Exploring Topological Materials for Hydrogen Evolution Reaction: Insights from Density Functional Theory

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Abstract

Hydrogen energy technologies offer a transformative shift toward reducing reliance on fossil fuels and creating a sustainable, low-carbon future. In this shift, topological materials, known for their strong electron interactions and unique physical properties, present promising opportunities in electrocatalysis. In this study, we performed a systematic density functional theory (DFT) analysis of over 100 topological materials and examined more than 1,000 adsorption sites. Our findings

reveal that topological materials possess abundant active sites, resulting in a wide range of hydrogen adsorption energy ranging from -1.5 to 0 eV. To identify the most promising catalysts for hydrogen evolution reaction (HER) in acidic media, we focused on the topological materials with hydrogen adsorption energies within -0.27 ± 0.1 eV. By evaluating their Gibbs free energy ΔG values for HER, we found that all selected materials had ΔG values between -0.31 and -0.16 eV, enabling the identification of 11 promising candidates with high potential for effective HER activity. Our study provides valuable insights and guidelines for further exploration of topological materials as high-performance HER catalysts.

1. Introduction

Hydrogen energy technologies have been recognized as a promising candidate to reduce dependence on fossil fuels and meet future energy demands [1, 2]. Currently, fossil fuels, including natural gas, coal, and oil, account for approximately 80% of the world's energy consumption.[3] The combustion of fossil fuels releases large amounts of greenhouse gases, leading to more severe weather events, rising sea levels, and declining biodiversity. Additionally, it also fuels geopolitical conflicts and energy security concerns due to the unequal distribution of reserves.[4, 5] In response to these growing environmental concerns and energy security challenges, hydrogen has the potential to drive the global transition toward a more sustainable, low-carbon future.[6]

The development of highly efficient, selective, stable, and cost-effective catalysts for the water-splitting process is the crucial step toward thriving hydrogen economy. Utilizing electrocatalysts along with electricity from renewable sources for hydrogen evolution reaction (HER) is one of the most promising approaches. Platinum-group metals, especially platinum and its alloys, have emerged as the most effective electrocatalysts for this process.[7-9] Among them, the ultralow-Pt-loading electrocatalysts, which can reach the balance of low cost and high HER performance, have attracted much attention. Wang *et al.* demonstrated that anchoring platinum clusters onto two-dimensional fullerene nanosheets (PtC_{60}) significantly boost platinum's activity for the alkaline HER. This PtC_{60} composite shows 12 times higher intrinsic activity compared to the traditional Pt/C catalyst in alkaline condition.[10] Hodnik *et al.* reported a novel composite catalyst consisting of Pt nanoparticles supported on $TiON_x$ ($Pt/TiON_x$), which outperformed the benchmark Pt/C catalyst

regarding both HER activity and stability in acid electrolytes.[11] Other transition metals (Co, Fe, Mo, Ni, *etc.*) have also been explored as effective electrocatalysts for HER in recent years to confront the scarcity and high cost of Pt. [12-15] At the same time, single-atom catalysts (SACs) are also receiving increasing attention due to the maximized atom utilization efficiency arising from their abundant active sites.[16-18] Yet, the search for electrocatalysts simultaneously combining high activity, selectivity, stability, and cost-effectiveness remains ongoing.

Topological materials, known for their strong electron interactions and distinctive physical properties, provide exciting new opportunities in the field of electrocatalysis.[19, 20] With their unique surface states and exceptional charge mobility, they emerge as highly effective electrocatalysts capable of addressing the limitations of current hydrogen production technologies.[21] Keong *et al*. found that Bi_2Te_3 topological insulator thin films, when having partially oxidized surfaces or tellurium vacancies, show high activity for HER, with a current density reaching up to 1.74 μA cm^{-2} for a 48 nm Bi_2Te_3 thin film.[22] Our group has explored the topological nodal-line semimetal $AuSn_4$, discovering that oxidized $AuSn_4$ can be an effective catalyst for HER in alkaline media.[23]

Despite numerous efforts, the search for the optimal electrocatalyst for HER remains ongoing. In this work, we conduct density functional theory (DFT) calculations to systematically screen topological materials, aiming to identify high-performance topological material catalysts specifically suited for HER. Our study screens 1,000 sites across nearly 100 surfaces of topological materials, and identifies 11 topological materials promising as superior electrocatalysts for HER. Our study not only helps better understand topological materials and how they relate to HER but also provides guidance for future research in material synthesis and electrochemistry towards developing more effective HER catalysts.

2. Calculational Method

The DFT calculations were performed by using the plane-wave-based Vienna Ab initio Simulation Package (VASP 5.4.1).[24, 25] The exchange-correlation interactions were modeled by the Perdew, Burke, and Ernzerhof (PBE) functional within the framework of the generalized gradient approximation (GGA),[26] while the core electrons interaction was described with the projector augmented wave (PAW)

method.[27-29] The force and energy convergence criteria were set at 0.02 eV $Å^{-1}$ and 10^{-6} eV, respectively. The first Brillouin zone was sampled with a 3 × 3 × 1 k-point grid using the Monkhorst–Pack scheme. The long-range van der Waals correction was performed by adopting Grimme's DFT-D3 method.[30] The adsorption energies (E_{ads}) of the proton were calculated as $E_{ads} = E_{total} - E_{surf} - E_H$, where E_{total}, E_{surf}, and E_H represent the energies of optimized adsorption configurations, empty model surface, and half of the H_2 molecule, respectively. The HER performance was evaluated by the Gibbs free energy of the reaction (ΔG_{H^*} was calculated by: $\Delta G_{H^*} = \Delta E_{H^*} + \Delta ZPE - T\Delta S$, where ΔE_{H^*} is the energy difference of E_{ads}, and ΔZPE and ΔS are the changes of zero-point energy and entropy of H* adsorption, respectively). In this study, TΔS and ΔZPE were obtained by following the scheme proposed by Nørskov *et al*.[31]

3. Results and Discussion

3.1 Adsorption sites

The intricate surface structure of topological materials provides rich reaction sites, which make the topological materials promising in the field of catalyst. Given that low crystal facets are more energy favorable that they are more friendly to synthesis, in this study, we focus on all the low-index crystal facets, include: (001), (100), (101), (110), and (111) surfaces (Figure 1). As expected, they provide rich reaction sites with various conditions, which may lead to more active sites available for enhanced activities.

To make the study more systematic, our investigation meticulously explores all potential reaction sites on each surface with all possible terminations, including top sites, bridge sites, hollow sites (Figure 1a). A comprehensive analysis of catalytic performance at each site was conducted to identify the most stable adsorption site.

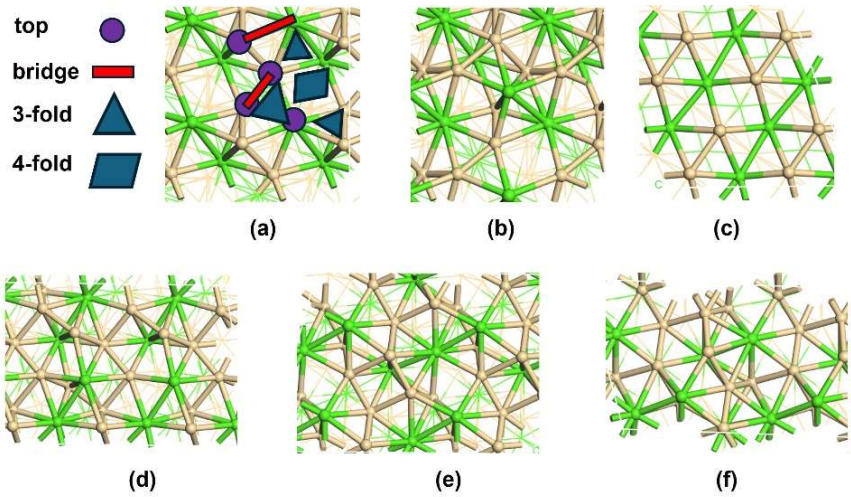


Figure 1. All the possible low-index facets and adsorption sites studied in this work. Panels a and b show Cr_1Ce_1 (001) surface with Cr and Ce termination, respectively; c ~ f :(100), (101), (110) and (111) surfaces. Green and ochre spheres represent Cr and Ce atoms, respectively. The different adsorption sites: top, bridge, 3-fold and 4-fold hollow sites are illustrated in Figure 1a.

3.2 Adsorption energies

Adsorption plays a crucial role in surface reactions, as an ideal catalyst should have an intermediate binding affinity for reactants. The adsorption needs to be strong enough to facilitate the reaction but not so strong that it prevents the easy desorption of the products.[32] The adsorption energy of hydrogen on topological material varies in a wide range, as summarized in Table 1. On Al_1Pt_1 (001), the hydrogen prefers the Pt-top site with an E_{ads} calculated to be 0.57 eV, which indicates that the adsorption of hydrogen on Al_1Pt_1 is endothermic that the adsorption is not energy favorable. As a result, Al_1Pt_1 (001) is expected to be nonactive towards HER because the adsorption is not energetically favorable, and this makes subsequent reactions hard to take place. While on Al_1Au_1 (110) surface, the hydrogen prefers the Al-top side with an E_{ads} calculated to be -2.22 eV, indicating a strong binding between hydrogen and Al_1Au_1(110) surface. However, such a strong binding corresponds to the high energy cost of release of hydrogen from the substrate. Thus, the activity of Al_1Au_1 (110) towards HER is expected to be nonactive either.

We have conducted a statistical analysis and found that the adsorption energies of hydrogen atoms on the surfaces of topological materials predominantly fall within the range of -1.5 to 0 eV. As a result, we selected candidates whose E_{ads} values satisfy

these criteria. This focus was also motivated by the observation that the systems with E_{ads} outside this range tend to bind hydrogen either too weakly or too strongly, making them unsuitable for further consideration. As summarized in Figure 2, the topological materials exhibit a well-distributed range of E_{ads} values, highlighting their potential to provide abundant active sites. In addition, most of the selected topological materials possess a moderate adsorption capacity for hydrogen atoms, making them promising candidates for efficient HER.

Table 1. The most favorable adsorption sites for hydrogen on various topological materials: the E_{ads} (in eV) values at the most favorable adsorption sites are listed. The suffixes _t, _b and _h at the column sites are short for top, bridge and hollow sites, respectively.

Material	E_{ads}	sites	Material	E_{ads}	sites	Material	E_{ads}	sites
Al_1Pd_1_001	-0.18	Al-Pd-bri	Al_1La_1_111	-0.88	Al-La_b	C_1Hf_1_111	-2.16	Hf-Hf_h
Al_1Pt_1_001	0.57	Pt-top	Ba_1Sn_1_111	-0.38	BaBaBa _h	C_1Ti_2_101	-1.21	Ti3_h
Au_1Be_1_001	-0.07	Au-Be_b	Ba_2Zn_1_111	-0.47	ZnZnZn_h	C_1Ti_2_110	-1.19	Ti-Ti_b
Co_1Ge_1_001	-0.18	Co_t	Bi_1Li_1_111	-0.14	Bi-Li_b	C_1Ti_2_111	-1.27	Ti3_h
Co_1Si_1_001	-0.48	Co-Co_b	Al_1Au_1_110	-2.22	Al_t	C_1V_2_101	-1.05	V-V_b
Cr_1Ge_1_001	-0.42	Cr-Cr_b	Al_1La_1_110	-0.61	Al-La_b	Cu_1Ti_2_001	-1.06	Cu3_h
Cr_1Si_1_001	-0.39	Cr-Cr_b	Al_1Sc_1_110	-0.75	Al-Al-Sc_h	Cu_1Ti_2_111	-0.94	CuTi_h
Fe_1Pd_1_001	-0.94	Fe_t	Al_1La_1_001	-0.50	La-La_b	Fe_1Pt_1_100	-0.49	Pt_t
Ga_1Pt_1_001	-0.29	Pt_t	Al_1Pt_2_001	-0.78	Al_t	Fe_1Pt_1_101	-0.52	Fe-Fe-Pt_h
Ge_1Mn_1_001	-0.13	Mn-Mn_b	Al_1Sc_1_001[2]	-0.51	AlAl_b	Fe_1Pt_1_110	-4.20	NA
Ge_1Rh_1_001	-0.03	Rh_t	As_1Rh_1_001	-0.15	Rh-Rh_b	Fe_1Pt_1_111	-2.45	Fe_t
Hf_1Sb_1_001	-0.54	Hf-Hf_b	As_2U_1_001	-0.31	As_t	Ga_1Mn_1_001	-0.84	Ga-Mn_b
Hf_1Sn_1_001	-0.66	Hf-Hf_b	C_1Ni_1_001	-0.01	Ni-Ni_h	Ga_1Sc_1_001	-0.55	Ga_t
Mn_1Si_1_001	-0.26	Mn-Si_b	C_1W_1_001	-0.71	W-W_h	Ga_1Sc_1_100	-0.41	Ga-Sc_b
Ni_1Si_1_001	-0.20	Si_t	C_1Zr_1_001	-1.34	Zr-Zr_h	Ga_1Sc_1_101	-0.95	Ga-Sc_b
Re_1Si_1_001	-0.54	Re_t	Ce_1O_1_001	-1.02	Ce-Ce_h	Ga_1Sc_1_110	-1.17	Ga-Sc_b
Si_1V_1_001	-0.52	V-V_b	H_1V_1_001	-1.34	V-V_h	Ga_1Sc_1_111	-0.72	Sc_t
Ga_2Sc_1_100	-0.31	Ga-Sc_b	Hf_1P_1_110	-1.03	Hf_t	Hf_2Rh_1_100	-0.92	Hf-Rh_b
Ga_2Sc_1_101	-0.58	Ga_t	Hf_1P_1_111	-0.84	Hf_t	Hf_2Rh_1_110	-2.25	HfHfHf_h
Ga_2Sc_1_110	-0.19	Ga-Ga_b	Hf_1Ru_1_001	-1.09	Hf-Ru_b	Ir_1Ta_1_001	-3.40	Ta_t
Ga_2Sc_1_111	-0.81	Sc_t	Hf_1Ru_1_100	-1.09	Hf-Hf_b	Ir_1Ta_1_101	-1.32	Ta_t
Ga_2Th_1_001	-0.43	Ga_t	Hf_1Ru_1_101	-1.02	Hf-hf_b	Ir_1Ta_1_111	-0.55	Ta-Ta_b
Ga_2Th_1_100	-1.13	GaThTh_h	Hf_1Ru_1_110	-1.02	Ru_t	Ir1V1_111	-0.82	Ir_t
Ge_2Pt_1_001	-0.41	Ge-Pt_b	Hf_1Ru_1_111	-0.59	Ru_t	Mg_2Pt_1_001	-0.48	Pt_t
Ge_2Pt_1_100	-0.10	Ge-Pt_b	Hf_2Hg_1_001	-1.15	Hf-Hf_b	Mg_2Pt_1_100	-0.75	Mg_t
Ge_2Pt_1_101	-3.88	Pt_t	Hf_2Hg_1_100	-0.84	Hg_t	Mg_2Pt_1_101	-0.34	MgMgMg_h
Ge_2Pt_1_110	-0.32	Pt_top	Hf_2Hg_1_101	-1.18	HfHgHg_h	Mg_2Pt_1_110	-0.67	Mg_t
Ge_2Ti_1_101	-0.57	GeGeTi h	Hf_2Hg_1_110	-1.03	Hf-Hf-Hf_h	Mn_1P_1_001	-0.38	Mn-Mn_b
Ge_2Ti_1_110	-1.61	Ti_t	Hf_2Hg_1_111	-1.27	Hg_t	Mn_1P_1_100	-0.85	P_t
Hf_1P_1_001	-0.33	Hf_t	Hf_2Ni_1_101	-1.18	Hf-Hf-Hf_h	Mn_1P_1_101	-0.43	MnP_b
Hf_1P_1_100	-1.47	HfP_b	Hf_2Ni_1_110	-0.98	Hf-Hf-Hf_h	Mn_1P_1_110	0.75	MnPP_h
Hf_1P_1_101	-0.83	Hf_t	Hf_2Ni_1_111	-1.18	Hf-Hf-Hf_h	Mn_1P_1_111	-0.33	P_t

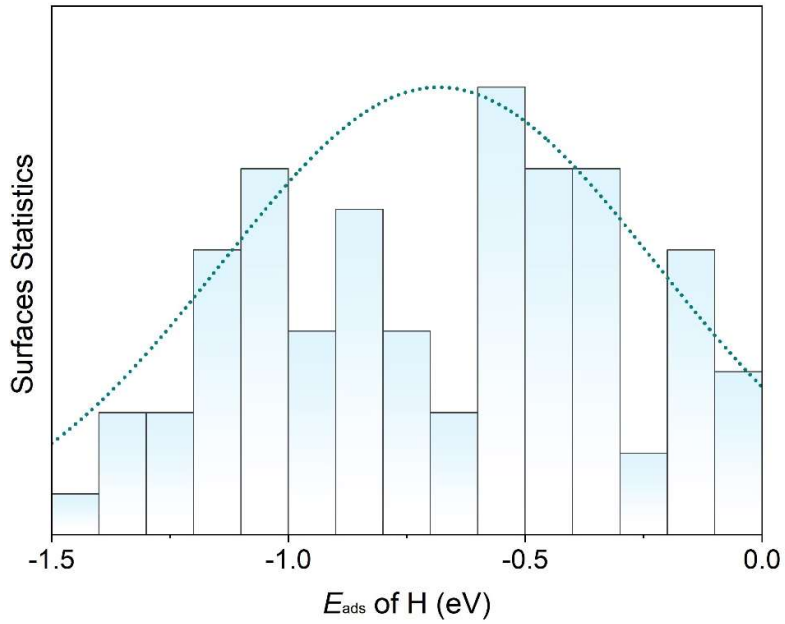


Figure 2. Normalized distribution of E_{ads} for hydrogen on various topological materials.

3.3 Preferred adsorption sites of the selected topological materials

It was reported that an optimal activity and selectivity can be achieved when E_{ads} of hydrogen is at −0.27 eV. [31, 33] This criterion is based on previous studies that adsorption energies close to -0.27 eV typically balance the hydrogen binding strength required for optimal HER activity. Nørskov *et al*. demonstrated that adsorption energy near -0.27 eV is often ideal for achieving high HER activity across a variety of catalysts, providing a balance between adsorption and desorption processes.[31] Similarly, studies by Greeley *et al*. have reinforced that an optimal adsorption range enhances catalytic efficiency and stability.[33] With this criterion, we have pinpointed 11 distinct surfaces, with each displaying E_{ads} of hydrogen within a 0.1 eV range of the optimal benchmark of −0.27 eV, as shown in Figure 3.

After identifying the promising topological materials for HER, we summarized the detailed structures of these surfaces in Figure 4. Interestingly, the favorable adsorption sites can be the top, bridge, and hollow sites, depending on the surfaces and the materials. For example, hydrogen prefers Al-Pd bridge sites on Al_1Pd_1 (001) surface, while it prefers Co-top sites with a slight tilt toward the neighboring Ge atom on Co_1G_1(001) surface. Both Ga_2Sc_1 (100) and (110) are the preferred hydrogen adsorption surfaces. However, hydrogen prefers the Ga-Sc bridge site on (100) while it prefers the

Ga-Ga bridge site on (110) surface. The details of other geometries can be found in Figure 4. As expected, these topological materials offer robust surfaces and adsorption sites, which can accommodate hydrogen with optimal adsorption strength.

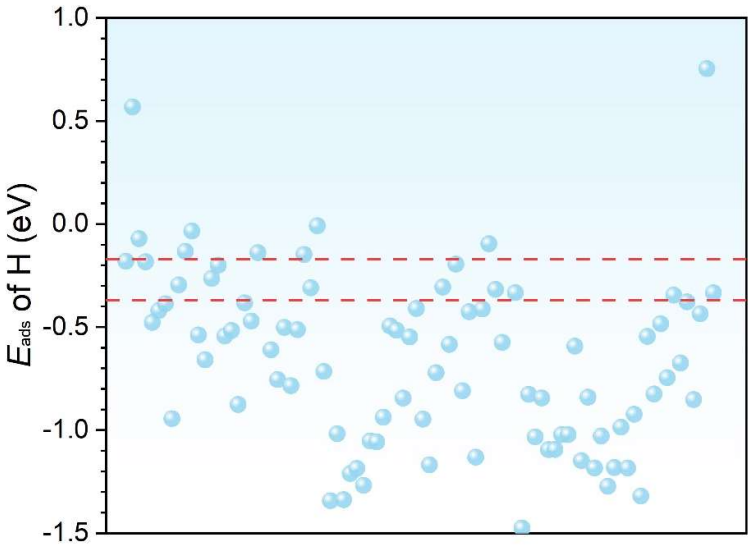


Figure 3. The adsorption energies of the most stable adsorption configurations of hydrogen atoms on different topological materials. The points in between the red dotted lines show those with E_{ads} of hydrogen within the −0.27 ± 0.1 eV.

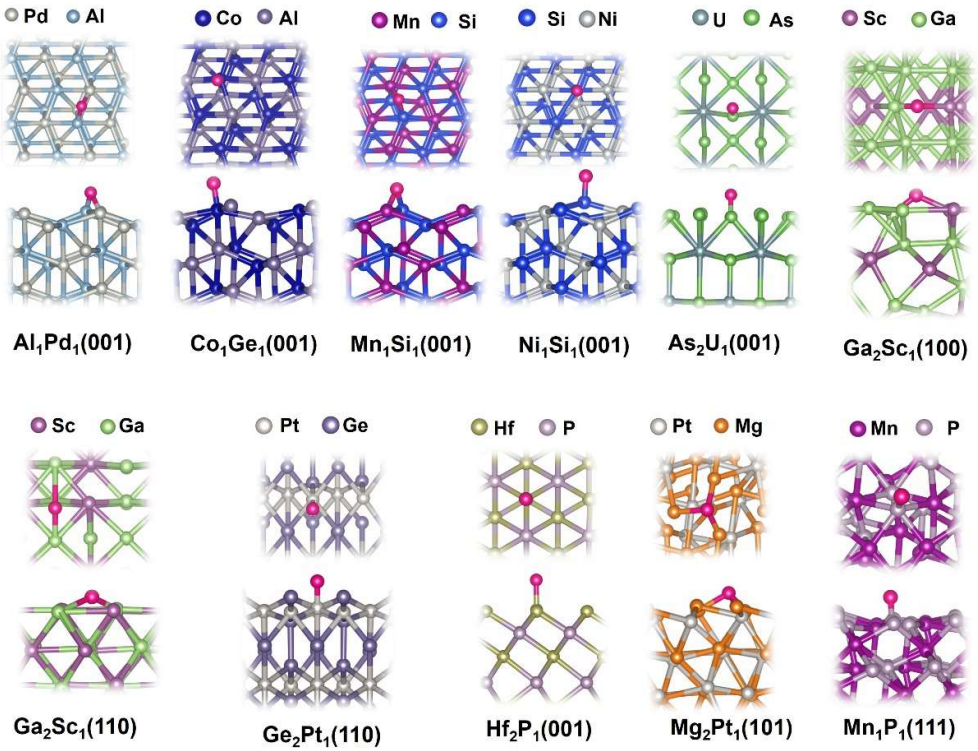
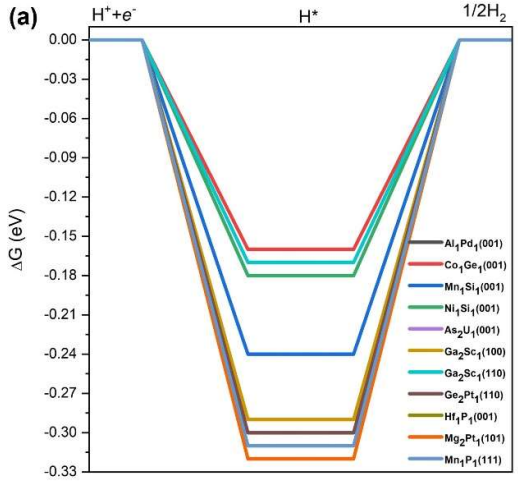


Figure 4. The top views and side views of the most stable hydrogen adsorption sites on 11 promising topological materials. The pink spheres represent hydrogen atoms, and the color

schemes for other atoms are also provided for each topological material.

3.4 Gibbs free energy calculations

The Gibbs free energy ΔG_H is a well-accepted descriptor that has been successfully applied to predict HER activities.[34] Previous studies have established that an ideal ΔG close to zero is a strong indicator of effective HER activity, as it suggests a balanced adsorption and desorption process, which is critical for optimal hydrogen evolution.[31,33] Focusing on these 11 topological materials, we further calculated the ΔG_H and the results are summarized in Figure 5. It is seen that the ΔG values range from -0.16 to -0.32 eV, suggesting that these surfaces have the potential to function as high-performance catalysts for HER. Among these 11 topological materials, $Al_1Pd_1(001)$, $Co_1Ge_1(001)$, $Ni_1Si_1(001)$ and $Ga_2Sc_1(110)$ demonstrate the ΔG of -0.16 eV, -0.16 eV, -0.18 eV and –0.17 eV, respectively. These four candidates are expected to possess the topmost HER performance. Interestingly, Ga_2Sc_1 possesses two active facets, that is, (100) and (110), both of which possess superior HER activity, highlighting its excellent catalytic performance.



(b)

Surface	ΔG_H (eV)
$Al_1Pd_1(001)$	-0.16
$Co_1Ge_1(001)$	-0.16
$Mn_1Si_1(001)$	-0.24
$Ni_1Si_1(001)$	-0.18
$As_2U_1(001)$	-0.29
$Ga_2Sc_1(100)$	-0.29
$Ga_2Sc_1(110)$	-0.17
$Ge_2Pt_1(110)$	-0.30
$Hf_1P_1(001)$	-0.31
$Mg_2Pt_1(101)$	-0.32
$Mn_1P_1(111)$	-0.31

Figure 5. ΔG_H values for HER on the 11 promising toplogical quantum materials and their corresponding adsorption surfaces.

3.5 Discussion

Experimental studies on topological materials have demonstrated favorable catalytic properties that align well with our predictions, particularly regarding adsorption energies and ΔG values. For example, Qu *et al*. reported that Bi_2Te_3, a topological insulator, exhibited significant HER activity, achieving a current density of

1.74 μA cm^{-2}, with partially oxidized surfaces contributing to enhanced catalysis.[35] Boukhvalov *et al*. demonstrated the HER activity of the topological nodal-line semimetal $AuSn_4$, attributing its performance to unique surface states that facilitated electron transfer.[23] These findings highlight that topological materials can possess intrinsically advantageous properties for HER, supporting our predictions regarding adsorption sites and ΔG in the materials we studied.

In the present study, we selected an adsorption energy range of -0.27 ± 0.1 eV to evaluate HER performance. This criterion is based on previous studies that adsorption energies close to -0.27 eV typically balance the hydrogen binding strength required for optimal HER activity.[31,33] By adopting this criterion, our study provides a robust approach that can be replicated and built upon in future HER research involving topological materials.

Our study relies on the Gibbs free energy of hydrogen adsorption (ΔG) as a primary descriptor for assessing HER activity. While ΔG has been widely used as an adequate descriptor for evaluating HER performance, it may not fully capture the complex mechanisms of catalytic performance, especially in topological materials, where unique surface states and electronic properties are integral to their functionality.[36] In topological materials, the presence of surface states and high electron mobility could affect HER performance by facilitating charge transfer, enhancing catalytic activity even if ΔG values are suboptimal. Furthermore, reaction kinetics, including hydrogen diffusion rates on the catalyst surface, are essential for understanding HER mechanisms and can vary significantly in materials with complex electronic structures. In the future, electronic structure calculations, such as projected density of states and Bader charge analysis, may be incorporated to further elucidate the charge transfer characteristics and reaction kinetics of the selected topological materials.

4. Conclusion

We conducted a comprehensive computational investigation of nearly 100 surfaces of topological materials to identify high-performance topological catalysts for efficient HER. We examined over 1000 adsorption sites, including top, bridge, and various multi-fold sites. Our findings reveal that these topological materials exhibit a broad range of hydrogen adsorption energies, primarily ranging from -1.5 to 0 eV. Since previous studies suggested an optimal adsorption energy of -0.27 eV for ideal HER

performance, we focused on materials with adsorption energies within -0.27 ± 0.1 eV. The computed Gibbs free energy ΔG values for these materials in HER range from -0.31 to -0.16 eV, and detailed configurations for hydrogen adsorptions are provided. Ultimately, we identified 11 topological materials as promising catalysts for superior HER catalytic activity. The findings offer valuable insights and guidelines for further theoretical and experimental exploration of topological materials as high-performance HER catalysts.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

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