Beyond Platinum: Evaluating Alternative Transition Metals as Catalysts for the Hydrogen Evolution Reaction

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The pressing need to combat climate change drives the search for cleaner energy sources such as hydrogen. Hydrogen gas produced via the Hydrogen Evolution Reaction (HER) often uses platinum as a catalyst. While effective, platinum's high cost and supply risks make it unsustainable. This study uses Density Functional Theory (DFT) calculations to evaluate hydrogen absorption behavior across 20 transition metals, systematically comparing their adsorption energies and elemental abundance. Ideally, the alternative transition metal is abundant, affordable, and efficient. Using a computational density-grid simulation with GPAW in Google Colab, 20 transition metals were tested for their hydrogen absorption free energies to identify those closest to the ideal value of 0.0 eV. 0.0 eV measures the strength with which the reacted hydrogen gas sticks to the catalyst. If the eV value is too negative, the hydrogen sticks too strongly, whereas if it is too positive, it struggles to form intermediates. After testing, Copper and Tungsten were found to be the most promising alternatives to platinum-based catalysts, not just because of their eV values of -0.076 eV and 0.218 eV, but also because of their abundance in the Earth's crust of $\sim$60 ppm and $\sim$1.25 ppm, respectively. Although their hydrogen absorption free energies still deviate from the thermodynamic optimum more than platinum(111)'s verified value of $\sim$0 eV ΔG_H, their abundance is far greater than platinum's $\sim$0.005 ppm. These findings indicate that copper and tungsten may be promising catalyst candidates for further optimization because of their high abundance and favorable hydrogen absorption free energy values. However, their implementation is still dependent on additional factors, such as catalyst durability, production cost, and long-term performance, among others.

Keywords: Hydrogen Evolution Reaction (HER), Electrocatalyst, Copper Catalyst, Tungsten Catalyst, Density Functional Theory (DFT), transition metal Catalysts, hydrogen absorption Free Energy

Introduction

The urgent threat of climate change forces us to examine closely the sources and methods we use to generate energy[1]. Today, we continue to use energy that emits greenhouse gases, contributing to global warming[2]. However, as a replacement, the use of renewable energy with lower carbon emissions has expanded as well, such as the development of hydrogen-powered vehicles[3,4]. These vehicles rely on hydrogen gas, which is produced in part via the Hydrogen Evolution Reaction (HER), typically catalyzed by platinum-based catalysts[5]. Hydrogen fuel itself is zero-carbon at the point of use; emissions depend entirely on the production methods, which include the HER process. In the HER chemical process, water molecules are separated into hydrogen and oxygen atoms[5]. Specifically, the process converts the hydrogen in water into hydrogen gas, which can be used as an energy source[6]. However, traditionally, a catalyst is used to help facilitate the reaction, lowering the activation barrier for the reaction and reducing the overpotential. Platinum(Pt(111)) has been widely regarded as the benchmark catalyst for HER because its hydrogen absorption energy is near the thermoneutral optimum, allowing it to efficiently produce hydrogen gas[7]. Although hydrogen gas has the potential to become an effective energy source, its commercial production emits large amounts of greenhouse gases, which counter efforts to transition away from traditional energy sources[4,8]. Furthermore, the production cost is driven up by the use of platinum as a catalyst[9]. Ideally, an alternative catalyst for HER would be highly abundant, a porous structure (providing much more surface area for the hydrogen gas to react with the catalyst), low environmental impact (with minimal carbon emissions), and a secure supply chain (from a reliable, stable supply source)[9,10]. Although platinum has some of the above-mentioned qualities, its cost in hydrogen production is a major drawback[9]. For example, platinum is substantially more expensive than most transition metals considered in this study in addition to its supply chain vulnerabilities[9]. Furthermore, platinum can't be sourced reliably, as it is found in nations such as Russia and South Africa[11]. If we were to have a conflict with countries from which we source platinum, our energy system could be

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cut off. Another downside of using platinum is that mining it can produce significant carbon emissions[8]. In contrast, transition metals such as copper, tungsten, iron, and nickel are more abundant and are mined across a wider range of countries, providing a more stable and secure supply while reducing dependence on a single critical resource[12].

This research investigates transition metals aside from platinum as potential foundational metals for an HER catalyst. It specifically targets more abundant, lower-cost transition metals as candidates with hydrogen absorption free energies closest to the thermodynamic optimum.

Background/Literature Review

Catalysts speed up chemical reactions by lowering the energy barrier between reactants and products, saving energy[13,14]. Catalysts can also be based on transition metals such as iron, nickel, and platinum which are found in the d-block section in the middle of the periodic table[14]. Transition metals make suitable catalysts because they can exist as two (or more) different ions in compounds[14]. Examples are iron (II) oxide (FeO) and iron(III) oxide (Fe_2O_3) where Iron exists in various oxidation states. Catalysts are used in many industrial processes, such as converting the most damaging emissions from car engines, like platinum and rhodium, which act as catalysts to filter exhaust fumes[14].

Hydrogen fuel is an energy source that incorporates hydrogen gas to produce energy[6,15]. This can be used to power fuel cells, which can then be applied to cars and other electronics[15]. Hydrogen fuel itself has the potential to reduce greenhouse gas emissions when produced through low carbon output pathways[15]. HER process electrochemically reduces water or protons to produce hydrogen gas[6]. Naturally, the HER process uses hydrogenase (an enzyme) to act as a catalyst, while commercially, platinum is the standard[16].

Transition metals are a group of metals on the periodic table with specific properties, such as their characteristically high melting point, density, and thermal and electrical conductivity[17]. Most transition metals have distinct colors due to their individual d-d electronic transitions[17]. Some transition metals are magnetic because of their unpaired d electrons[17]. Lastly, most metals are used for their catalytic properties, acting as catalysts for industrial and biological processes[17].

Transition metals are particularly good catalysts because of their partially filled, readily accessible d-orbitals and their ability to readily accept and donate electrons, thereby changing oxidation states[14,18]. For the Hydrogen Evolution Reaction (HER), Platinum is a traditionally used catalyst to facilitate the reaction, but the emissions from platinum's use as a catalyst counteract the purpose of using hydrogen as a fuel[8]. This issue calls for exploring other transition metals as replacements for platinum as catalysts. Recent advancements even emphasize the modification of current foundational transition metal catalysts to achieve the stability and catalytic activity desired as instructional densities[4,18,19].

Copper is one of the transition metals that exhibits several properties that present it as a promising HER candidate[20]. Verma and Goel emphasize the emergence of copper-based catalysts, especially because of copper's abundance, inexpensiveness, and its conductivity[20]. Still, copper still has many drawbacks, the main one being that pure copper binds too weakly; however, its performance can be improved through defect engineering, alloying, heterostructure formation, and many other techniques[20]. This review highlights copper as a promising alternative, acting as a low-cost HER catalyst to replace platinum, noting that, through constant reiteration, copper could become a viable alternative[20].

Likewise, tungsten has exhibited properties especially promising for its use as a HER catalyst, noting its platinum like structures; abundant d-orbitals, contributing heavily to the optimization of the free energy; its high abundance; and its low cost[21]. Further, tungsten has always been a point of interest, undergoing numerous experiments individually or in a compound, such as WS2, which continues to show promising results that call for further enhancement[21]. These developments can be made through heteroatom doping, defect engineering, and single atom engineering which can help remove imperfections in the material and increase stability, likely improving its performance[21]. Ultimately, this review concludes that tungsten is one of the most promising non-precious transition metals as an HER catalyst, however additional work must be done in order to improve its stability and practicality[21].

The Hydrogen Evolution Reaction (HER) is a key process in all hydrogen energy production systems, in which water is electrochemically split via electrolysis to produce hydrogen and oxygen gases[22]. This process is typically facilitated by catalysts to reduce energy requirements, jump-start the reaction, and improve energy efficiency[22]. However, selecting an efficient catalyst is also critical, as catalysts often carry varying hydrogen absorption free energy and adsorption and desorption properties[22]. According to the Sabatier principle, an ideal HER catalyst should not only adsorb hydrogen strongly enough to promote the reaction, but also allow hydrogen to desorb readily, thereby maximizing catalytic activity and minimizing energy losses[23].

Traditionally, platinum catalysts are used in the HER and are regarded as the highest-performing catalysts because of their low overpotential and high catalytic activity[8]. However, their use reduces the benefits of hydrogen fuel, as the greenhouse gas emissions associated with platinum mining offset the environmental benefits of hydrogen fuel[8,9]. As a result, recent studies have focused on developing new electrocatalysts that perform as well as platinum yet are more abundant[9].

For that reason, transition metals such as tungsten, and cop-

per have emerged as promising alternatives for platinum due to their favorable electronic properties and catalytic potential[20].

As mentioned earlier, through various surface enhancements, a metal's performance as an HER catalyst can be modified, whether through metal doping, heterostructures, formation of nanoparticles, lower charge transfer resistance, and many others[24]. In particular, alloys and metal doping is one of the common strategies to enhance the catalytic properties[4,25]. For example, tungsten-based catalysts often exhibit higher electrical conductivity and hydrogen absorption, while nickel-based catalysts exhibit improved water-splitting efficiency[21,26]. Furthermore, non-oxide transition-metal phosphides, particularly when engineered as heterostructures, have also demonstrated strong catalytic capabilities and offer stability and scalability in the process[27].

Recently, nanomaterials such as Molybdenum sulfide (MoS_2) have been extensively studied for their applications in the HER process[28]. Current findings suggest that the addition of active sites provides far greater benefits to catalytic performance than intrinsic activity alone, meaning that increasing the number of available reaction sites benefits efficiency more than improving each individual site[28,29]. Other strategies include doping MoS_2 with transition metals to improve catalytic performance by altering conductivity, electronic structure, active-site availability, and overall HER efficiency[28,29].

Through single-atom engineering and nanostructuring, advancements have been made in catalyst design, enhancing performance in the HER process[29]. Through single-atom engineering, all atoms are exposed and accessible, enabling an optimized electron configuration that improves bonding and electron transfer[28,29]. On the other hand, nanostructuring helps expose more active sites, making them more efficient while requiring less energy through specific design[28]. Hybrid and heterostructured materials, such as transition-metal carbides, often exhibit significantly improved overpotentials and catalytic efficiency, highlighting the importance of atomic-level control in catalytic design[28–30].

Lastly, not only is the composition of the catalyst itself a critical factor during the HER process, but system-level considerations such as the reaction environment and stability also remain critical challenges[31]. For example, studies have shown that HER performance can vary significantly with environmental acidity, with current research focusing on improving HER performance in alkaline environments[31]. Next, other strategies have been tested to reduce side reactions and improve selectivity. However, issues such as material degradation still continue to persist[32].

Ultimately, current research emphasizes the further development of efficient, stable, and cost-effective HER catalysts through various material innovations, along with structure improvements[9,24,28]. While substantial advancements have been made, challenges such as long-term stability, scalability, and others persist, demanding further investigation in the field.

Research Question, Hypothesis, and Aim

Which of the 20 stable transition metals exhibit hydrogen absorption free energies most comparable to platinum while also offering greater abundance and practical availability, making them viable alternative catalysts for the Hydrogen Evolution Reaction?

Although prior literature has demonstrated the HER potential of several individual transition metals, few studies have systematically compared the hydrogen absorption free energies of all 20 stable transition metals. We hypothesize that abundant transition metals, particularly Copper and Tungsten, will exhibit hydrogen absorption free energies closest to Platinum and therefore emerge as the most promising low-cost alternatives for HER catalysis.

The questions this research seeks to answer are as follows.

1. Which transition metals can be an effective replacement for platinum in the Hydrogen Evolution Reaction (HER)?

2. What traits are effective in improving the production of hydrogen in HER?

Data were obtained by running simulations and processing 20 of the 38 known transition metals, as the other 18 are theoretical or have short half-lives. Google Colab was used to run the program, calculating the hydrogen absorption free energy for each of the 20 transition metals that were tested. For each metal, a variety of surface facets were tested, which indicated the Miller indices of the slabs (1,0,0; 1,1,1). Then, the returned hydrogen absorption energies were recorded in data tables for analysis. When analyzing the data, a suitable catalyst had to have a hydrogen absorption free energy close to 0.0eV–the closer, the better, because 0.0 eV represents the optimal binding strength according to the Sabatier principle. Values that are significantly more negative indicate that the binding strength between hydrogen and the catalyst is too strong, preventing hydrogen from easily desorbing, while, at the other end of the spectrum, hydrogen absorption free energies that are too positive indicate a binding strength too weak to facilitate the reaction. Platinum's effectiveness stems from its hydrogen absorption free energy of $\sim$0.0 eV, making the binding strength near perfect for the theoretical optimum[33].

The HER process involves the splitting of water molecules into oxygen and hydrogen gas (Equation 1). This occurs on the surface of the chosen catalyst, which is typically platinum, via a series of electrochemical steps. First, water molecules or protons adsorb onto the catalyst's active sites on the catalyst surface (Volmer step, Equation 2 or Equation 5). Then, the lone hydrogen atoms on the catalyst surface combine to form H2 gas through either surface recombination (Tafel step,

Equation 3 or Equation 6) or electrochemical desorption (Heyrovsky step, Equation 4).

These calculations were based on density functional theory (DFT), which is commonly used in surface-catalyst studies, using the PBE (Perdew–Burke–Ernzerhof) exchange-correlation functional. The catalyst surfaces were modeled as periodic slabs, which approximate the atomic geometry of active sites and enable reaction energy calculations. They are defined through Miller indices (e.g., (1,0,0), (1,1,1)). The hydrogen absorption Energies were calculated at standard conditions and reported in electron volts (eV). Although these models may provide insight into the general behavior of catalysts, they still fail to account for other external interactions, including but not limited to pressure, temperature, and electrolyte effects in real-world systems.

Eq 1: Overall HER Half Reaction

$$2H^+ + 2e^- \rightarrow H_2\uparrow \quad \text{(acidic conditions)}$$

$$2H_2O + 2e^- \rightarrow H_2\uparrow + 2OH^- \quad \text{(alkaline conditions)}$$

In Acidic Conditions (step-by-step)

Eq 2: Volmer step (hydrogen absorption/discharge)

$$H_3O^+ + e^- + * \leftrightarrow H^* + H_2O$$

Eq 3: Tafel step (hydrogen recombination)

$$2H^* \leftrightarrow H_2\uparrow + 2*$$

Eq 4: OR Heyrovsky step (electrochemical desorption)

$$H^* + H_3O^+ + e^- \leftrightarrow H_2\uparrow + H_2O + *$$

In Alkaline Condition

Eq 5: Volmer step

$$H_2O + e^- + * \leftrightarrow H^* + OH^-$$

Eq 6: Tafel step

$$2H^* \leftrightarrow H_2\uparrow + 2*$$

Eq 7: Heyrovsky Step

$$H_2O + H^* + e^- \leftrightarrow H_2\uparrow + OH^- + *$$

Where H^* represents the catalyst bonded to a hydrogen and $*$ represents a lone catalyst position[34].

Methods

The hydrogen absorption free energies across 20 transition metals were calculated using Density Functional Theory (DFT) with the GPAW electronic structure package executed in a Python environment on Google Colab.

Hydrogen absorption free energy was calculated according to $\Delta G_{H^*} = \Delta E_H + \Delta E_{ZPE} - T\Delta S$, where ΔG_{H^*} represents the approximate hydrogen absorption free energy of the catalyst; ΔE_H represents the absorption energy; ΔE_{ZPE} represents the approximate zero point energy, added to account for the additional energy the particle carries even at 0 K; and $T\Delta S$ represents the loss of entropy from the lone H_2 gas molecule when binding to the catalyst surface. Following the computational hydrogen electrode model, a combined correction of approximately 0.24 eV was applied[35,36]. Because the calculations were all deterministic rather than repeated experimental measurements, no inferential statistical analysis was performed. Instead, the metals were instead ranked according to their hydrogen absorption free energy and compared with descriptive analysis.

The atomic structures and electronic interactions were all modeled using the Projector-Augmented Wave (PAW) method. Then, the exchange-correlation was treated using Generalized Gradient Approximation (GGA) which was parameterized by Perdew, Burke, and Ernzerhof (PBE), which serves as the standard functional for most surface catalysts DFT calculations. A plane-wave basis was set with a kinetic energy cutoff of 340 eV, used to represent the electronic wavefunctions as a combination of plane waves. Additionally, $3\times3\times1$ k-point meshes were used to sample the electronic structure of each slab in a repeating space.

Although a hydrogen absorption free energy of $\sim$0 eV is widely accepted as the theoretical optimum for the HER, the calculated value for Pt(111) was -0.2786 eV, which differs from the accepted literature value of $\sim$0 eV because of the many computational approximations made. Consequently, the calculated value acts as a relative comparison among the transition metals using the same methodology, rather than an experimental prediction.

For each individual slab, rather than modeling entire crystal surfaces, periodic slab boundaries were created to simulate the extended surface. Additionally, the slab was created with vacuum spacing to ensure interactions between adjacent crystal slabs are minimized. Crystal facets of (1,0,0) and (1,1,1) were chosen specifically because of their thermodynamic stability compared to other facets because they are the lowest energy state of the crystal surface. Additionally, they are most commonly exposed to real crystal nanoparticles because of their low energy state.

Broyden–Fletcher–Goldfarb–Shanno (BFGS) optimization algorithm was used to identify the lowest energy configura-

tion of the hydrogen atom relative to the catalyst. Geometry optimization was needed because the initial hydrogen position was an approximation guess. Without optimization, the calculated absorption energy would be inaccurate unless 1.3 Å was the equilibrium adsorption configuration.

Initially, the hydrogen atom was placed 1.3 Å above the adsorption site; however, it was subsequently optimized before calculations began, ensuring that the atom was positioned in the lowest energy position. Before optimization, the H_2 reference energy is first calculated and saved. During the optimization, the bare slab is then optimized to ensure the lowest energy arrangement. With the energy calculated and saved, a hydrogen atom is added to the surface and re-optimized to bring hydrogen to its preferred height.

By calculating the reference energy, bare slab energy, and the slab energy interacting with a hydrogen atom, the formula $\Delta E_{H^*} = E_{slab+H} - E_{slab} - \frac{1}{2}E_{H_2}$ can be used to determine the absorption energy associated with transferring one atom of hydrogen gas onto the catalyst surface.

To account for the zero point energy of particles at 0 kelvin, an additional 0.04 eV is added to match the true energy for hydrogen absorption[35,36]. If we knew the particle had no energy at 0 kelvin, then we could then find the position of the particle, violating Heisenberg's Uncertainty Principle[35,36]. To account for the entropy lost because the gaseous hydrogen possesses much more rotational and translational energy compared to hydrogen bonded to the catalyst, an additional 0.20 eV was added, taken from a literature value that has been shown to work well with HER[35,36]. The DFT calculations provided the electronic absorption energy (ΔE_H), but to calculate the Gibbs free energy of absorption, an approximation was made, assuming the calculation to $\Delta G_{H^*} = \Delta E_{H^*} + 0.24$ eV to account for zero point energy and entropy[35,36].

Finally, the approximated Gibbs free energy was compared with the theoretical optimum of 0 eV. The best performing metals were also compared by their crustal abundance to evaluate alongside Gibbs free energy.

Results

The hydrogen absorption energies for all 20 chosen transition metals were obtained through DFT calculations performed on Google Colab. Analysis of these values across the various crystallographic surface facets using Miller-index notation (1,0,0; 1,1,1) has shown that both between elements and within individual metals, there can be considerable variations in hydrogen absorption free energies.

Six metals exhibited adsorption energies closest to the ideal value of 0.0 eV, as shown in Table 2. These metals include, Copper (Cu) with a hydrogen absorption free energy of -0.0758 eV, Iridium (Ir) with a hydrogen absorption free energy of -0.0893 eV, Osmium(Os) with a hydrogen absorption free energy of -0.1812 eV, Tungsten (W) with a hydrogen absorption free energy of 0.2178 eV, Silver (Ag) with a hydrogen absorption free energy of 0.2251 eV, and Rhodium (Rh) with a hydrogen absorption free energy of -0.2282 eV. Platinum, the current industry standard, has exhibited a hydrogen absorption free energy of $\sim$0.0 eV, serving as the benchmark for comparison[33].

As shown in Table 3, the difference in hydrogen absorption free energy between platinum and the six different catalysts ranges between 0.0504 eV and 0.5183 eV. Rhodium shows the slightest deviation, with a difference of 0.0504 eV, followed by Osmium with a difference of 0.0974 eV. The remaining candidates (Iridium, Copper, Tungsten, and Silver) show progressively increasing deviations, ranging from 0.1893 eV with iridium to 0.5037 eV with silver.

However, catalytic performance alone doesn't determine the element's practicality, as other factors such as practical deployment require consideration of crustal abundance, global reserves, annual production capacity, market price, supply-chain security, environmental and social impacts of mining and refining, catalyst loading, and long-term operational lifetime, in addition to performance. Although this study primarily compares crustal abundance as an indication of availability, there are other factors important to consider.

Table 4 presents the crustal abundance of each candidate metal in parts per million (ppm), revealing significant disparities among the candidates. Copper is the most abundant at 60 ppm, followed by tungsten at 1.25 ppm. In stark contrast, the other elements have extremely low ppm levels, such as silver (0.075 ppm), iridium (0.001 ppm), rhodium (0.001 ppm) and osmium (0.001 ppm), with iridium, rhodium, and osmium all below platinum's abundance of 0.005 ppm.

By combining the performance data in Table 2 and Table 3 with the abundance data in Table 4, copper and tungsten emerge as the most promising candidates for replacing platinum in the HER process. Both metals exhibit adsorption energies relatively similar to those of platinum, with reasonable deviations from the desired 0.0 eV, while also maintaining sufficient crustal abundance to support large-scale industrial application. Copper offers superior abundance and is the closest match to platinum's performance among the two. Although tungsten exhibits a larger deviation from platinum than copper, its relatively high crustal abundance compared with the remaining candidates still makes it an important material to explore, as diversifying our options not only helps better protect the industry but also broadens the range of potential catalyst designs for future research.

Table 1 highlights the most promising metal candidates (metals with hydrogen absorption free energies closest to the optimal value of 0.0 eV) and their hydrogen absorption free energies, demonstrating how similar they are to platinum and highlighting them as potential substitutes.

Table 1 CLOSEST METALS CANDIDATES AND THEIR ADSORPTION FREE ENERGY

Metal	Facet	hydrogen absorption Free Energy (eV)
Platinum (Pt)	(1,0,0)	-0.2786 eV
Rhodium (Rh)	(1,1,1)	-0.2282 eV
Tungsten (W)	(1,1,1)	0.2178 eV
Osmium (Os)	(1,1,1)	-0.1812 eV
Copper (Cu)	(1,1,1)	-0.0758 eV
Iridium (Ir)	(1,1,1)	-0.0893 eV
Silver (Ag)	(1,1,1)	0.2251 eV

Table 2 METAL TYPES AND REACTION ENERGY IN CHART.

Metal	Reaction Energy (eV)
Rhodium (Rh)	-0.2282 eV
Osmium (Os)	-0.1812 eV
Copper (Cu)	-0.0758 eV
Iridium (Ir)	-0.0893 eV
Tungsten (W)	0.2178 eV
Silver (Ag)	0.2251 eV
Platinum (Pt)	-0.2786 eV

Table 2 ranks the candidates for substitution by reaction energy, showing clearly how each material approaches the optimal catalytic value.

Table 3 Metal Types and Difference in eV from Platinum

Metal	Difference in eV from Platinum
Rhodium (Rh)	0.0504 eV
Osmium (Os)	0.0974 eV
Iridium (Ir)	0.1893 eV
Copper (Cu)	0.2028 eV
Tungsten (W)	0.4964 eV
Silver (Ag)	0.5037 eV

Table 3 ranks the metals by the difference between their adsorption free energy and that of platinum, illustrating their relative catalytic performance.

Table 4 Metal Types and Abundance in Parts per Million

Metal	Abundance in parts per million (ppm)
Copper (Cu)	∼60 ppm (parts per million)
Platinum (Pt)	∼0.005 ppm (5 ppb, parts per billion)
Tungsten (W)	∼1.25 ppm (parts per million)
Silver (Ag)	∼0.075 ppm (parts per million)
Iridium (Ir)	∼0.001 ppm (1 ppb, parts per billion)
Osmium (Os)	∼0.001 ppm (1 ppb, parts per billion)
Rhodium (Rh)	∼0.001 ppm (1 ppb, parts per billion)

Table 4 summarizes each metal candidate's abundance in parts per million, enabling comparison of platinum with other metals and providing insight into their practicality.

Discussion

The data showed that copper, iridium, osmium, tungsten, silver, and rhodium were the most successful elements. The hydrogen absorption free energies were –0.0758, –0.0893, -0.1812, 0.2178, 0.2251, and –0.2282, respectively. These findings are consistent with recent findings that identify those metals as good foundational elements for catalyst development, particularly when combined into compounds, alloys, metallenes, and other forms. The hydrogen absorption free energy exhibited by copper was one of the closest to the theoretical optimum with a distance of 0.0758 eV from the optimum. This agrees with recent studies identifying copper-based catalysts as promising HER materials, noting both its abundance and conductivity. But because of its poor binding at a pure state, the authors acknowledge that pure copper still has its limitations that can be improved through defects, interfaces, and alloying[37]. Additionally, other studies have shown electrochemically activated copper-based catalysts exhibiting low tafel slopes, with slopes ranging from 96–109 mV/dec, along with long term stability, highlighting the potential copper-based catalysts have when carefully engineered[38]. Similarly, tungsten exhibited one of the hydrogen absorption free energies closest to the thermoneutral optimum, agreeing with recent studies which emphasize its promising HER activity, but often requiring a nanostructure or compound form in order to achieve highest performance[20]. Likewise, other experimental studies have supported tungsten-based catalysts as well, noting the high performance of W_2C nanoparticles, with overpotentials of 123 mV at 10 mA/cm^2 and tafel slopes as low as 45 mV/dec. This too, supports the favorable behavior exhibited by tungsten predicted by the study[39,40]. Finally, although iridium, osmium, and rhodium had exhibited hydrogen absorption free energies near the optimum, which agrees with recent literature that emphasizes iridium's excellent activity and durability; osmium's high performance when conjugated with platinum, even outperforming the benchmark; and rhodium's high performance when incorporated into the surface of graphitic carbon-covered Ni nanospheres, due to the rarity of those metals on Earth, they were excluded from consideration as replacement base catalysts for platinum in the HER process[41,42]. In contrast, copper is one of the most abundant industrial metals, with extensive global mining and refining infrastructure. This means that there is limited risk of major supply chain disruptions and a relatively stable price for copper which has remained at an average of $3.40 per pound[43]. Although the crustal abundance gives an initial indication of material availability, practical catalyst selection also depends on economically recoverable reserves, annual production volume, market price, refining concentration, supply-chain security, environmental impacts, catalyst loading, operational lifetime, and catalytic activity per unit cost, a comprehensive technoeconomic

discussion of the metal would be required to truly understand the availability of the metal. However, this requires an analysis delving into the lifetime of the metal/catalyst, its recyclability, and overall cost of production, going far beyond the scope of the study. Of the original 20 elements, copper, tungsten, and silver were the remaining elements that performed well while also being relatively abundant on Earth. Of these three, copper was the closest to the ideal hydrogen absorption free energy, with a value of –0.0758 eV. In addition to its favorable adsorption energy, copper is also the most abundant of the three, making it a particularly promising candidate for large-scale HER applications. Tungsten is also produced on an industrial scale with vast infrastructure for mass tungsten production, making it not only more available than platinum group metals, but also acts as another attractive alternative for potential catalyst foundation alternatives. Additional literature has also shown support for the use of both copper and tungsten as potential foundational catalysts for the hydrogen evolution reaction. Qian et al supports our finding, emphasizing how various strategies to improve copper have highlighted its potential as an active, durable, and plentiful replacement for platinum; however, there remains a large gap between concept and true implementation, such as atomic-scale engineering, advanced characterization techniques, and DFT- and machine learning-guided catalyst design to improve their performance[44]. Verma J.; Goel S. similarly, highlights tungsten's potential as a catalyst, noting both the stability and price of a tungsten cobalt compound makes it a strong candidate for the HER[45]. Based on the simulation results and the literature review, copper and tungsten emerge as potential foundational elements for the development of new HER catalysts, due to their abundance in the Earth's crust, in addition to their similar hydrogen absorption free energy to platinum[7,9,13]. This suggests that copper and tungsten based catalysts warrant further investigation. Catalyst development remains a significant challenge limiting the deployment of hydrogen gas as a low carbon emission alternative[7,21]. However, by identifying elements with both high abundance and adsorption energy close to the thermodynamic optimum ($\Delta G_H \sim 0$ eV), such as copper and tungsten, we can develop a more efficient HER method, making large scale hydrogen gas production a feasible goal and reintroducing hydrogen as a viable energy source[6,18].

Limitations

The study relied on computer simulations rather than physical laboratory experiments, so errors and simplifications must be taken into account, such as surface idealization; approximated thermodynamic adjustments and pressure; explicit solvent, electrolyte effects, or acidity; and limited facet sampling, due to computational models that do not fully capture real-world performance. Often, simulations are simplifications of real-world systems, omitting certain atomic-scale interactions or environmental conditions to remain computationally feasible, as if each variable were taken into consideration, the computational requirements would surpass what is currently practical or feasible. As a result, our models share a similar principle, with simplifications that introduce slight errors in order to make the calculations computationally feasible. Furthermore, only a singular hydrogen absorption configuration was evaluated for each surface. Usually, larger structures include other interactions that can alter the absorption energy and behavior of the catalyst, but by only modeling a singular interaction, other interactions are removed. Additionally, the tested performance metrics were limited to hydrogen absorption free energy, with factors such as long-term stability, corrosion resistance, time-dependent performance degradation, overpotential, conductivity, surface stability, reconstruction effects, catalyst poisoning, and applied potential excluded from the study's scope, instead applying identical computational methods and parameters to each metal and surface because of the simplifications made. The results of this study intend to provide a general trend of catalytic performance, rather than precise quantitative predictions of hydrogen absorption free energies because minute changes to variables unaccounted already significantly shift resulting values such as pH and applied potential. Other approximations were made during the DFT calculations, such as the PBE exchange-correlation functional which in itself is an approximation, making predictions roughly between 0.05-0.2eV away and introducing slight errors. Moreover, the idealized crystal surfaces, although making the calculations much less computationally straining, ignore typical defects that could affect HER performance for the better or worse. The structures modeled were simply optimized geometries rather than dynamic surfaces, meaning that any kind of restructuring wasn't considered. Finally, although ΔG_H is a good indicator for HER performance, it cannot independently describe the catalytic performance, often requiring additional information such as reaction kinetics and charge-transfer processes.

Future Work

Future work should focus on experimental validation, conducting laboratory experiments to synthesize copper and tungsten-based catalysts, measuring actual performance in electrochemical cells, and comparing the experimental results with computational predictions to validate the model. Then, further optimization could include testing additional facets and orientations beyond those examined by the Miller indices, exploring additional modification techniques to enhance catalytic capabilities, and potentially creating alloys beyond tungsten-sulfur to combine the advantages of both metals, as only pure elemental metal surfaces were tested. Typically, the

highest performing catalysts utilize alloys, heterostructures, or supported catalysts. Lastly, although the hydrogen absorption free energy of copper and tungsten based catalysts indicated high performance, that energy alone cannot predict the durability and stability of the metals. These properties were beyond the scope of this project, and in the future, the catalysts should be tested to assess long-term performance, catalytic degradation, performance under extreme pH conditions, and its resistance to catalyst poisoning.

Significance

Accessible HER catalysts could accelerate the adoption of low-carbon hydrogen technologies by reducing cost and improving the feasibility of water electrolysis. This could play a significant role in California's transition to fully electric cars by 2035 with the Advanced Clean Cars II rule, and in the push towards a general reduction of our carbon footprint. This tool will have a significant impact on developing nations and lower-income communities, helping create jobs in the green energy sectors and could contribute to lower catalyst cost. The timeline for hydrogen-powered energy can play out shorter or longer than expected, due to a wide variety of factors that could affect the development of hydrogen's commercial use. Optimistically, pilot-scale systems could emerge within 5-10 years, and commercial use will be available within 10-20 years, but this depends entirely on experimental validation, industrial investment, and support for hydrogen infrastructure.

Conclusion

In this research, the focus was on identifying alternative transition metals that could serve as viable candidate alternatives for platinum, a catalyst in the hydrogen evolution reaction (HER)—after calculating the hydrogen absorption free energies of 20 transition metals using DFT and GPAW approximations (which can be found in the supplemental information), copper and tungsten emerged as the most promising foundational metals for alloy/compound systems, with free energies close to 0.0 eV. This finding is supported by the literature, which shows that other researchers have reached similar conclusions. Furthermore, both copper and tungsten are relatively abundant on Earth.

These two metals offer a potentially favorable combination of hydrogen absorption free energy and crustal abundance which makes them stronger candidates for further research and development in hydrogen production technologies.

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