalent bond with a localised electron (Song, *et al*., 2019). ELF is utilised in DFT investigations to determine the kind and strength of the bond that exists between the catalytic surface and the adsorbate (Ying, *et al*., 2020).

Density of states

When using orbital analysis to study the orbital interaction of solids, the density of state (DOS) is a crucial tool. In contrast to insulators and semiconductors, which have a band gap at the Fermi level, it describes electrocatalyst as having metallic conductivity and electronic states that cross the Fermi level with no band gap (Deng, *et al*., 2019; Liang, *et al*., 2018). The DOS close to the Fermi level, as well as the high activity of an electrocatalyst being related to the abundance of states close to the Fermi level, and also related to the evolution and transfer of electrons on the electrocatalyst surface (Vojvodic, *et al*., 2014; Wang, *et al*., 2019). According to this theory, the peaks that have appeared in the DOS profile represent atoms with increased catalytic activity, making the profile spike a standout feature in the plot (Lu, *et al*., 2017).The d-band centre that describes the electrocatalytic activity of transitional metals is another extensively used method for DOS. As the intrinsic interactions are revealed by the coupling of molecular orbitals, the process that occurs during the interaction of the electrocatalyst surface and the adsorbate is typically investigated using the projected density of state. This proves there is a hybridisation taking place as different orbitals interact. In conclusion, the tools listed above assist with electrocatalyst development and understanding the catalytic mechanism that occurs during the interaction of the adsorbate and the electrocatalyst surface.

Classification of Hydrogen Evolution Electrocatalysts (HER)

In this section, different classes of HER electrocatalyst are presented, each class presents a modified electrocatalyst. The performance of an electrocatalyst against pristine material is compared by overpotential required to produce a current density of 10 mA.cm^{-2}; the lower the overpotential, the better the performance.

Transition metal sulphides

MoS_2 is one of the transition metal sulphides (TMS) materials that has been studied the most. MoNiS@NiS/CC demonstrated great performance and excellent stability, requiring, respectively, 68 mV and 33 mV overpotential to produce a current of 10 mA.cm^{-2} in 1M KOH and 0.5 M H_2SO_4 (Xie, *et al.*, 2020). According to the study, excellent performance was brought about by the metals' (Mo and Ni) interactions and synergistic effects. The performance may also be attributed to the defects on the heterointerface, which promotes the movement of electrons during the surface catalytic reaction and the release of generated gases. Other investigations using TMS for the development of hydrogen are summarised in Table I, and the overpotential was obtained experimentally with DFT as a tool to give fundamental insight.

Table I. HER transitional metal sulphide electrocatalyst

Pristine material	**Doped material**	**Overpotential and current density of pristine material (mV) and (mA.cm^{-2})**	**Overpotential and current density of doped material (mV) and (mA.cm^{-2})**	**Prediction technique/ study**	**Additional information**	**Reference**
$NiCoS_4$	N- $NiCoS_4$	210 and 10	41 and 10	X-ray photoelectron spectroscopy (XPS), synchrotron-based X-ray absorption spectroscopy (XAS), and (DFT)	-	(Wu, *et al.*, 2018)
FeS_2	Ni-FeS_2	260 and 10	126 and 10	XPS, XAS AND DFT	**DFT modelling** - CASTEP package in Materials Studio - PBE AND GGA exchange correlation	(Ye, *et al.*, 2021)
MoO_2/Ni_3S_2	P-MoO_2/Ni_3S_2/NF	-	95 and 10	-		(Jin, *et al.*, 2022)

Transition metal oxides (TMOs)

One of the most researched TMOs in HER is MoO_2. According to a study by (Kou, *et al.*, 2020) carboned doped NiO is now the best-performing TMO, with an extremely low overpotential of 27 mV to drive 10 mA.cm^{-2} in 1 M KOH solution. The doping enables advantageous intermediate H adsorption to the undercoordinated Ni sites. The stability of the materials and their potential for use on an industrial scale is not discussed in this paper. Other studies on TMOs are included in Table II below, and the overpotential was obtained experimentally with DFT as a tool to give fundamental insight.

Table II. HER transitional metal oxides electrocatalyst

Electrocatalyst	Electrolyte	Overpotential and current density of material (mV) and ($mA.cm^{-2}$)	Tafel Slope (mV. Dec^{-1})	Reference
NiO/Ni-CNT	1.0 M KOH	~90 and 10	~75	(Gong, *et al*., 2014)
NiO NRs-m-Ov	1.0 M KOH	110 and 10	100	(Zhang, *et al*., 2018)
Ni/NiO-250	1.0 M KOH	145 and 10	43	(Yan, *et al*., 2015)
Ni, Zn dual doped CoO	1.0 M KOH	53 and 10	47	(Ling, *et al*., 2019)
NiOx@BCNTs	1.0 M KOH	79 and 10	119	(Wang, *et al*., 2017)

Transition metal dichalcogenides

Free energy is utilised as the description for transition metal dichalcogenides (TMDs), which are well known and extensively studied due to their high performance and inexpensive cost in HER development and production. It is crucial to make it clear that TMDs are transitional metals that contain group 16 elements like sulphur and oxygen, among others. These consist of MoS_2 and MoO_2, which were previously covered in the sections on TMS and TMO, respectively. Other studies on TMDs are included in Table III below, and the overpotential was obtained experimentally with DFT as a tool to give fundamental insight.

Table III. HER transitional metal dichalcogenides electrocatalyst

Electrocatalyst	Electrolyte	Overpotential and current density of material (mV) and ($mA.cm^{-2}$)	Tafel slope (mV. Dec^{-1})	Reference
P-MoS_2 NSs	0.5 M H_2SO_4	43 and 10	34	(Liu, *et al*., 2017)
Ni-Co/1T-MoS_2	0.5 M H_2SO_4	70 and 10	38	(Li, *et al*., 2017)
$FePSe_3$/NC	0.5 M H_2SO_4	70 and 10	53	(Yu, *et al*., 2019)
MoS_2/Ni_3S_2	0.5 M H_2SO_4	98 and 10	61	(Yang, *et al*., 2017)

Carbon-based materials

When compared to other metal-based electrocatalysts, carbon- or carbo-based materials have features such as corrosion resistance, inertness, and oxidation resistivity, making them one of the most commonly investigated materials in HER studies (Zheng, *et al.*, 2014). It demonstrates that doping engineering activates the catalytic activities in carbons under the guidance of DFT. Graphene co-doped with N and P has shown improved HER performance, according to studies like Zheng *et al*., (2014). The works that reported on carbon-based materials in the HER field are summarised in Table IV below, and the overpotential was obtained experimentally with DFT as a tool to give fundamental insight.

Table IV. HER carbon-based materials electrocatalyst

Electrocatalyst	Electrolyte	Overpotential and current density of material (mV) and ($mA.cm^{-2}$)	Tafel slope (mV. Dec^{-1})	Reference
N,P-doped C NWs	0.5M H_2SO_4	163	89	(Zhang, *et al*., 2015)
g-C_3N_4/graphene	0.5M H_2SO_4	207	54	(Zhao, *et al*., 2014)
C_3N_4@NG	0.5 M H_2SO_4	240 and 10	51.5	(Zheng, *et al*., 2014)

Single-atom electrocatalysts

Single-atom electrocatalysts (SACs) were designed to use all of the active catalytic atoms in an electrocatalyst, thereby lowering the cost. Tong, *et al.*, (2021) anchored single Pt atoms on a porous nickel foam (Pt_1/N-Ni/NF), and obtained a low overpotential of 33 mV at 10 $mA.cm^{-2}$. Pt_1/N-Ni/NF andPt_1/FeO_x, a material created by inserting a single Pt atom, showed increased HER activity as a result of this SAC (Qiao, *et al.*, 2011). According to the DFT calculations, the excellent performance was caused by charge transfer between Pt and FeO_x or N-Ni/NF, which led to more unoccupied d orbitals in Pt and reduced the activation energy barrier. This method is also frequently applied in HER investigations; Cheng *et al.*, (2016) anchored single and clusters of Pt atoms in N-doped graphene nanosheets, which outperformed commercial Pt/C catalysts in terms of performance (higher HER activity and stability). The Pt charge transfer in the d orbitals also contributed to this spectacular performance. The charge transfer of a single atom, which directly impacts the electrons in the d orbitals, may be inferred as the basis for SAC. Table V summarises various studies of SAC in HER, and the overpotential was obtained experimentally with DFT as a tool to give fundamental insight.

Table V. HER single-atom electrocatalysts

Electrocatalyst	**Electrolyte**	**Overpotential and current density of material (mV) and ($mA.cm^{-2}$)**	**Tafel slope (mV. Dec^{-1})**	**Reference**
Pt–MoS_2	0.1 M H_2SO_4	~150 and 10	96	(Deng, *et al.*, 2015)
Pt SAs/DG	0.5 M H_2SO_4	23 and 10	25	(Qu, *et al.*, 2019)
Pd–MoS2	0.5 M H_2SO_4	78 and 10	62	(Luo, *et al.*, 2018)
400-SWMT/Pt	0.5 M H_2SO_4	27 and 10	38	(Tavakkoli, *et al.*, 2017)
PtSA-NT-NF	0.1 PBS	24 and 10	30	(Zhang, *et al.*, 2017)
Ru@Co SAs/N-C	1.0 M KOH	7 and 10	30	(Yuan, *et al.*, 2019)

Transition metal carbides or nitrides (MXenes)

MXenes, which were first proposed by Naguib *et al.*, (2011) are the newest class of material used in electrocatalysts for HER. The fact that these materials exhibit graphene-like characteristics led to the creation of the moniker MXene. In actuality, the term begins with MAX, where M stands for transitional metals, A for predominantly group 13 or 14 elements (Ga or Al), and X for mostly carbon or nitrogen. Ti_2C, V_2C, and Ti_3C_2, among many other compounds, are MXene-based. Conclusion: these materials are conductive under normal circumstances, allowing charge transfer during HER (Gao, *et a*l., 2016).

Table VI. HER transitional metal carbides or nitrides electrocatalyst

Electroatalyst	**Electrolyte**	**Overpotential and current density of material (mV) and ($mA.cm^{-2}$)**	**Tafel slope (mV. Dec^{-1})**	**Reference**
$Mo_2TiC_2T_x$-Pt_{SA}	0.5 M H_2SO_4	30 and 10	30	(Zhang, *et al.*, 2018)
$Ni_{0.9}Co_{0.1}$@Nb-$Ti_3C_2T_x$	1.0 M KOH	43.4 and 10	116	(Du, *et al.*, 2019)
Pt/$Ti_3C_2T_x$-550	0.1 M $HClO_4$	32.7 and 10	32.3	(Li, *et al.*, 2019)
Mo_2CT_x	0.5 M H_2SO_4	189 and 10	75	(Handoko, *et al.*, 2018)
CoP@3D Ti_3C_2T	1.0 M KOH	168 and 10	58	(Xiu, *et al.*, 2018)

CONCLUSION

In this review paper for the conference proceedings, we highlighted the importance of green hydrogen as an alternative for alleviating environmental concerns regarding the use of fossil fuels. Findings also showed that the South African government supports the United Nation's commitment to decarbonisation. DFT is the technology that can be employed to gain an insight about the electrode for water splitting to green hydrogen, and it also helps in developing a new electrocatalyst. The DFT descriptors include formation energy, adsorption energy, scaling relations, *d*-band model and e_g orbital occupations. A range of different electrocatalysts has been presented, and the search for an efficient and cheap electrocatalyst for HER that will allow a viable water electrolysis process that can be implemented to meet country/global energy demands is still underway. DFT is the technique that can facilitate the new development of such an electrocatalyst.

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