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Short Review Article

Overview of Borophene as a Potential Candidate in 2D Materials Science for the Energy Applications

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Abstract:

Energy problem is one of the serious concerns in modern society; therefore, we have to take hastily an effective action. Hence, researchers are looking for some attractive materials with low-cost, lightweight, and environmentally effective. Recently, 2D materials have taken notable recognition in the field of materials science for multiple energy application, because of its unique electronic and optical properties; and borophene is one of the 2D material which is commendatories than graphene. However, it has not much experimentally explored yet. This review discusses the synthesis process of borophene and discussed energy-related application such as energy storage, optoelectronic, photocatalytic activity, and hydrogen storage. Moreover, this work provides a summary of each application that could help to understand the importance of borophene materials for energy applications.

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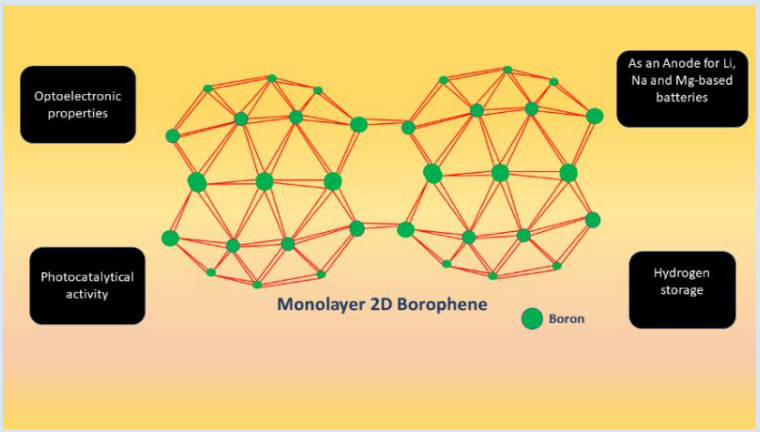
Keywords: Borophene; Energy storage; Optoelectronic; Hydrogen storage, Photocatalytic activity

Graphical Abstract:



Biography:

Niket Powar has completed M.Sc in Organic chemistry from Yashwantarao Chavan Institute of Science, Satara, Shivaji University, Kolhapur, Maharashtra, India. Afterwards, he has worked as Junior Research Fellow (JRF) in Ahmedabad university at Gujarat, India. Whereas, he has worked on the synthesis of bimetallic nanocomposite and demonstrated the catalytical activity for an organic transformation reaction. Recently, he has pursued M.Tech in nanotechnology and renewable energy and as part of M.Tech project, worked on the energy-related topic including the 2D materials. Moreover, his area of research interest is in the photocatalytic activity, water splitting, quantum dots based solar cell and 2D based materials for energy application. Now he is working as a research co-worker with Dr Rajkumar Pandav.

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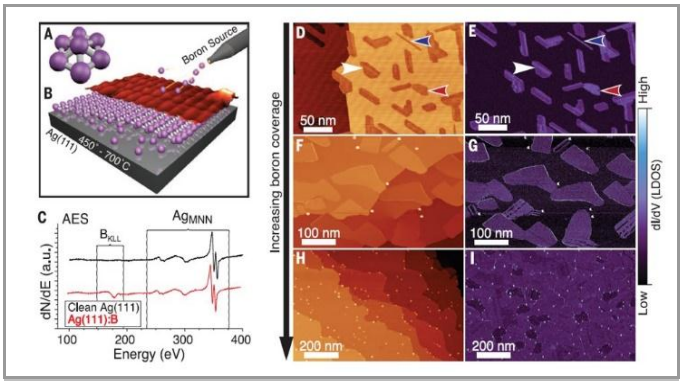
Dr. Rajkumar Pandav has completed his PhD in chemistry in 2016 from Shivaji University, Kolhapur, Maharashtra, India. During his PhD, he has worked on Synthetic, Characterization and Investigation of catalytic activity of mixed metal oxides and published 12 research paper in reputed journals. Since form 2012, he is working Assistant professor in Yashawantrao Chavan Warana Mahavidyalaya, Warananagar. Recently, he has been focusing widely for research in materials chemistry, such bimetallic nanocompsite, metal oxide and 2D based materials for photocatalytical activity.

1. Introduction

Nowadays, an emerging trend of 2D based inorganic materials [1-5] have been expanded hastily for application of energy conversion [6,7] and storage, [8,9] After graphene was discovered, researchers have found astonishing electronic [10,11], mechanical [12,13] and thermal [14] properties. Afterwards, discovered several 2D based materials such as Silicene [15,16] Germanene [17-19], Phosphorene [20,21], Arsenene [22,23], Antimonene [24] and transition metal dichalcogenides [25-27]. In Periodic table Boron comes nearest to Carbon element and Boron has an ability to form of polyhedral cluster structure, impact of that in 1996, Boustani [28] has done some computerized based calculation and proved that quasi planner cluster of Boron has remarkable properties resemble to the Graphite**,** we will discuss this papers in details, because of in this first time has mentioned about the 2D Boron based materials. Moreover, provided different structure with certain numbers of Boron atom and denoted point group symmetry, in addition to that derived structures has obtained stability, because of the presence of interaction pi-orbital out of a plane, a result of that formation of electron cloud sequent prevail stability. Besides, double layer Boron atomic layer highly stable, a consequence of that Boustani concluded that aforementioned contexts give an idea about possibilities for Boron polyhedral cluster having analogous properties to the Graphite [29]. After nine years in 2015, Andrew from Argonne laboratory ,USA has published an article commenting that, prepared first time grown atomically thin layer of Borophene sheets under ultra-high vacuum condition on top of Ag(111) substrate [30]. And claimed, at atomic cluster scale, pure form of Boron behavior like carbon, which created similar to simple planner and cage-like fullerenes [31] Bororphene shows metallic characteristics, in their papers have reported scanning tunneling microscopy images, which has shown that flakes kind of nature, follow Figure 2. In experimental and theoretical studies lead to systematic understanding structure of borophene, it has taken attention for 2D atom-thin sheet of boron found to be honeycomb structure like to Graphene, with hexagonal vacancies, which is highly stable that could possible to make boron nanotube with multiple sheets. The Piazza *et al*. have first time demonstrated experimental experience about hexagonal vacancies and it can vary with the deposition substrate [32]. In this present review article, it gives an idea about how borophene can overwhelm to graphene application, and moreover, we will address a few synthesis methods. Furthermore, in the case of application borophene has numerous applications, we have introduced a few of them, that includes energy conversion and storage, besides, that photocatalytic for CO_2 reduction and water splitting. And the concerning hydrogen storage can be enhanced of storage capacity. Therefore, it gives a wide perspective towards new 2D material which is analogs properties to graphene or we can mention better than that.

2. Synthesis of 2D atomic-thin layer Borophene

The Borophene has synthesized first time by Andrew J. Mannix *et al*. in 2015 at the USA. The Borophene has grown on the top of Ag(111) as substrate under ultra-high vacuum condition and used solid boron precursor. A substrate provided an inert surface to grown boron and maintained 450^{oC} to 700^{oC} substrate temperature. After deposited of boron, discovered that two phases have developed, that was a homogenous and striped phase, those depended on deposition rate, it has shown in figure 1. The slow rate ended in the striped phase and higher rate dominated the homogenous phase [30]. Afterwards, they have done characterization and found gapless (metallic) characteristics, and this study motivated for scientist to work in future.



Scheme 1. Synthesis of 2D- thin layer borophene on top of Ag(111) substrate

Figure 1A Showed that distorted B_7 cluster, B) Growth set with atomic structure model and STM topography, C) This AES spectrum graph showed Ag(111) before and after deposition of boron. D) to I) illustrated STM topography and closed-loop dI/dV images of borophene sheet left and right side respectively. In details, D and E showed that low coverage, F and G medium coverage, H and I has high coverage. Moreover, homogenous, striped, island and nanoribbon has shown with red, white and blue arrow correspondingly. Reproduced and reprint with permission [30].

Qing Zhong *et al*. came with similar substrate Ag(110), however, crystal lattice was different. And they have successfully prepared a single-layer atomic thin layer of borophene nanoribbon. Moreover, inferred about the substrate that, in beforehand Ag(111) crystal lattice substrate a growth of borophene formed triangular shape and edges are along three crystallographic orientation of Ag(111). In their investigation stated that self-assembly grows of borophene nanoribbon along [-110] direction of Ag(110), further appeared four periodic structure on borophene nanoribbon, additionally studied and confirmed properties with DFT(density functional theory) [33]. In 2013, Yuanyue Liu and co-workers explained the penetrating synthesis of 2D boron sheet with first-principle calculation. The 2D boron grown on the Au(111) and Ag(111) and Cu(111), this metals does not have reactivity, its leads formation compound with them. However, these metals provide extremely good for the nucleation process. Also, high nucleation [34,35] rate barrier avoids the 3D formation of boron. Additionally, Mg offers reactivity with boron and forms metal borides, [36] in that case, a saturation of atoms impedes further growth of sheet [37]. Wenbin Li *et al*. have synthesized honeycomb borophene used as Al(111) substrate with help of molecular beam epitaxy(MBE) and concluded that, Al has stable substrate for boronphene formation. And noticed, effective charge transfer in Al with compared to Ag, resultant claimed that it could help for intensification of electronic properties [38]. The substrate encouraged flexibility of the borophene has described by the Zhuhua Zhang *et al*. deposited on Ag(111) [39] and added elastic plate theory [40].

3. Applications

After, synthesized the borophene in 2015, it has widely explored for energy application such energy storage and conversion. However, in current review article gives outlook and brief explanation about a few application of borophene.

3.1. Energy Storage

The modern world is going to suffer sooner because of the energy crisis, therefore, we need to have some low-cost and higher performance materials to enhance the energy capacity and outstanding cycle performance in energy storage devices. Recently, 2D based materials have been significantly growing. And 2D based materials electrode have shown remarkable electrochemical performance in energy storage capacity [41-43]. Graphene has played a pivotal role in energy storage, [44,45] as an excellent electrode system, however, beyond the graphene, also there are some 2D materials such as MoS_2 [46,47], WS_2[48], VS_2 [49] this are transition metal dichalcogenides, further in transition metal carbides so-called Mxene for an example Mo_2C [50,51] and Ti_3C_2 [52] etc. Here, we have focused that borophene as a potential candidate for energy storage. Researchers already have done details study of properties for borophene and found one step ahead than graphene, therefore, this ideology has motivated to introduce this kind of materials for energy storage in different based ion batteries such Li, Na and Ca. Yang Zhang and co-worker Studied Li and Na ion adsorption and diffusion rate, used spin-polarized density function. And registered observation as Li atoms can bind effectively to borophene without energy barriers during the process, borophene and resultant adsorbed complexes exhibited the metallic characteristics, this necessary for an electrode. Borophene layer has corrugated structures, noticed that borophene itself might provide a channel facility for Li-adsorption. However, diffusion of Li-ion occurred in an uncorrugated direction, which has registered 10^4 and 10^5 faster than MoS_2 and graphene respectively [53-55]. In 2016, has noticed the performance of Li-ion battery with two different structure, that was β12 and χ3. Xiaoming Zhang *et al*. have improved Li and Na ion adsorption sites, also, found good electrical properties of before and after adsorption of host materials. And storage capacity has noticed significantly as 1984 $mAhg^{-1}$ in β12 and 1240 $mAhg^{-1}$ in χ3, therefore, it has much time better performance than current 2D materials electrode [56]. In Li-S batteries [57-61] has hurdle for the suppress the shuttle during a performance, after, investigated understand the lacking in the adsorption energy on the carbon surface of lithium polysulfides with compared to the electrolyte molecules, consequently, lithium polysulfide is easy to dissolve and transfer to the anode. The result of that effort has been taking to developing the anchoring group for enhancement of large adsorption energy in Li-S based batteries. To solve that problem, H.R. Jiang and co-worked came with borophene material and exhibited ultra-higher adsorbent capacity as anchoring material for Li-S batteries. However, in borophene found a decomposition of Li-S during cycling, the effect of that

loss of sulfur has noticed. The solution for that defective borophene, which has found effectively enhancing the adsorption energy, moreover, it stopped the decomposition of Li-S [62].

Table 1. Use of borophene for the batteries

Borophene	Theoretical capacity(mAh/g)	References
p-doped	1732	[63]
Li0.75B	1860	[64]
Novel boron nanosheets	3306	[65]
For Na-ion batteries	1240	[66]

3.2. Optoelectronic Applications

The light modulation is a crucial aspect in the photonics [67] and optoelectronics field [68,69], therefore, we could regulate control of light in various channels such as optimizing materials attributes and effective novel materials. Nowadays, 2D materials have been dominating in the field of optoelectronic [70,7] area, because of unique optical and electronic [72,73] characteristics. So far there are many 2D materials, assuredly, its start with graphene, that has confirmed optical properties to a great extent. Yonder graphene [74], also registered 2D materials, for an examples WS_2 [75], $MoSe_2$ [76], MoS_2 [77], this are transition metal dichalcogenides and it has notified extraordinary optical properties because we can optimize the band gaps from monolayer to bulk as high to low E_g respectively. Furthermore, metal carbide [78] and metal nitride also found significantly great properties, notwithstanding, this is mostly more than two atoms, hereabouts, we are centring to a single element based 2D materials, currently, the new materials which have analogous features to graphene that is borophene as also attained extremely effective optoelectronic properties. Lyudmyla Adamska [79] *et al*. have confirmed fine-tuning the optoelectronic properties, two-dimensional boron synthesized of different crystal structure, its dependent on which substrate has used. While developing the borophene sheet typically, it uses to induced strain, accordingly, demonstrated two different structure that was β_{12} and δ_6, under appeared strain, resultant change in the band structure and charge density delocalization properties as tuneable because of few percentages of strain in borophene material. Furthermore, as we knew that changing band structure with monolayer to bulk, here also investigated by same research group that borophene as transparent electrode using density functional theory [80]. In 2017, J.W. Jiang and research group have observed that van der Waals heterostructure of tunable Schottky barrier and electronic properties in borophene/g-C2N and concluded that electronic properties of borophene/gC2N Van der Waal heterostructure used first-principle calculations, noticed effective charge transport in heterostructure while applied external electric field. The consequence, of we, have an opportunity to tune carrier concentration and Schottky barrier with the help of tuning in the Van der Waal heterostructure [81]. This insight can be useful in nanophotonic and optoelectronic devices. L. Z. Liu *et al*. have concluded that effectively elimination of Schottky barrier as well as strong electrical field effect using monolayer borophene electrode [82]. This all facts have benefit for the electronic, nanophotonic and optoelectronic devices.

3.3. Borophene Based Photocatalytic Activity

Recently, this field has taken widely attention for water splitting to the production of hydrogen as fuel. In 1972, first demonstrated photocatalytic activity for water splitting by Honda-Fujishima using TiO_2 as photo-catalysis [83-86], however, TiO_2 band gap comes under the UV region [87], therefore, resultant activity was not that great. To overcome this problem we should have semiconductor materials, which as bandgap in the visible region, afterwards many materials have discovered, nevertheless, now it has been great demanding for 2D based materials because of its tunable bandgap so that we could overcome the previous hurdle. Besides, 2D material has high surface area that provides active sites for catalytical activity [88]. The graphene [89,90] is having high catalytical activity and showed for water splitting as well. However, currently, 2D transition metal dichalcogenides have been drastically highlighted for the photocatalytic activity due the long-time stability, tunable bandgap and available active sites for the reaction are existing effectively such WO_3 [91], TiS_2 [92], SnS_2 [93,94], WSe_2 [95,96], one more remarkable properties of this materials has conversion of indirect to direct band followed with bulk layer to monolayer correspondingly. Additionally, one more group of 2D materials based groups acquiring attention that is MXene [97]. So borophene also has similar properties likewise graphene, therefore, it has also as interesting photocatalytic activity. In 2016 Li Shi *et al*. [98] have demonstrated that boron monolayers as electrocatalyst properties for hydrogen evolution (HER) so-called water splitting, have used the first principle calculation to understand it. And concluded that boron monolayers show that approximately zero free energy (ΔG_H) for hydrogen adsorption because of it similar to the metallic properties such Pt. Moreover, proved the silver has a suitable efficient substrate for the HER activity because mismatch during the growth of borophene leads to enhancement of electrocatalytically activity. The borophene is weightless materials for the HER and Oxygen evolution reaction (OER), after doping of C,

N, P, and Li element into borophene, the resultant effect has studied by Showkat H. Mir and co-worker, calculated the adsorption free energy for Oxygen and hydrogen. And resultants have examined that enhancing that catalytical activity, so its newly open window for lightweight 2D materials for HER and OER [99]. Recently in 2018 Chuangwei Liu *et al*. [95] claimed that borophene could be a metal-free catalyst. Aforementioned, many researchers [100-102] have proven that all this significant characteristics and evidence prove that highly possibility of having a remarkable change in HER and OER field because of the borophene as novel electrocatalyst.

3.4. Hydrogen Storage

In future hydrogen fuel will prominent source for energy, however, there are several challenges have been existing and researchers have been always fascinating to solve this obstacle. Suppose, if we are looking according to priorities safety is most important things in hydrogen storage, as we knew that energy density of hydrogen gas is excessive, hydrogen is very reactive with oxygen, it is an exothermic reaction. Moreover, solid-state hydrogen storage remains a major challenge. The metal hydrides [103,115] have extensively been used in hydrogen storage, however, unfortunately, stability and sluggish kinetics [104] are major drawbacks of this kind of materials. In the current situation, new families have been coming into hydrogen storage science, which has immense potential to overcome most of the problems that so far exists. The 2D materials are one of them have arrived in hydrogen storage and become useful in a great extent, there are numerous example such as graphene [105,106] has used majorly, however, nowadays, new family materials also been used such transition metal dichalcogenides [107,108] and alkali based 2D materials such as metal carbides and nitride [109]. The 2D materials are mechanically robust and it has a profoundly catalytical activity to enhance the kinetics for adsorption and desorption of hydrogen gas [110]. Moreover, it gives highly active sites that are high surface energy, that provides a large amount of adsorption of hydrogen gas. Recently, new material has been introduced in hydrogen storage, which as an analogue to graphene, that is borophene. In borophene found that has several steps ahead significant properties than graphene, and as we know that boron has extremely reactive with hydrogen, forms stable compounds. So far experimentally has not applied as expected, calculated storage capacity using first principle calculation, Chun-Sheng Liu *et al*. [111] have reported that reversible hydrogen storage in metallic hexagonal B_{36}, explained the curvature and ionization. Borophene has coated with Li-metal to enhance the adsorptions and found adsorption energy has suitable for room temperature. Furthermore, several hydrogen molecules have measured by using negative differential resistance behavior at different bias voltage region. However, Li-atom has a problem that it adsorbs with low binding energy, therefore, Jianchuan wang *et al*. [112] have came with a solution, Calcium coated boron sheet, and registered that six molecules have captured at 0K with binding energy as -0.20 to -0.32 eV/H_2. The mechanism of adsorption has appeared from not only the polarization effect but also the orbital hybridization and noticed 12.58 wt% gravimetric hydrogen density. Moreover, Ca-decorated [113-115] boron sheet at room after adsorption of hydrogen all structures were stable, this kind of materials could be useful for the vehicle application. Some of the researchers have tried with Na- decorated [116] as well instead of Li-atoms. Therefore borophene is having an immense potential for hydrogen storage, however, there are some challenges, to overcome that we need to have further modification.

4. Conclusion

Based on the concise illustrated above information about the borophene, we have inferred that it has enormous potential for the materials science field applications, notably for energy applications. Furthermore, borophene has not been examined much in an experimentally, because still, synthesis has to optimize. Nevertheless, recently for Li, Na and Mg ion-based batteries has reported borophene is a potential candidate for the anode. The borophene has high surface energy, consequently, it has shown that high photocatalytic activity for water splitting. In the case of hydrogen storage, borophene has the most stable material than any other that so far available today. Sooner in future, will have tremendous attention in the materials science field, particularly in Li-ion batteries and hydrogen storage.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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