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Review

Borophene: Synthesis, Properties and Experimental H_2 Evolution Potential Applications

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Abstract

Borophene, a two-dimensional (2D) allotrope of boron, has emerged as a highly promising material owing to its exceptional mechanical strength, electronic conductivity, and diverse structural phases. Unlike graphene and other 2D materials, borophene exhibits inherent anisotropy, flexibility, and metallicity, offering unique opportunities for advanced nanotechnological applications. This review presents a comprehensive summary of recent progress in borophene synthesis methods, highlighting both bottom–up strategies such as chemical vapor deposition (CVD) and molecular beam epitaxy (MBE), and top–down approaches, including liquid-phase exfoliation and sonochemical techniques. A key challenge discussed is the stabilization of borophene's polymorphs, as bulk boron's non-layered structure complicates exfoliation. The influence of substrates and doping strategies on structural stability and phase control is also explored. Moreover, the intrinsic physicochemical properties of borophene, including its high flexibility, oxidation resistance, and anisotropic charge transport, were examined in relation to their implications for electronic, catalytic, and sensing devices. Particular attention was given to borophene's performance in hydrogen storage and hydrogen evolution reactions (HERs), where functionalization with alkali and transition metals significantly enhances H_2 adsorption energy and storage capacity. Studies demonstrate that certain borophene–metal composites, such as Ti- or Li-decorated borophene, can achieve hydrogen storage capacities exceeding 10 wt.%, surpassing the U.S. Department of Energy targets for hydrogen storage materials. Despite these promising characteristics, large-scale synthesis, long-term stability, and integration into practical systems remain open challenges. This review identifies current research gaps and proposes future directions to facilitate the development of borophene-based energy solutions. The findings support borophene's strong potential as a next-generation material for clean energy applications, particularly in hydrogen production and storage systems.

Keywords: borophene; 2D materials; H_2 evolution reaction; H_2 production; electrocatalysis

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1. Introduction

Borophene, a potentially groundbreaking one-atom-thick layered nanomaterial, has emerged because of research on 2D boron materials, and was firstly experimentally reported by A. J. Mannix et al. in 2015 [1], although parallel work was published by B. Feng et al.

in 2016 [2], submitted in Mannix's prior publication. Both works present the molecular-beam epitaxy growth of borophene on the surface of Ag (111) but from two different perspectives: Mannix aimed to study the impact of flow control of the precursor on phase tuning, while Feng's research relied on temperature impact on the phase during and after synthesis, demonstrating a temperature-dependent phase transition. Due to boron's position between nonmetallic carbon and metallic beryllium on the periodic table, boron possesses only three valence electrons, giving it both metallic and nonmetallic characteristics [3]. The electronic structure of bulk boron allows for the formation of a wide variety of chemical bonds, including some unusual and complex types [1–3]. To date, borophene represents the lightest 2D material discovered [4,5], and is expected to share properties with graphene due to their close relationship, although with more complex bonding [6] in bulk. Compared with graphite, which has a layered structure (Figure 1a), boron has a B_{12} icosahedron as the basic structural unit (Figure 1b), thus making it difficult to synthesize using common top–down methods. Moreover, borophene demonstrates superconductivity [7], with σ and π electrons occupying electronic states on the Fermi surface. Its mechanical properties, such as high anisotropy [5], Young's modulus [8,9], Poisson's ratio [9,10], fracture strength [9], and stress–strain [11] are equally compelling. Despite its low bulk density, borophene exhibits high ideal strength and in-plane stiffness, making it suitable for composite material design. Its flexibility against out-of-plane deformation makes it ideal for flexible nanodevice fabrication.

Moreover, its anisotropic structure allows for control over magnetic and electronic properties, opening doors to a myriad of applications. In essence, borophene intrinsic properties, including its low atomic weight, lightness, affordability, and high electronic conductivity, make it an attractive prospect for various technological advancements [12]. The development of borophene in theoretical models (Figure 1c) began with the prediction of its triangular structure in 1997 [13]. Subsequently, a new single-layer boron structure, known as the α-sheet, was identified through calculations [14]. This structure features a triangular lattice with hexagonal honeycomb holes. The boron atoms in the α-sheet lie in the same plane, resulting in lower energy compared to the buckled triangular structure, which had been previously considered the most stable. Between 2007 and 2014, various classical borophene structures emerged, such as the β-sheet, snub sheet, α-1-sheet, structure-1/8-sheet, β1-sheet, pmmn-sheet, and pmmm-sheet [15]. These structures were formed through different arrangements of hexagonal and triangular lattices, all possessing very low and nearly equal energy levels.

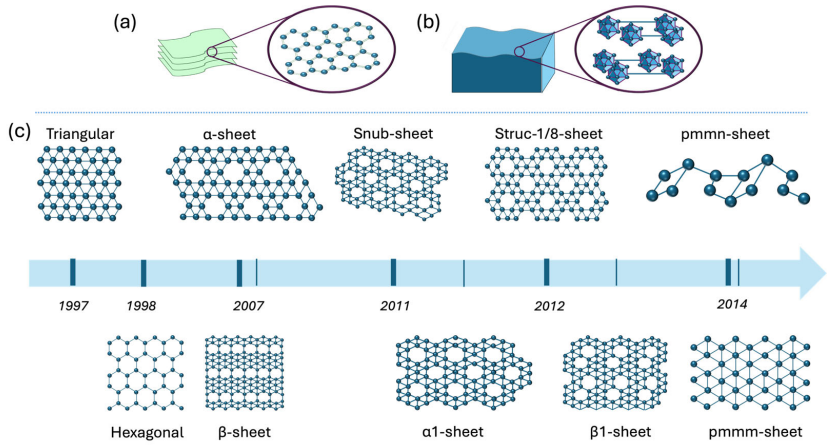


Figure 1. Bonding of (**a**) bulk graphite and (**b**) structured of bulk boron, and (**c**) timeline of borophene theoretical models. Adapted with permission [16]. Copyrights 2021, Wiley.

As mentioned before, the high capacity and excellent electronic conductivity [17] of borophene, combined with outstanding ionic conductivity [18], demonstrate that this novel material can be used as a catalyst for a hydrogen evolution reaction (HER) [19,20], and oxygen reduction and oxygen evolution reactions [21], with high catalytic performance. Studies on these applications are further relevant since the global environmental and energy crises have sparked intense interest in researching sustainable energy harvesting materials; thus, borophene may be a key promising avenue to produce hydrogen (H_2) [19,20], i.e., a renewable and eco-friendly energy source.

Over the past century, various production techniques for hydrogen have emerged, but among them, HER stands out for its effectiveness and affordability. Consequently, there has been a significant focus on developing HER catalysts with high efficiency, both experimentally and theoretically [22]. One crucial factor in evaluating HER catalysts is the H-adsorption free energy, which indicates the strength of the bond between hydrogen and the catalyst. So far, only a handful of metals, such as platinum (Pt) and ruthenium (Ru), along with certain noble metal-based materials, have demonstrated optimal catalytic efficiency for HER [23]. These findings underscore the importance of ongoing research in this field to address the pressing energy and environmental challenges we face globally.

Although precious metal catalysts such as Pt [24–26], Au [26], Pd [27], Ir [28], and Ru [28,29] among others, have demonstrated great performance in HER, the high cost and limited storage are the main drawbacks of their large-scale production and applications. Thus, two-dimensional (2D) materials, with an emphasis on borophene, have gained attraction as low-cost catalysts, and their potential applications in energy conversion and hydrogen storage due to high activity of the surface [30,31]. It has been proven that, due to its good adsorption kinetic, large surface area, hydrogen storage reversibility [32], and metallic properties, borophene has HER activity comparable to that of Pt [31].

Although in recent years, review reports have been collated to exhaustively sum up the theoretical studies, synthesis, properties, and electrochemical applications of borophene and borophene-based materials, their coverage toward a fully understandable mechanism of hydrogen evolution reaction (HER) has been briefly mentioned. Ajmal S. et al.'s [33] and Yildiz O. G. et al.'s [34] reviews provide general aspects of electrochemical energy conversion regarding the theoretical prediction of the HER activity of pristine and doped borophene by ab initio calculations; moreover, both cite only one of the most up-to-date experimental research projects of HER. Conversely, Pratihar B. et al. [35] have carried out excellent work in summarizing the few and novel research on borophene HER studies and applicability, with an outstanding report of the proposed electrochemical mechanism of the 2D material; nevertheless, its scope is limited to only mentioning the overpotential and Tafel slopes of each experiment, and does not integrate the stability, stabilization, and deeper discussion of the phase influence. To address these gaps, this review is primarily focused on enlightening the methods for the stabilization of borophene, and the role of structural phases, and electronic properties of HER to provide a reference for guiding the future research of borophene in energy conversion.

In this review, firstly, the past focus on the development of borophene synthesis, to the theoretical prediction to the recent progress concerning the optimization of the synthesis methods are presented. Then, physicochemical properties such as anisotropy, high thermal conductivity, and high electronic density are discussed for the further understanding of the potential applications of borophene. Afterward, the hydrogen evolution mechanism of borophene and comparison with other 2D materials such as graphene, silicene and phosphorene regarding the hydrogen evolution reaction (HER) application and viability were carried out, as well as comparison with noble metals such as Pt and Ir, among others. Finally, the challenges in overcoming the mass production and application of

borophene-based materials, as well as outlooks and perspectives are discussed for a better understanding of the future of 2D boron for HER applications (Figure 2).

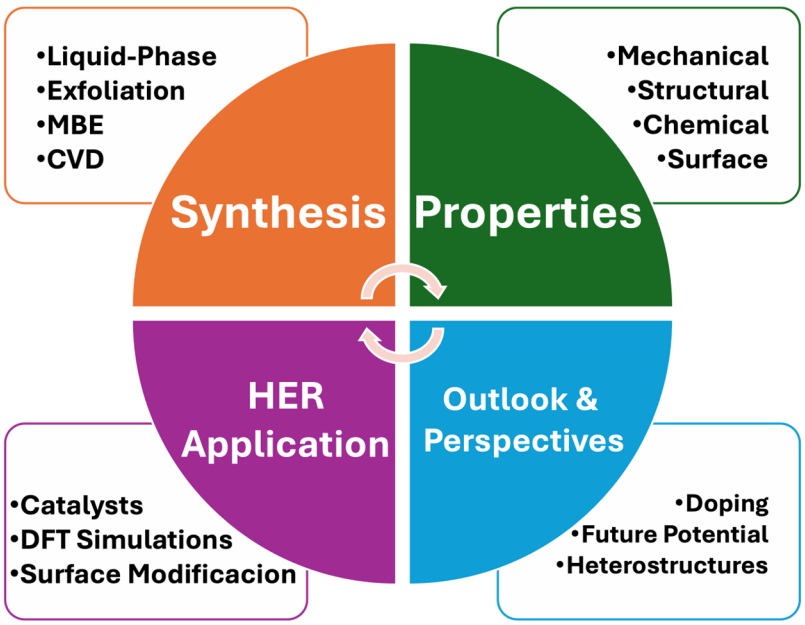


Figure 2. Roadmap of the review article.

2. The Phases of Borophene Predicted Theoretically and Obtained Experimentally

It is well known that borophene fabrication represents a major challenge due to bulk boron bonding configurations [5]. Boron, located between beryllium (Be) and carbon (C), has metallic and nonmetallic properties [2,36], and due to the three valence-electrons (1 s^2, 2 s^2, 2 p^1) can be capable of creating extensive covalent networks; the property that allows for the creation of the low-dimensional structure of boron, such as fullerenes, nanotubes, and 2D boron, is the compact covalent radius that can undergo sp^2 hybridization. Two-dimensional boron is given the name of borophene since its structure, akin to that of graphene, has been theoretically studied intensively [37]. In 1997, Boustani et al. [12] first predicted the triangular network of boron clusters with a quasi-planar structure by ab initio calculations. Long after, in 2014 Piazza et al. [38], predicted that the monoatomic layer B_{36} clusters, now referred α-sheet, were stabilized by hexagonal vacancies and could be grown on Cu (111), thus demonstrating that hexagonal hole vacancies in the triangular lattice could impact on the stability of 2D boron. Also, in this work, the concept of borophene was introduced for the first time.

In 2015, theoretical research by Zhang et al. [39] about the growth of borophene structures onto different metallic substrates such as Au, Ag, Cu, and Ni demonstrated that borophene could be grown and stabilized by different substrates. Theoretically, a triangular lattice would be more stable if it has periodic voids and can grow on metal surfaces such as Ag (111), Au (111), Al (111), and Cu (111). As far as it is known, the successful boron phases that have been synthesized are β_{12} [1,31,36], χ_3 [1,2,40,41], graphene like [42,43], χ_6 [44], and γ-B_{18} [45] on metal substrates (Figure 3).

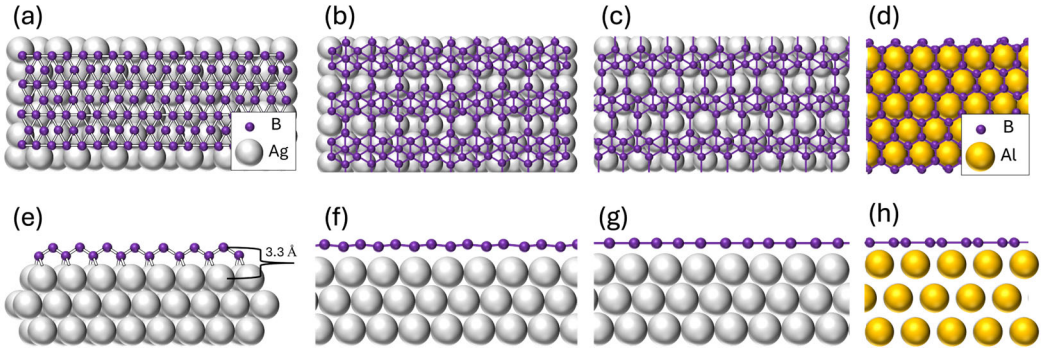


Figure 3. Top view (**a**–**d**) and side view (**e**–**h**) structure models of 2-Pmmn, β_{12}, χ_3, and graphene-like borophene, respectively, on Ag (111) and Al (111) substrates. (**a**,**e**) Adapted with permission [1]. Copyright 2015, AAAS. (**b**,**f**) Adapted with permission [46]. Copyright 2017, IOP Publishing, Ltd. (**c**,**g**) Adapted with permission [2]. Copyright 2016, Springer Nature. (**d**,**h**) Adapted with permission [43]. Copyright 2018, Elsevier.

As seen in Figure 3a,e, 2-Pmmn borophene has a corrugated configuration due to its vertical undulations, as theoretically predicted by computational calculation, with average height between atoms at around 0.91 Å. This monolayer is the lowest-energy structure constructed by B_7 clusters, with lattice constants a = 5 Å and b = 2.89 Å, with a rectangular unit cell. It is now known that the substrate (Ag (111), Au (111), Cu (111), Ir (111) or Al (111)) helps with the stabilization of the one-atom boron sheet. Moreover, due to the structure formation, this phase is highly anisotropic owing to the strong and highly coordinated B–B bonds. Moreover, the 2-Pmmn borophene phase has a Young's modulus larger than graphene (398 N/m and 170 N/m along the armchair and zigzag direction, respectively [47,48] (Figure 4)). As a result of the corrugated structure, Poisson's ratios are negative, with values of −0.04 and −0.02 along the armchair and zigzag direction, respectively. Finally, to know the applicability of 2-Pmmn borophene thermal conductivity is a key parameter to consider [49–52], thus thermal conductivity was measured, and, as expected, this parameter was anisotropic, with values of ~75.9 and ~147 W/mK [53], along with the zigzag and armchair directions of the lattice, respectively.

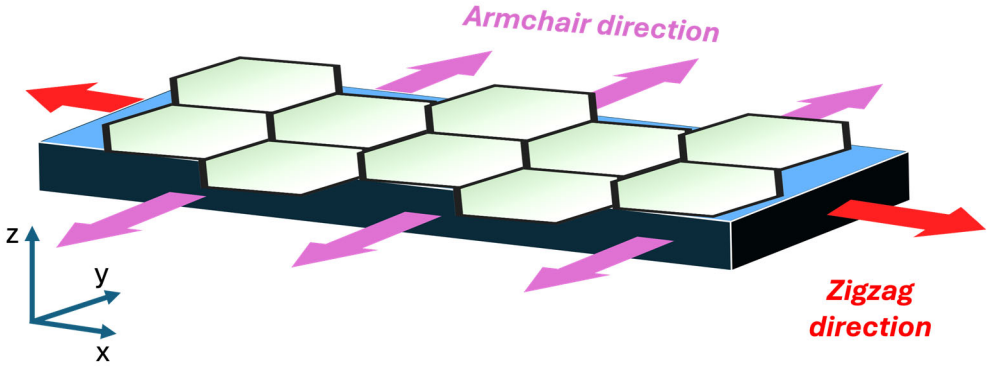


Figure 4. Armchair and zigzag direction of the 2D boron sheet. Adapted with permission [48]. Copyright 2013, Elsevier.

On the other hand, the β_{12} phase is a planar sheet for which the model exhibits a hole chain separate by hexagonal boron rows (Figure 3b,f). The lattice constants are a = 5 Å and b = 3 Å, also with a rectangular unit cell. The planar nature of this sheet comes after the relaxation on the substrate, which, again, is Ag (111). The χ_3 phase (Figure 3c,g) consists of a zigzag boron row separated by hole arrays on the substrate Ag (111). Young's modulus for β_{12} and χ_3 was smaller than the 2-Pmmm phase, with values of 179 and 198.5 N/m, respectively. Along the zigzag direction is relatively close to the

armchair values [47]. The metallic behavior of β_{12} and χ_3 was observed [54], although it has been demonstrated that shear strain affects the bandgap value. For example, with a 6% strain, β_{12} has a bandgap value of 0.7 eV [55–58]. The anisotropic nature of the χ_3 phase shows semiconducting character, with values of 0.6 eV and 1.2 eV in zigzag and armchair directions, respectively [55–58].

Finally, the honeycomb borophene phase was predicted to be unstable in a Ag (111) substrate due to the low energy transfer [57]; therefore, Al (111) plays a key role in the formation of phase-stabilizing the lattice and transferring one electron of Al to the borophene sheet. Then, after relaxation, the honeycomb borophene adopts a 1:1 lattice matching the Al (111), and the sheet obtained is flat, making it more stable than those synthesizes onto Ag (111) and Au (111), thus being more energetically stable (Figure 3d,h).

Borophene has allotropes that rely on the hexagon boron vacancy concentration which is the ratio between the number of the hexagon boron vacancies and the number of atoms in the original triangular sheet. The polymorphism of the 2D boron is peculiar and different from other materials such as graphene, silicene, and boron nitride, among others. Another factor that affects the borophene formation is the substrate, as mentioned before, since the electron interaction between the substrate and the boron sheets implies the stabilization of the lattice structure. The most used is Ag (111), but for the formation of graphene-like borophene, Al (111) is suitable; Cu (111) is being studied for the stabilization of all three phases of borophene mentioned before.

3. Synthesis Methods for Borophene

Several synthesis methods have been studied ever since the first experimental growths of borophene back in 2015, which include a wide variety of bottom–up and top–down methods, each with its benefits and drawbacks, as further discussed.

Bottom–up methods (Figure 5a) involve two of the most used routes to synthesize atom thin films: molecular-beam epitaxy (MBE) [1,2,42–44,59] and chemical vapor deposition (CVD) [41,45,60–62]. These were the first methods studied that resulted in the growth of borophene sheets onto Ag, Al, and Au, although high-cost and low yield are the main drawbacks of these methods.

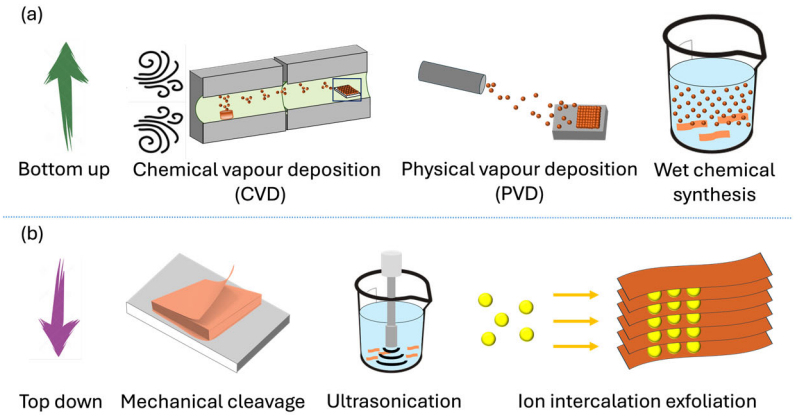


Figure 5. The main synthesis methods for 2D borophene sheets: (**a**) bottom–up and (**b**) top–down. Adapted with permission [16]. Copyrights 2021, Wiley.

On the other hand, top–down methods (Figure 5b) are more diverse, such as liquid-phase sonochemical exfoliation [40,63–66] and oxidative etching [67], among others, which demonstrates the difficulty of exfoliating non-layered bulk boron, thus requiring more complex processes and a high amount of energy and time, making the lamination process of bulk boron more challenging (Figure 5).

3.1. Bottom–Up Synthesis

3.1.1. Molecular Beam Epitaxy (MBE)

The MBE technique has been widely used for the synthesis of 2D materials owing to the evaporation of elemental boron onto the surface of a selectively chosen substrate, under ultra-high-vacuum conditions. In 2015, A. J. Mannix et al. [1] demonstrated the growth of an atomically thin borophene on an inert Ag (111) surface with the morphology of striped-phase nanocrystals using MBE. Controlling the deposition rate (flux between ~0.01 to ~0.1 monolayer per minute) and substrate temperature at 550 °C, the first successful synthesis of borophene was achieved, with the formation of the two phases: a homogeneous pattern (2-Pmmm phase) and striped pattern. Furthermore, the borophene structures were demonstrated to be more complex rather than most common 2D materials due to the transition metal interaction of the material with the substrate. It is worth mentioning that the resulting 2D sheet is highly mechanically anisotropic due to the highly coordinated B–B bonds [52,53]. Contrary to theatrical predictions in which it is forecast that borophene has metallic properties [53], 2-Pmmm boron has shown semiconductor properties under standard conditions, but gained metallicity under extremely high pressures [54]. This work establishes the groundbreaking research on borophene not only in the theatrical but also the experimental area, which unveils the potential applications of the material and its polymorphs for the property studies of it.

In 2016, B. Feng et al. [2] in parallel showed that borophene grows by the direct evaporation of a pure boron source on a Ag (111) substrate. In contrast with the work carried out by Mannix et al. [1], the substrate temperature was only 300 °C, at which the obtained phase was β_{12}. The ordered pattern observed by STM images showed parallel stripes in the direction of Ag (111). Afterward, an annealing was carried out to the sample at 380 °C in which the β_{12} phase had a transition to the χ_3 phase. This research confirms that the two phases tend to coexist in the 380–530 °C temperature range, and at higher temperatures, the 2-Pmmn phase is formed [1]. The best conclusion to this work is the impact that the temperature of the substrate has on the formation of the borophene phases.

In 2018, Li et al. [43] successfully obtained graphene-like borophene with a pure honeycomb structure by using an Al (111) surface as the substrate. The synthesis route was MBE; therefore, ultra-high vacuum was used in order to obtain monolayered borophene. Evaporated boron was deposited on an Al (111) substrate at 230 °C. In contrast, low temperature was used, as seen from previous works (which start at 550 °C [1] and 300 °C [2]). The honeycomb-like borophene was energetically firm and almost one electron charge shifted from aluminum (due to its high electron density) to each boron atom of the borophene/Al (111) phase and stabilized the honeycomb borophene structure [57]. This work establishes that a borophene lattice can be manipulated by controlling charge transfer from the substrate to the borophene, thus giving a hint for the basic study of noble metals to stabilize the borophene structure.

In 2019, B. Kiraly et al. [58] reported, differently from growth on Ag substrates, that borophene islands can be generated at high temperatures on Au. For this, a boron flux of ~0.02 mL/min was guided onto a Au (111) substrate at ~550 °C for 30 min to 3 h. As mention in the work of Li et al. [43], it was concluded that the nucleation and growth of borophene on Au were due to energy minimization and stress release at the substrate surface. Also, by increasing the boron coverage, borophene changed from small well-defined islands to longer sheets, making it a suitable method for large-surface area borophene-based materials.

3.1.2. Chemical Vapor Deposition (CVD)

CVD growth was achieved by the usage of gaseous precursors rich in boron which are decomposed at a high temperature into boron atoms and flowed onto a substrate to

form the 2D layer, becoming a promising technique for the mass production scale up. In 2021, Tai et al. [60] grew borophene on a carbon cloth using sodium borohydride ($NaBH_4$) as the precursor and H_2 as the carrier gas. α′-borophene was successfully obtained at 973 K for a synthesis time of 30 min. A study on the growth parameters demonstrated that this temperature and reaction time provide the optimal energy for the nucleation and further growth of the borophene sheet.

In 2022, Abdi et al. [61] reported a novel strategy for borophene growth on an Al-coated Si wafer as the substrate with diborane (B_2H_6) as the boron source. In this work, the growth was achieved at 830 K with continues H_2 flow, and as a result, a few angstrom boron nanosheets were obtained, demonstrating the atomically thick nature of the material. Physical characterization, such as atomic force microscopy (AFM), revealed nanosheets with an average area of 6 μm^2 and others with 50 μm^2; it is worth mentioning that the nanosheets had the χ_3 phase with some signs of the β_{12} phase.

Another interesting CVD synthesis approach was carried out by Guo et al. [62] in 2024, where they developed 2D tetragonal borophene. The substrate selected was a polycrystalline copper foil and, as the precursor, a 5:1 mix of boron powder and boron oxide (B_2O_3), respectively. Regarding the CVD parameters, temperature was kept at 1373 K and the flow of the precursor in the presence of mixed Ar and H was fluxed to the substrate. Nanosheets with a thickness of 15 nm and area of 1 μm × 1 μm were obtained.

3.2. Top–Down Synthesis

As several works have demonstrated, top–down synthesis such as the exfoliation method has been used for the large-scale production of 2D materials, and is therefore suitable for borophene synthesis. Sonication-assisted liquid-phase exfoliation has been proven to be more effective than chemical exfoliation, since there are not intermediate chemical reactions, and it is a promising option for the synthesis of a 2D B-sheet. For exfoliation, the material must present a layered structure in the bulk precursors, which is not the case for bulk boron due to the bonding configurations among B atoms. To solve this, a novel combination of exfoliation and etching technologies was proposed to synthesize ultrathin borophene.

3.2.1. Liquid-Phase Sonochemical Exfoliation (LPE)

In 2018, Li et al. [63] presented a scalable and novel method to produce few-layer borophene sheets. In this work, B powder was added to 100 mL of N, N-Dimethylformamide (DMF) and then sonicated at 350 W for 4 h with a 1 s-start/2 s-pause pulse by a probe-type sonicator. DMF was used since it has proven to be an excellent solvent for graphite exfoliation, and for this reason, experiments were carried out to determine the performance of the solvent applied to borophene. The obtained B sheets have an average area of 19,827 nm^2 and average thickness of 1.8 nm. By analyzing the results, it was evident that they have given a route for B-sheet synthesis that help with the development of thin films and composites. Exploring the routes for liquid-phase exfoliation, Yasaei et al. [64] conducted studies to determine the optimal parameters, and, for this reason, a probe bath sonication was carried out with isopropanol, 2-butanol, DMF, and N-methylpyrrolidone (NMP), whereby it was concluded that polar solvents are appropriate for the uniform and stable dispersions of borophene.

Also, in 2018, Ji et al. [65] coupled liquid-phase and thermal oxidation. This synthesis has an advantage that after the first liquid-phase exfoliation step, the B–B bonds of the boron sheets can be oxidized at high temperatures to obtain B_2O_3 which induces the stabilization of the B sheet; the B_2O_3 can be dissolved into water after a second LPE. Then, the layer size and thickness of the boron sheet were around ~100 nm and ~5 nm, respectively. Although

the experiments conducted were successful, the yield production was lower than 1%, making it difficult for a scalable attempt.

In 2022, Fu et al. [66] explored a sonochemical exfoliation route by using pure B powder added in an NMP solution in a probe-type sonicator at 600 W for 4 h with a start/pause pulse of 4 s. Afterward, the mixture was further sonicated in a sonochemical bath for 72 h at 10 °C. Then, after the cleaning process, boron nanosheets with height of 5 nm were observed by AFM with areas of 5 nm × 5 nm. Although a good amount of B nanosheets were obtained with a high yield, the synthesis time was around 80 h in total, which resulted in a high amount of energy consumption, being the main drawback.

3.2.2. Chemical Etching (CE)

In 2022, Xie et al. [67] developed a unique method for the etching of aluminum diboride (AlB_2) by chlorohydric acid (HCl). The experiment carried out consisted of the addition of HCl or hydrofluoric acid (HF) onto bulk AlB_2. Interestingly, the experiments showed that with the usage of HF, Al sheets can be obtained, while, on the other hand, the reaction with HCl promotes the high-yield production of borophene sheets with thickness of 4 nm and length of 600 nm. This work demonstrates, for the first time, the synthesis of borophene by oxidative etching and the use of diboride as a precursor, opening the path to a wide variety of boride precursors.

In Table 1, a sum up of the synthesis methods, and the achievable sizes and thickness of borophene sheets demonstrates the advantages and disadvantages of each method. It is easy to see that with the MBE methods, although the first to be studied, the obtained borophene sheet was difficult to manipulate for further applications or studies; moreover, the technique was more reliable for laboratory applications or analysis. In contrast, the CVD methodology had a more scale-up nature that could help in mass production, although the usage of highly toxic precursors, as well as the difficult extraction of the samples from the substrate complicated its further applications. Top–down models, on the other hand, showed high-yield production and not a complex environment for the synthesis, though it was notable that the long reaction time from a couple of hours up to 80 h demonstrated a high-energy consumption model that, for environmental applications, is the main drawback. In this manner, chemical etching showed the most reliable synthesis route for a short-time and environmentally friendly method, although mechanism optimization must be carried out for further applications and to truly understand the borophene etching mechanism.

Table 1. Borophene synthesized via different bottom–up and top–down methods, and their sizes.

		Precursor	Substrate/Medium	Synthesis Time	T [°C]	Phase	BP Size (Thickness and Size)
Bottom–Up Methods	MBE	[1] B	Ag (111)	N/A	550	2-Pmmn	thk = 0.38 nm l = 100 nm
		[2] B	Ag (111)	N/A	300	β_{12} and χ_3	thk = 0.44 nm l = 20 nm
		[40] B	Al (111)	N/A	230	Honeycomb	thk = 230 pm l = 100 nm
		[59] B	Au (111)	3 h	550	$\nu_{1/12}$	thk= 0.44 nm l = 5 nm
	CVD	[60] $NaBH_4$	C cloth	30 min	700	α'	N/A
		[61] B_2H_6	Al-coated Si	1 h	560	χ_3 and β_{12}	thk = N/A A^2 = 6 μm^2
		[62] B/B_2O_3	Cu foil	1 h	1000	tetragonal	thk = 15 nm l = 1 μm

Table 1. *Cont.*

		Precursor	Substrate/Medium	Synthesis Time	T [°C]	Phase	BP Size (Thickness and Size)
Top–Down Methods	LPE	[63] B	DMF	4 h	RT	β-rhombohedral	thk =1.8 nm l = 200 nm
		[65] B	NMP/EtOH	5 h	RT	β-rhombohedral	thk = 3 nm l = 100 nm
		[66] B	NMP	76 h	10	β-rhombohedral	thk = 5 nm l = 5 nm
	CE	[67] AlB_2	HCl	N/A	RT	β_{12} and χ_3	thk = 4 nm l = 600 nm

4. Structural and Chemical Properties of Borophene

As mentioned in the previous section, borophene phases rely on the synthesis method and the selected precursor; thus, properties may change due to the nature of each phase, such as atom arrangement, and therefore, the applications of each phase vary depending on its structural and chemical properties. It has been cleared that borophene cannot form graphene-like structures due to the lack of one electron in its valence band [68,69] and rather exhibits a triangular lattice with hexagonal vacancies, making the arrangement of the vacancies a key factor for the phase formation [70].

4.1. Structural Properties

4.1.1. β_{12} Phase

As one the well-known borophene phases, β_{12} has demonstrated high atomic density on its ridgelines, which leads to substantial orbital overlapping and, therefore, excellent electron density [70]. As such, β_{12} phases have a highly metallic behavior [64] with regular triangular unit arrangements [71].

4.1.2. χ_3 Phase

Another widely known borophene phase is the χ_3 structure which, as the β_{12} phase, exhibits directional metallic behavior and has mechanical plasticity and higher carrier mobility [72]. Compared to the earlier-mentioned phase, the χ_3 phase consists of a complex hexagonal lattice [71,73].

4.1.3. α Phase

Given to the anisotropic behavior of borophene phases, an interesting shift was observed in the α phase, since it has been demonstrated to have a semiconducting property [74] compared to that of the χ_3 and β_{12} phases.

A novel characterization technique that has gained popularity is near-field Raman spectroscopy, with an emphasis on tip-enhanced Raman spectroscopy (TERS) since it has enabled the simultaneous acquisition of the morphology and optical response of materials at the nanoscale, resulting in a powerful tool for studying 2D materials like borophene, where nanoscale features and their optical signals are critical for their performance [75]. TERS has been applied to probe near-field heating effects on monolayer MoS_2 photoluminescence, demonstrating its ability to investigate localized phenomena in 2D materials [76]. For borophene, this study has helped demonstrate the vibrational properties of the 2D boron for the correct differentiation of the structural phases due to commensuration and strain [77].

4.2. Chemical Properties

Unlike 3D bulk boron, which is prone to oxidation, 2D boron has been found to be inert to oxidation due to the differences in atomic arrangements [2]. While boron typically has three valence electrons, the promotion of an electron from the 2s to the 2*p* orbital allows boron to have four available valence orbitals. However, this still results in electron-deficient boron atoms because the number of valence electrons is less than the number of valence orbitals, preventing the electronic orbitals from being fully filled when forming chemical bonds. Both bulk 3D boron and 2D boron atoms at the periphery form classic two-center two-electron bonds. However, the inner atoms of 2D boron exhibit delocalized multicenter two-electron bonds, which contributes to their difference in oxidation stability [50]. In a boron sheet, the boron atoms at the center of hexagons act as "donors," compensating for the electron deficiency in boron, while the HHs serve as "acceptors." This unique bonding pattern makes boron sheets inert to oxidation [78].

Feng et al. [2] utilized X-ray photoelectron spectroscopy (XPS) to analyze monolayer borophene, revealing two distinct low-binding energy peaks (188.2 and 187.1 eV) corresponding to different B–B bonds in the 2D boron sheets. In contrast, the binding energy of the bulk boron 1s peak in 3D bulk boron generally falls within the range of ~189–190 eV. Additionally, a higher energy peak, at 191.5 eV, suggests the presence of oxidized boron atoms, with a calculated ratio of oxidized boron atoms-to-unoxidized boron atoms at approximately 0.23, indicating a significant stability against oxidation for most boron atoms on the borophene surface. Moreover, oxidized atoms predominantly localize at the edges of the borophene film, as confirmed by in situ scanning tunneling microscopy (STM) experiments.

Oxygen exposure resulted in oxidation primarily at the edges of boron islands, while the boron sheets themselves remained stable. Even with continued oxygen exposure, the boron sheets retained stability against oxidation, emphasizing the inherent inertness of 2D borophene compared to 3D bulk boron. Further, chemical properties of the different phases of borophene will be discuss.

4.2.1. β_{12} Phase Characteristics

Oxygen molecules can be adsorbed on free-standing β_{12} borophene, which lowers the system's energy [40]. However, β_{12} borophene has an energy barrier for O_2 dissociation of about 0.36 eV [40], making it relatively inactive. At this phase and prepared with other materials for heterojunctions [79], the β_{12} phase shows good catalytic properties, though the instability of borophene limit its applications at a large scale.

4.2.2. χ_3 Phase Characteristics

As in the previous phase, the χ_3 phase easily adsorbs oxygen molecules and reduces system energy. The energy barrier for O_2 dissociation is about 0.3 [56], which is similar to that of β_{12}, making the phases similar in properties but not in applications. Studies conducted on this phase were photoexcited carrier dynamic-oriented for optoelectronic and photovoltaic devices.

4.2.3. α Phase Characteristics

The high stability of the α phase and its electronic properties make it useful in semiconducting and hydrogen storage applications [80]. The doping of a phase with Al and Ga has demonstrated enhancement of the structural, mechanical, and chemical properties aiming at an anisotropic nature and structural dependency [81].

To sum up, the structural and chemical properties of borophene allotropes make them an outstanding 2D material of which the properties can be tuned to apply them for a specific

performance, and thus, a wide variety of applications can be developed with one material. However, the main drawback is the instability of the material that prevent it for further scalable applications and research due to the lack of reproducibility of experiments.

4.3. Stabilization of the Synthesized Borophene Sheets

Despite the vast experimental research and efforts, the main drawback for the potential applications of borophene comes from its high chemical reactivity and sensitivity to ambient conditions, limiting studies to ultra-high-vacuum conditions [2]. In addition, borophene's stability is affected by structural defects and polymorphisms arising from the synthesis route; thus, recent research has focused on stabilization methods by substrate engineering, encapsulation, and doping [82,83]. With the previous discussion of borophene anisotropy and its highly influenced electronic and mechanical properties by the obtained phase that deepens on the substrate, the low stability of borophene sheet arises from the low out-of-plane stiffness and high surface energy that tends to oxidize and degrade [37]. Due to the electron deficiency of boropehene, the structure is prone to defects such as vacancies, atoms, and dislocation [84]; thus, grain boundaries and vacancy defects could stabilize polymorphs under specific conditions [84], making some phases more stable under particular thermal and chemical environments [85]. Strategies and methods for the stabilization of borophene include the following:

- Substrate engineering: Selective choice of substrate helps strong interactions between borophene through charge transfer and epitaxial locking. Further, macroscopic single-phase borophene has been achieved using this strategy by choosing Ir (111) [86].
- Alloying and doping: Alloying with nitrogen or hydride to form boron–nitride analogs improves stability significantly [9]. On the other hand, doping with Ag^+ has been demonstrated to enhanced the stability of the lattice [83].
- Hydrogenation: To make a long-term stable borophene, hydrogenation to produce borophene can be induced [87].
- Functionalization: Via molecular adsorption, borophene can be passivated in its reactive sites. For instance, borophene oxide sheets can be produced by oxidation-assited exfoliation [88].
- Control of the growth parameter: As previously discussed, studies on the synthesis of borophene have demonstrated that the precise tuning of temperature, pressure, and deposition rates allows for the synthesis of selective borophene phases and, therefore, controlled defects can be achieve to stabilize the nanosheet [89,90].
- Defect engineering: Introduction of specific defects such as line defects in χ_3 borophene can enhance the stability of this phase [91].

The discussed methods show that scientific efforts aim to address the intrinsic instability of borophene, although further research is needed to optimize and approach long-term stability.

5. Borophene Applications for H_2 Evolution Reaction and H_2 Storage

Currently, energy sources for generation and storage potential come from fossil fuels such as oil, coal, and natural gas, which provide 85% of all energy used in the world [92]. These resources are being depleted and cannot be replaced in a reasonable period because they are non-renewable. In addition to being finite, the production of energy with fossil fuels results in the generation of highly dangerous gases and by-products due to combustion, such as CO_2 and nitric oxides that threaten the environment, living beings, and human health, and cause climate change [92].

The use of renewable energies, such as solar and wind, provides opportunities to electrify and provide heating systems to remote areas due to the global accessibility of

the resources on which they are based. It is worth noting that in 2013 [92], 16% of energy consumption came from renewable sources and, comparing the years 2012 and 2017, a higher investment in renewable energies has been observed, with a 13% increase, the most researched being solar with photovoltaic panels [93]. The major problem with renewable energy is that it is volatile, regional, and intermittent, so two methods have been applied to overcome this drawback.

The first, standby power, requires additional sources in which the power can be adjusted to the total instantaneous power of the generators; if the systems cannot operate or their total power is not sufficient, standby power can be activated. The second method is the use of accumulators in which low-energy storage is used in stand-alone generation systems, such as high-capacity storages: subway high-pressure-compressed air storage cavities, hydroelectric plants, and gravity energy storage devices, among others [94]. Hydrogen itself is a way of transporting and storing energy from the source to the end user. Unlike renewable sources available in nature, which must be converted to electricity to be transported efficiently, hydrogen must be produced.

Thus, hydrogen can be produced from renewable sources and converted into electricity using fuel cells. In addition, an attractive feature of hydrogen is that the only product of its combustion is water. Thus, combining hydrogen production with renewable energies and its use in fuel cells is a new route toward a completely environmentally friendly system, and reducing carbon emissions and dependence on fossil fuels [93,94].

5.1. Borophene Applied in Electrocatalysis HER

As theoretically predicted, borophene has been shown to be an active catalyst for the hydrogen evolution reaction (HER). In the work carried out by Wang et al. [95], borophene has demonstrated to have a higher catalytic activity compared to bulk boron. Moreover, borophene-supported single-atom catalysts are being explored for electrocatalytic nitrogen reduction reactions [96].

In 2021, Tai et al. [60] grew α'-borophene sheets on carbon cloth by the CVD method. The electrocatalytic activity for HER was about 142 mV at 10 mA cm^{-2} with a Tafel slope of 69 mV dec^{-1}. They also highlighted enhanced performance to the highly active area and low resistance of charge transfer; further analysis established that the α' phase is a crucial factor for the applicability of borophene.

In 2024, Can et al. [97] studied in a novel article the HER activity of electrochemically exfoliated β-rhombohedral borophene (see Figure 6). This study enlightens the further applicability of boron nanosheets, since they report an overpotential of 480 mV at 10 mA cm^{-2} with a Tafel slope of 163 mV dec^{-1}. Although the results are far from those of materials such as P_tO [80], its main reason for the applicability of the borophene is due to the low cost of the optimized synthesis methods, as well as the reagent precursor and furthermore, with decent stability. Double-layer capacitance (C_{dl}) and electrochemical surface area (ECSA) values were determined with outstanding results due to the increase in the surface area modifying the atomic structure, and therefore, the intrinsic activity was improved and reducing the overpotential of boron.

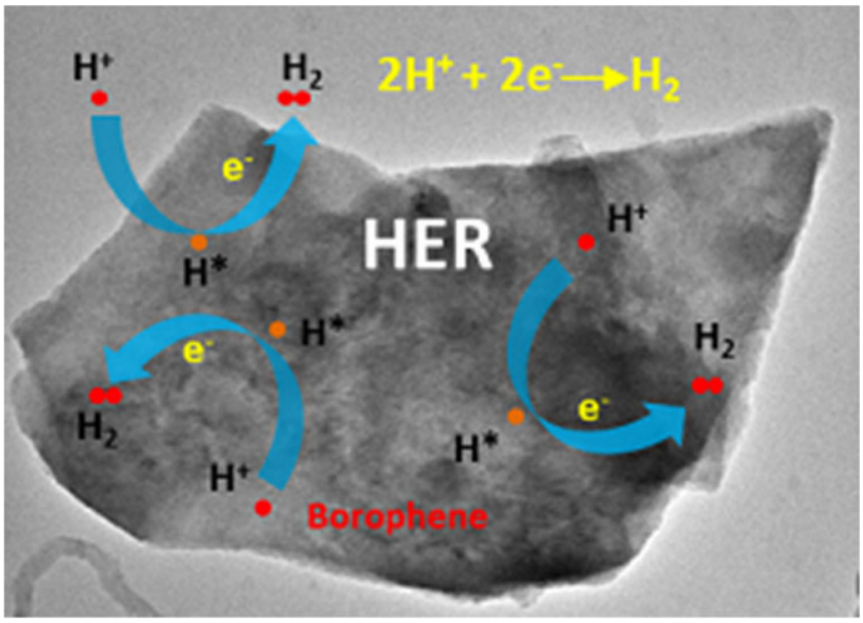


Figure 6. Schematic HER activity of borophene obtained by the electrochemical exfoliation. Reproduced with permission [97]. Copyrights 2024, Springer Nature.

The proposed active sites of HER on the surface of different borophene sheet phase surface such as β_{12}, α_1, χ_3, and β_1 are presented in Figure 7. It can be observed that the activation energy was 0.11, 0.55, 0.63, and 0.56 eV for each phase, respectively. Additionally, for H_2 evolution, the paths were different through the bond exchange mechanism that is favor by a H_2O-assited bond-exchange mechanism [98].

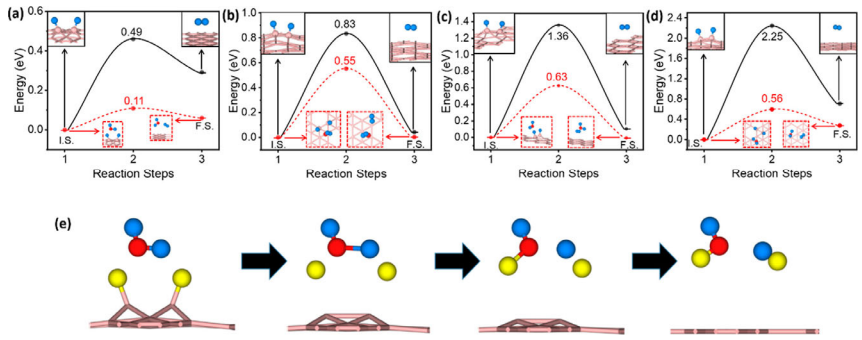


Figure 7. Activation energy for H_2 evolution with and without the bond exchange mechanism on (**a**) β_{12}, (**b**) α_1, (**c**) χ_3, and (**d**) β_1 borophene sheets. I.S. and F.S. represent initial and final states, respectively. The solid black line and dashed red lines are a visual guide only. (**e**) Schematic showing H_2O-assisted H_2 evolution through the bond exchange mechanism. A red circle indicates the O atom. Blue and yellow circles indicate the H atom from H_2O molecule and H atoms adsorbed on the surface. Reprinted with permission from [98]. Copyright 2023 American Chemical Society.

A comparison of borophene against other 2D materials such as graphene, MoS_2, phosphorene, and silicene can be observed in Table 2, which outlines the importance toward further research on borophene in electrochemical conversion.

Table 2. Comparison of studies carried out for the evaluation of the HER activity of several 2D materials against borophene sheets.

Material	HER Activity Prediction and Advances
Borophene	Theoretically predicted to be active; experimental studies revealed intrinsic activity and enhanced electrocatalytic activity.
Graphene	Due to its inert surface, HER activity is limited and can be carried out by using the 2D material as a support or by doping [99].
MoS_2	Although presented as a promising HER catalyst, for applicability combination with other materials must be performed [100].
Phosphorene	Poor HER activity that has only been reported by the formation of heterostructures [100].
Silicene	Lack of studies oriented to HER, although modification by doping or surface modification has demonstrated to modify its electronic and structural properties [101].

5.2. Borophene Applied in Electrocatalysis OER

As mentioned in Section 4.3, pristine borophene applications remain a challenge due to the poor stabilization and facile oxidation in ambient conditions. Thus, efforts to stabilize a 2D boron sheet have led to its usage as support for metallic and transition metal oxide nanoparticles. Saad et al. [102] showed the interesting synergetic effect that arises with the addition of Ag nanoparticles on the borophene structure; firstly, the metallic nanoparticles facilitate the growth of Co_2O_4 nanoplates by increasing the electrical conductivity of borophene. Additionally, interactions between B, Co, an O atoms reduce the oxygen evolution reaction (OER) barrier and further increasing stability of borophene. This work shows an OER overpotential of 270 mV at 10 mA cm^{-2}, with a Tafel slope of 62 mV dec^{-1} that outstands the performance of the pristine materials.

Borophene as a support material has conducted several research lines such as the work performed by Zeng et al. [103], aimed toward efficient and durable catalysis. In this regard, the hydrogenation of borophene was carried out to obtain further complex catalysts such as Pt/B/C in the nano range. The main reason is that the Pt–B bond gives stability to the borophene sheet and allows for an increased activity of OER.

Wenelska et al. [104] conducted a study for the deposition of NiO nanoparticles onto borophene sheets to overcome the drawbacks of water splitting limited by sluggish OER. This work shows an overpotential of 191 mV at 10 mA cm^{-2}, with a Tafel slope of 44 mV dec^{-1} with a long-term stability up to 99.9%. In contrast, Zielinkiewicz et al. [105] demonstrated that the addition of NiO nanoparticles in the borophene sheets induce lattice defects by the rapid dehydration/reduction, and thus stabilizing the structure; their electrochemical evaluation agrees with the work carried out by Wenelska, with an overpotential of 169.56 mV at 10 mA cm^{-2} with a Tafel slope of 31 mV dec^{-1}. In the same nickel route, addition of Ni_2P was conducted by Maslana et al. [106] at different B: Ni_2P ratios such as 1:1, 100:1, 10:1, 1:100; the most active was demonstrated to be 1:1 ratio with an overpotential of 299 mV at 10 mA cm^{-2} with a Tafel slope of 53.6 mV dec^{-1} at long-term testing.

Other material incorporations have been studied; for example, Dymerska et al. [107] evaluated the OER of zircon-doped borophene. As previously discussed, doping helps with the stabilization, and improves both OER and HER, with electrochemical results of 252 mV at 10 mA cm^{-2} with a Tafel slope of 43 mV dec^{-1} and of 240 mV at 10 mA cm^{-2} with a Tafel slope of 203 mV dec^{-1}, respectively. As an addition, the stability test highlights the outperforming of this material compared to Pt/C or RuO_2 in HER and OER.

5.3. Borophene for H_2 Storage

The H_2 storage of borophene relies on key properties mentioned before, such as large specific surface area which provides ample sites for the enhanced adsorption of the hydrogen molecule [108]. The key properties that make borophene a potential candidate for this application are the large surface area that proves more sites for hydrogen molecules to attach or adsorption, high H_2 storage capacity, no defects required for H_2 adsorption simplifying the structure production, and finally, the borophene's lightweight that improves the energy efficiency and overall system performance [109].

Although very promising, the advances of H_2 storage remain theoretical rather than experimental, and are based on the density functional theory (DFT) to determine H_2 storage. To have a great potential, the borophene-based system should have a reversible adsorption energy for hydrogen uptake, and then release physically and chemically the binding interactions at ambient temperature. This must be reversible and available for several cycles.

Thus, borophene H_2 storage has been focused on decorated 2D boron sheets. For instance, Ji et al. [110] made theoretical predictions regarding Li-decorated borophene, which can be adsorbed onto the surface lattice. They reported a H_2 biding energy of 0.35 eV/H_2, which is in the middle of the reversible adsorption energy range (0.1–0.8 eV/H_2). Furthermore, a maximal theoretical hydrogen storage of 9.22 wt.% was reported.

Another interesting work regarding borophene decoration was carried out by Wang et al. [111] with alkali metals such as Li, Na, and K. This work shows how although Na and Li decoration led to strong H_2 adsorption due to high gravimetric hydrogen density (between 8.36 wt. and 13.96 wt.%), the Na- and K-doped borophene are unsuitable for hydrogen storage due to the unfavorable adsorption energy between -0.14 and -0.19 eV/H_2. With this, it was concluded that interactions between substrate and metal atoms determine H_2 storage. Not only that, but Li-doped borophene also shows outstanding results compared to carbon-based storage mediums; thus, borophene could be expected to be a promising host material for H_2 storage by the modulation of interactions between metal atoms and borophene.

Doping has raised interest due the optimization of borophene with, for example, titanium. Dong et al. [112] make an outlook regarding the B_{40} fullerene dope with titanium in the resulting Ti_6B_{40} structure which demonstrates an adsorption energy of 0.37 eV/H_2 with the holding of up to 34 H_2 molecules. Moreover, the results show reversible storage under ambient conditions.

To sum up, a comparison table of the addressed borophene phases is presented in Table 3 for further discussion.

Table 3. Comparison of theoretical studies on borophene for hydrogen storage.

Metal Added	Borophene Phase	Adsorption Energy	Hydrogen Storage Capacity
		eV/H_2	wt.%
Li	α [113]	0.11	10.75
	2pmmn [114]	0.15	6.8
	χ_3 [110]	10.39	10.79
	β_{12} [115]	0.22	10.85
Ca	α [116]	0.19	12.68
	2pmmn [109]	0.11	7.6
	χ_3 [113]	0.23	7.2
	β_{12} [117]	0.24	9.5

Table 3. *Cont.*

Metal Added	Borophene Phase	Adsorption Energy	Hydrogen Storage Capacity
		eV/H_2	**wt.%**
N	α [118]	0	6.22
Na	α [111]	0.11	9
	2pmmn [119]	0.007	8.36
K	α [111]	0.06	2.36
Ti	χ_3 [120]	0.199	15.065

6. Challenges and Perspectives

In this review, we discussed the strategies to stabilize borophene structures and highlight the importance of developing large-scale methods for producing stable semiconducting borophene. The proposed strategies include sonication and substrate assistance. While some progress has been made in synthesizing borophene via the CVD and MBE methods, stable semiconducting borophene remains limited. There is still the necessity of advancing preparation techniques to meet the demands of boron-based nanomaterials for potential applications in energy conversion and production since yield production, growth rate, and cost remain highly dependent on the synthesis route limiting the tests only to a laboratory environment, and no benchmarking can be performed for an economical model regarding its worldwide application. The possible approaches include elemental doping, the thermal decomposition of borohydrides, and the one-pot heating of boron sources with various materials. Hydrogenation is identified as a viable route for growing stable semiconducting borophene, exemplified by the synthesis of α′-4H-borophene, which not only suggests a method to open the band gap, but also provides experimental direction. It underscores the importance of continued research combining theoretical insights with experimental efforts [121].

Based on successful experiments, it is crucial to explore the physical, chemical, and biological properties of borophene for potential device applications. Borophene has been investigated for use in chemical sensors, nonvolatile memory devices, supercapacitors, electrochemical hydrogenation production, and cancer therapy and imaging. However, there is still much to uncover, particularly in advanced information storage devices, photodetectors, and sensors. Despite progress, borophene research remains in its early stages, presenting both challenges and opportunities. The systematic exploration of borophene preparation, properties, and applications is needed. The controlled synthesis of crystalline and semiconducting borophene requires further effort to explore novel physical properties. This review aims to break traditional thinking and pave new paths in borophene research, both theoretically and experimentally. There is a strong belief that borophene holds vast potential to drive research and development in the realm of 2D materials.

7. Conclusions

Borophene, an emerging two-dimensional material, has garnered significant attention due to its exceptional physicochemical properties, diverse polymorphic structures, and potential for a wide range of advanced technological applications. This review summarized and analyzed the recent advances in borophene synthesis, the stabilization of its polymorphs, its mechanical and electronic properties, and especially its promising role in hydrogen storage and energy-related technologies.

One of the primary challenges in borophene research is the development of scalable and reliable synthesis methods that yield stable and high-quality monolayers. While bottom–up methods like chemical vapor deposition (CVD) and molecular beam epitaxy

(MBE) have demonstrated success in controlled environments, their scalability remains a limitation. On the other hand, top–down approaches, including ultrasonic-assisted liquid-phase exfoliation, have offered a pathway for bulk synthesis, albeit constrained by the non-layered nature of bulk boron. Innovations that combine etching and sonication have opened new possibilities, particularly for producing ultrathin boron sheets suitable for practical applications. The review also emphasizes that the substrate plays a critical role in stabilizing borophene, influencing not only its phase, but also its crystallinity and conductivity. Substrate-assisted growth on metals like Ag (111), Al (111), and Cu (111) remains a vital area of investigation for achieving the controlled synthesis of different borophene phases. Furthermore, emerging strategies such as elemental doping, hydrogenation, and the use of boron hydride precursors provide new avenues for tailoring borophene's properties to enhance stability and functionality. Mechanically, borophene stands out due to its low bulk density, high flexibility, and anisotropic behavior, which endow it with potential for integration into flexible electronics, sensors, and composite materials. Its delocalized bonding configuration and resistance to oxidation—particularly in 2D form compared to bulk boron—further support its viability in harsh environments and long-term applications. Most notably, borophene shows remarkable promise in energy storage and hydrogen evolution. Its high surface area, strong adsorption energy for hydrogen, and significant hydrogen storage capacity, especially when functionalized with alkali and transition metals, highlight its utility in future hydrogen-based energy systems. The data gathered so far underscore borophene's suitability as a high-performance material for hydrogen storage, electrocatalysis, and potentially in fuel cell technologies. Despite this progress, borophene research remains in its nascent stage. Critical gaps persist in understanding long-term stability, precise control over phase selection, and integration into device architectures. Addressing these challenges will require an interdisciplinary approach, combining theoretical predictions with experimental validation. A systematic exploration of borophene's structure–property relationships, functional modifications, and interface behavior with other materials is essential. Borophene is poised to become a transformative material in the next generation of nanotechnology and energy applications. Continuous investment in fundamental research, novel synthesis pathways, and application-driven investigations will be crucial to unlocking its full potential. The insights provided in this review are intended to serve as a foundation for further innovation, guiding both the scientific and engineering communities in shaping the future of borophene-based technologies.

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