Proceedings of the 5th International Conference on Materials Chemistry and Environmental Engineering
DOI: 10.54254/2755-2721/2025.29820

Transformative Potential of Borophene: Revolutionizing Energy Storage

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Abstract. Borophene is a new two-dimensional material with several outstanding properties. Since it consists of boron atoms, it would be widely utilized in energy storage applications. This review primarily focused on mechanical flexibility, superior electrical conductivity, and high reactivity, which allows it to be used in supercapacitors, lithium-ion batteries, hydrogen storage, and enlightening the unique atomic structure of borophene. Among all the properties, hydrogen storage is the most noteworthy of all, considering the fact that borophene has a high surface area with strong hydrogen binding, which perfectly matches the need to dope with lithium. Being lightweight with tunable electronic and thermal properties, this makes it the perfect material for creating future energy devices that could eventually enhance charging cycles together with higher energy densities. Although challenges on its synthesis and stability remain, many further developments, in particular deposition techniques and protection methods continue to improve its prospects. The main emphasis of the review is especially dedicated to the transformation role played by borophene in energy storage, underlining at the same time its potential applications in different areas, such as hydrogen storage and solid-state batteries.

Keywords: Borophene, Energy storage, Hydrogenated molecule, Synthesis

1. Introduction

Borophene is a two-dimensional substance comprising a crystalline monolayer of elemental boron [1]. The existence of borophene was first predicted by theory in the mid-1990s. Computational studies by I. Boustani and A. Quandt revealed “that small boron clusters do not form icosahedral geometries like boranes but instead adopt quasi-planar structures”, leading to the prediction of borophene (boron sheets) [2]. Experimental confirmation of boron cluster planarity came from L.-S. Wang's research team, who found that the B36 cluster, with sixfold symmetry and a hexagonal vacancy, could serve as a basis for 2D boron sheets [3]. The synthesis of silicene, a highly reactive 2D material, led researchers to predict that borophene could also be realized using a metal surface as support [4]. In 2015, two research teams succeeded in synthesizing different borophene phases on silver (111) surfaces under ultrahigh-vacuum conditions [5]. Different from some familiar 2D substances like graphene, the atomic structure of borophene consists of mixed triangular and

DOI: 10.54254/2755-2721/2025.29820

hexagonal motifs. The cause of such atomic structure is the interplay between two-center and multi-center in-plane bonding, which is typical for elements like boron, elements with electron deficiency [6].

As borophene has various exceptional properties, it is particularly applicable for many energy storage applications [5]. It has a unique two-dimensional (2D) structure, as its atoms are arranged in different polymorphic structures, like triangular, and hexagonal, and even more complicated patterns like parquet lattices [5]. These different types of structure make borophene mechanically strong, and even with a variety of Young's modulus and Poisson's ratio, as it consists of many different types of phases or orientations, it's still flexible and exceeds graphene's properties, therefore making it ideal for stretchable electronics [5]. Due to its metallic nature, it has a high level of both electrical conductivity and density of states, which is close to the Fermi level [7]. Additionally, borophene hosts Dirac fermions, which leads to its distinctive electronic behaviors like high levels of electron mobility [7]. It also exhibits direction-dependent electrical conductivity, which varies conductivity in different crystallographic directions [5]. Therefore, some of its electronic properties like band gap and carrier mobility, could be tuned by changing atomic structures, applying strain, or doping. This further makes it suitable for electronic and optoelectronic applications. Also, borophene demonstrates high thermal conductivity, ranging from 14.34 to 150 W/m·K, and anisotropic thermal conductivity, which makes it suitable to help electronic devices to dissipate heat [5]. Borophene's optical transparency and wide absorption range across the visible and ultraviolet spectra further suggest its potential in optoelectronic applications [5].

Some of the chemical properties of borophene also contribute to their ability to energy storage, for instance, due to their electron-deficient nature, they are highly reactive, hence making them suitable for catalysis and chemical applications [7]. However, borophene could become too reactive, and therefore difficult to control, this is when its oxidation sensitivity helps to balance its reactivity [8]. When borophene is exposed to ambient environments, it would be prone to oxidation, and thus degrade its properties to some extent, making it easier to use and control [7]. Furthermore, in heterostructures, the interaction of borophene with graphene, something that is essential when synthesizing the substance, increases electron density and minimizes electron interactions [8]. Also, borophene will find wide applications in various catalytic uses that range from Hydrogen Evolution Reactions (HER) to oxygen reduction reactions because of its large surface area with high reactivity [5]. Particularly, borophene will find wide applications in hydrogen storage technologies due to its excellent hydrogen absorptivity [5]. Moreover, borophene could be used in another wide range of applications, as it could stabilize different types of bonds, like the three-centre two-electron (3c-2e) bonds and σ bonds, which both lead to the formation of 2D sheets [5].

Both the recent development of borophene and its potential in transformative energy storage are explored in this review, specifically focusing on supercapacitors and hydrogen storage. Reflections are also made on its atomic structure, electronic properties, and high surface area, it highlights the possible application of borophene, for instance, offering faster charge cycles, improving energy density, and increasing the durability of batteries and supercapacitors [7]. That suggests the important role borophene may play in the future energy storage field and perhaps even electric or hydrogen vehicle developments.

2. Development and advancements in borophene

During the 1990s, the seminal work of the researcher Boustani and coworkers originally modelled boron clusters using advanced computational techniques such as the Density Functional Theory (DFT) and predicted the possible existence of two-dimensional boron sheets [5]. Using these

DOI: 10.54254/2755-2721/2025.29820

models, the team proposed that the electron deficiency property of borophene would enable the possibility to form various stable, quasi-planar structures, such as triangular, hexagonal, and mixed triangular-hexagonal lattices [9]. Indeed, these theoretical studies state that borophene could exhibit extraordinary electronic, mechanical, and thermal properties [5]. Among these, its ability to conduct high electricity and mechanical flexibility is highly desired for energy-related applications, like electrodes in batteries and supercapacitors [5]. As borophene has the capability to form lightweight, metallic structures with a high surface area, it suggests its strong potential in fields like hydrogen storage and as material for energy-efficient devices [7].

The other aspect of the early stage theoretical work was the prediction of borophene's polymorphism, which is the ability to adopt different structural phases depending on the external conditions [9]. Phases like the buckled triangular and the distorted hexagonal sheets had been theoretically predicted to have different electrical and chemical properties, thereby making borophene highly tunable for specific applications [7]. Predictions of borophene's strong interaction with lithium and other metal ions supported the idea of its potential to become an energy storage material with high energy capacity for lithium-ion batteries [5].

The first successful experimental synthesis of borophene was realized in 2015 by two independent groups that successfully grew borophene monolayers on silver (Ag) (111) substrates assisted by molecular beam epitaxy (MBE), which was led by Guisinger and Wu [5]. This breakthrough was considerable because, unlike graphite, which is the precursor of graphene, boron does not form any natural layered structure, and further causes difficulties for borophene synthesis [5]. The synthesis process was assisted using the silver substrate to stabilize it, thus enabling the growth of different structural phases depending on temperature and deposition rates [7]. The experimental realization of borophene not only confirmed these theoretical predictions but also showed the polymorphic nature of this material, as reflected in structural phases such as sheets of β12- and χ3 [5]. The possibility of controlling borophene structure by conditions of synthesis opened a new way for tailoring properties to fit the application, especially in energy storage and flexible electronics.

These early works and predictions laid the foundation for further explorations of properties and applications of borophene in energy storage technologies. The abilities of borophene, the combination of high electrical conductivity, flexibility and tunability has positioned it as a strong candidate for possible future applications in supercapacitors, lithium-ion batteries, and hydrogen storage, where the performance could considerably surpass other 2D materials like graphene.

Significant advances have been made in the optimization of the synthesis of borophene, primarily due to deposition methods and the development of improved substrates for high-quality films [5]. Techniques like molecular beam epitaxy (MBE) and chemical vapour deposition (CVD) were optimized in a way to allow researchers to manage the growth of borophene in a more controlled and homogeneous way [5]. Advances in MBE now make it possible to deposit layers of borophene with tailored stoichiometries that yield optimized electronic properties capable of being tuned for specific applications [5]. The new development in atomic layer deposition (ALD) has improved layer-by-layer growth, enhancing structural integrity and uniformity of the boro sheets further; thus, it allows the incorporation of various dopants and functional groups that can be used to improve performance in energy storage applications further [7]. Modifications have also been done to substrates, and research into new substrates involves silver, gold, and even flexible substrates of polyimide and graphene for better growth of large-scale and defect-free free borophene films [5]. Such substrates offer better lattice matching, hence reducing the strain and defects, especially important to maximize the electrical and mechanical properties of the material [5].

DOI: 10.54254/2755-2721/2025.29820

Despite these advances, the stabilization of borophene stands out as one of the biggest challenges due to its vulnerability to oxidation when exposed to air and moisture, therefore, it's required to be handled and stored under extremely inert conditions [7]. Currently, various protective coatings, encapsulation methods, and environmental adjustments are being investigated in an attempt to enhance its stability in ambient conditions [7]. Other recent studies explored the use of boron nitride or other types of two-dimensional materials as protective layers that can shield borophene from degradation while still maintaining its electronic properties [5]. Besides that, industrial application of borophene requires upscale synthesis of the material, thus, researchers have been working on making suitable techniques more efficient and cost-effective on a large scale [9]. Liquid-phase exfoliation, solution-based synthesis, and even roll-to-roll manufacturing processes are being investigated with the view of easing the way toward bulk quantities of borophene without sacrificing quality [7].

Early exploratory studies have shown great promise for borophene in energy storage applications due to its lightweight structure, such as extremely high surface area, and its unique electronic properties [5]. These attributes mentioned make it an attractive candidate to enhance energy storage device performance, especially lithium-ion batteries and supercapacitors [5]. Most of the initial studies have focused on feasibility rather than specific comparisons with other materials and most of the research has shown the high theoretical capacitance and charge storage capacity of borophene, which proves to be highly improved compared to conventional materials [9]. Its unique configurations can lead to a variety of intercalation sites for better ion mobility, which becomes very important for enhancement in charge and discharge rates [9]. More significantly, researchers have been actively investigating the electrochemical behaviour of different borophene-based composites, where borophene is integrated with conventional electrode materials in hybrid systems to make use of their respective advantages [7]. These continuous improvements in borophene synthesis methodologies and possibilities to integrate it with practical devices would assess its feasibility for a wider range of applications, and future studies would reveal more of its potential in the energy storage field in the future [5].

3. Synthesis of borophene

3.1. Top-down approach

The top-down approach mainly involves mechanical and chemical methods for deriving borophene from bulk boron [4]. The most studied technique is mechanical exfoliation, where physical forces are applied to detach the layers from bulk boron [7]. During this process, sonochemical exfoliation may get involved, in which boron powder is dispersed in solvents like acetone, dimethylformamide, or isopropyl alcohol [7]. It will then be placed in an ultrasonic bath and undergoes ultrasonic treatment for several hours, which is typically up to 24 hours. This process helps in exfoliating the boron into few-layered borophene sheets [5]. After that, the separation of the resulting borophene flakes from the solvent is done by centrifugation, hence the isolation of the material for further studies [4].

Chemical vapour deposition (CVD) is another technique within the top-down approach. In this process, the precursors of boron are vaporized and then deposited on a substrate at controlled temperatures, usually in the range of 300 to 1100 °C [5]. Thus, CVD can ensure very tight control over the growth conditions with respect to temperature, pressure, and substrates to be used, thereby enabling the production of borophene into desired structural configurations and properties [7]. However, the usually implemented CVD synthesis may be successful only at the rigid conditions of

DOI: 10.54254/2755-2721/2025.29820

environmental control and choice of compatible substrates like silver or copper, which are highly expensive and have limited size [7].

3.2. Bottom-up approach

On the other hand, the bottom-up approach synthesizes borophene using its constituent atoms or molecules, building up the material layer by layer more effectively. One proven technique is the molecular beam epitaxy (MBE). During MBE, ultra-high vacuum conditions deposit boron atoms on a substrate [7]. Hence, it offers total control over the final composition and thickness of the resulting borophene layers. The growth technique has produced high-quality crystalline structures, exhibiting very good electronic properties, making it suitable for further advanced applications in electronics and optoelectronics [5].

One of the latest methods currently under research for the bottom-up synthesis of borophene is an electrochemical exfoliation technique [4]. In this instance, controlled electric current and adjustment of temperature for boron can facilitate electrochemical exfoliation of borophene from the substrate of boron [4]. By applying a controlled electric current and adjusting the temperature of the boron, researchers can promote electrochemical exfoliation of borophene from the boron substrate [4]. This technique therefore seems very promising for large-scale production due to the relatively simple setup, reduced chemical waste, and high-yield borophene sheets [4]. Due to the incorporation of temperature control, this method allows the enhancement of boron conductivity, therefore overcoming the challenges of using boron at low temperatures as an insulating material [7].

When synthesizing borophene, there stands a series of obstacles in the way of realizing it through both top-down and bottom-up techniques. The top-down approach is easier to conduct and more accessible, and results are immediate from the build materials [5]. However, it suffers from the limitation of quality and purity of borophene produced at the same time [5]. Whereas the bottom-up technique offers better control over material properties, it may well produce higher-quality borophene for more advanced applications [5]. Both of these methods require special requirements and have very specific environmental needs, and hence complicated to make and resource-consuming

Ultimately, the synthesis route that is followed will depend on the application intended, the scalability of the process, and the properties that should be present in borophene. In due course, further studies are going to result in improvement in both techniques by increasing yield, enhancing quality, and hence broadening applications of borophene as a material of great importance for future generations in energy storage, nanotechnology, and electronics [5]. Presently, the bottom-up or top-down approach-based hybrid methodologies are also being studied constantly to optimize the synthesis process for use in other applications, thereby overcoming some of the challenges and realizing the full potential of borophene.

4. Borophene properties for energy storage

One of the key properties of borophene is its exceptional mechanical strength [10-13]. It could withstand high levels of stress and strain, with a high range of Young's modulus, between 100 to 400 GPa. Therefore, might lead to advanced materials development for structural application.

Its exceptional strength is ascribed to the unique covalent bond within the hexagonal structures [5] and its crystallographic structure [7], which improves the performance of batteries while undergoing mechanical stress. In terms of electrical conductivity, borophene is highly conductive, and depending on the structure and doping, it shows metallic and semiconducting behaviours. This

DOI: 10.54254/2755-2721/2025.29820

flexibility makes it a perfect candidate for applications in electronics, such as the fabrication of high-performance transistors and nanoscale circuits. Besides, since it is able to transport ions and electrons fast, it perfectly fits in to improve energy storage device efficiencies, in particular batteries and supercapacitors.

Moreover, borophene shows interesting optical properties. It has the ability to absorb and emit light at certain wavelengths, thereby opening more perspectives for its application in optoelectronic devices [5]. It also exhibits a wide optical absorption spectrum, which makes it very useful for application in the case of photodetectors and solar cells, which can be used later in energy storage [5]. Besides, due to its anisotropic nature, borophene has relatively good thermal conductive ability; its conductivity value is approximately 266 W/mK, which may find applications for heat management, as it outperforms most of the known materials and therefore is very suitable for dispersing heat in such devices as lithium-ion batteries [5, 7]. At the same time, this reduces the possibility of any danger that could be caused by overheating and enhances the safety and longevity of batteries.

Furthermore, because of its unique structure and low dimensionality, borophene has a large surface area, which can be availed for applications in catalysis. For instance, this material has the potential to act as a catalyst in many different chemical reactions or as electrode material in batteries and supercapacitors, as the rate of ion transportation in those devices could increase and further enable better interaction with electrolytes present in a battery [7,13]. More importantly, it allows batteries to have a faster charging rate, which is essential for efficient energy storage systems. Lastly, borophene also contains a tunable bandgap, which allows modulation through strain and its tunability to enhance the performance of semiconductors, and at the same time, be able to adapt different electronic properties [7, 9].

New developments in the research studies would explore and understand the diversified properties of borophene. With the outstanding combination of mechanical, electrical, optical, and thermal properties, it indeed holds great potential for the improvement and innovation of various fields in science and technology.

During our research, we found that borophene has the most significant properties in regard to storage, for example, it's the lightest known two-dimensional material, which has superior electrical and thermal conductivity, and a higher tendency toward chemical reactions, which makes it suitable for storing metal ions in batteries. Therefore, amongst all the different types of batteries, like lithium, sodium and magnesium, borophene is the most suitable electrode material, which could be used as either a negative electrode or added to the electrolyte. Borophene has good electrical conductivity, and in particular, its ionic conductivity enables fast charge transport and ion diffusion. That makes the borophene in the battery capable of fast charging and discharging and hence improves the efficiency of the battery.

5. Borophene in energy storage applications

On account of the multitude of properties of borophene, this 2D material has different potential applications in the field of energy storage, including alkali metal ions batteries, hydrogen storage, solid-state batteries and supercapacitors.

5.1. Alkali metal ion batteries

For electrochemical energy conversion and storage, metal-ion batteries use a single type of ion to move between the positive and negative electrodes during charge and discharge [14]. Alkali metal

DOI: 10.54254/2755-2721/2025.29820

ion batteries (AMIBs), including lithium, sodium, and potassium-ion batteries, are crucial rechargeable battery technologies for decarbonizing electricity supply and transportation systems [15]. Because of its special qualities, borophene has been investigated as a very promising anode material for alkali metal ion batteries. Take lithium as an example, during lithium adsorption, it provides exceptional structural stability, small diffusion barriers, and high electrical conductivity. Theoretically, borophene-based anodes can store up to 1984mAhg^{-1}, which is a significant increase over conventional graphite anodes [16].

5.2. Hydrogen storage

For a material to be used for hydrogen storage, it must have a strong binding capacity for hydrogen (use the unit wt% to show H's weight percentage) and the ability to release and store hydrogen repeatedly in a reversible manner [17]. Compared with other research areas, borophene material for hydrogen storage rapidly grows [18]. Due to its high surface area, tunable electronic properties, and strong interaction with hydrogen atoms, borophene stores hydrogen by forming strong bonds and Van der Waals' force(VDW) between H and B particles. According to Ji et al., the solid binding capacity and reversible hydrogen storage ability of Li-doped χ3 and β12 borophene materials make them promising for hydrogen storage [19]. Furthermore, Liu and colleagues conducted Density Functional Theory (DFT) calculations on Li-decorated β12-borophene, and their findings indicated that a maximum of three hydrogen atoms can be absorbed by each doped Li atom [10]. Because Li-doped borophene can adsorb hydrogen molecules on both sides, it has a high potential hydrogen storage capacity of up to 13.7 wt% (at room temperature) or 9.1 wt% (at ambient temperature) [17].

5.3. Solid-state batteries

Unlike conventional batteries, which use liquid or gel polymer electrolytes for ionic conductions between the electrodes, solid-state batteries use solid electrolytes [20]. Compared to conventional lithium-ion or lithium polymer batteries, solid-state batteries have the potential to provide a significantly higher energy density [21]. Intrinsically, the enhancement of interaction between the additives and the host polymer chains is the key to boosting the ionic diffusion and transport of polymer-based solid-state electrolytes [22]. It has been discovered that the greatest surface area of two-dimensional (2D) materials can be used as nanofillers to optimize their interaction with polymer chains and subsequently control the binding strength of cations with adjacent anions [22]. Hydrogenated Borophene (HB) nanosheets are a unique class of two-dimensional materials with a flexible structure and crystalline/amorphous coexistence character that can enhance the interaction force between the HB nanosheets and the polymer host [22]. The ultra-lightweight, ultra-stable, and semiconductor qualities of HB nanosheets are further advantages [22]. Moreover, boron has an inherent flame-retardant quality. Thus, from a theoretical perspective, HB nanosheets can be a promising functional filler for quasi-solid-state electrolytes based on polymers. However, HB is limited to its initial use in the memory device field. As far as we know, HB is still not applied in the battery field [22].

There are some similarities between these applications. Overall, all the applications above have not been used in a wide range, either limited by the difficulty of synthesising borophene or the technology is still theoretical. The multiple applications reveal the promising future of borophene usage in the field of energy storage in the future. Some differences shown above may be that according to the different natures of borophene, hydrogen storage may be the most practical and realizable application that is likely to be achieved in the near future.

DOI: 10.54254/2755-2721/2025.29820

6. Conclusion

In conclusion, borophene, owing to its unrivalled combination of properties, is a very promising material for energy storage applications. Its light weight, combined with very high electrical and thermal conductivity and very high reactivity, turns this material into an ideal one for application in batteries, supercapacitors, and hydrogen storage [5]. Thus, thanks to a wide range of polymorphic forms included in the atomic structure of borophene, its mechanical and electronic properties could be tuned within very large ranges [5]. The material can thus be tailored for specific uses, ranging from fast charge and discharge cycles in batteries to improved ion transport in energy storage devices [7].

Applications involving hydrogen storage accordingly emerge as one of the most viable among those which involve borophene due to its high surface area and strong interaction with hydrogen atoms. In particular, the high capacity of borophene for hydrogen storage after doping with such elements as lithium positions it as a leading candidate among future hydrogen storage technologies [5]. The outstanding mechanical strength and conductivity also assured the potential use of borophene in solid-state batteries, where its flexible and flame-retardant properties could significantly improve both the safety and performance of energy devices [7].

Further challenges related to synthesis and stability may be conquered with the further development of better deposition techniques and protective coatings for scalable and practical applications of borophene. Due to the wide possibilities it holds in many fields, borophene is sure to create a revolution in the energy sector, especially in hydrogen storage and advanced battery technologies.

Author's contributions

Jiawei Ye contributed to the main idea, drafted the Introduction, sections on Development and Advantages in Borophene, Synthesis of Borophene, and Conclusion. Jiawei Ye edited the whole report, formatted the report, and ensured all citations were correct. Tianye Zhang wrote the section of Application of Borophene in Energy Storage Applications. Chengyi Shao contributed to writing about properties of Borophene for Energy Storage. All authors reviewed and discussed the manuscript before submission.

Acknowledgement

We would like to express our deep gratitude to our professor, Dr. David Zacks, who provided lots of feedback and helpful suggestions throughout this essay, helping us refine our ideas and enhance our arguments. Also, thanks to NeoScholar and Shanghai Jiaotong University that provided this chance to us. Furthermore, thanks to Ms Li, Kiki and Kennis who helped us with constructing the structure and always be helpful and supportive whenever we are facing challenges. Finally, thanks to all the efforts that our team members, Jiawei Ye, Chengyi Shao and Tianye Zhang, have put into this essay, the collaboration and hard work involved made this project a rewarding and enriching experience for us all.

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