Pure and Silicon Doped Boron Carbide (BC_3) Monolayer as Electrode Material for Li and Na-Ion Batteries - A DFT Examination

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Abstract*: In this work, density functional theory calculations are performed to study Pure and Silicon doped boron carbide (BC_3) as electrode material for alkali metal batteries. The structures of Pure and Silicon doped boron carbide (BC_3) monolayer have been optimized using M06-2X/6-31+G*. Our calculations show that, the energy gap of BC_3 is significantly reduced due to doping with Si. The adsorption of Li/Li^+ and Na/Na^+ on pure and Silicon doped BC_3 are also investigated. Our adsorption energy calculations indicate that the Li/Na atom adsorbed on Pure and Silicon doped BC_3 having high adsorption energy than Li/Na ion adsorbed on Pure and Silicon doped BC_3. This is because of the smaller charge transfer in Li/Na ion adsorbed on monolayer compared to Li/Na atom adsorbed on monolayer. The calculated specific capacity values for Li^+ adsorbed on Pure and Silicon doped BC_3 are 215.77 mAh/g and 207.89 mAh/g while the Na^+ adsorbed BC_3 has specific capacity value to be 208.34 mAh/g and 200.98 mAh/g respectively. Since, Li^+ adsorbed on BC_3 has high Cp values than Na^+ adsorbed on BC_3, which shows that Li^+ is suitable for charge storage application than Na^+.

Keywords*: boron carbide, metal-ion batteries, DFT, adsorption energy, Specific capacity.

I. INTRODUCTION

After the first discovery of graphene in experiments [1], substances such as graphene and similar materials are under extensive experimental as well as theoretical investigations. This is due to their innovative physicochemical properties [2], [3]. Further, these new systems have huge potential in many areas because of its interesting electronic properties [4]–[6]. Earlier studies have shown that the carbon-based systems, such as radiation-refined graphite and other carbon nanostructures have defects like monovacancies or multivacancies. Therefore, it is necessary to understand the characteristic of intrinsic or artificial defects of above system is must for their applications in many areas for example, nanoelectronic devices, and graphene-based Li batteries. In general, the boron is used as dopant in carbon nanostructures for preparing nanoscale material. It is not surprising that the BC_3 monolayer is synthesized in the laboratory [7], [8]. Its molecular structure is identical to graphene but few boron atoms replace carbon atoms in graphene.[9], [10]. Pontes et al. have found that, no activation barrier is needed for substituting carbon atoms with boron atoms [11]. Though, graphene layers have semiconductor with zero gap behavior, the honeycomb BC_3 behaves like semiconductor with an indirect band gap [12]. Thus, the tunable electronic properties of h-BC_3 have been studied previously [13], [14]. In addition, earlier Ding et al. suggest that the hydrogen atom adsorption in hexagonal boron carbide gives Semiconductor to metal transition takes place [14].

Tuning the physical and chemical properties in heterogeneous catalysts remains one of the challenges in surface chemistry. The adsorption behavior of graphene-like materials leads to their usage as gas sensors as well as energy storage devices [15]–[20]. Nowadays, the researchers are studying h-BC_3 as electrode for alkali metal ion battery applications. For instance, Bhauriyal et al. [21] have studied h-BC_3 for the application as an electrode material for metal ion (Al) battery. Recently, Jia et al. [22] and Li et al. [23] have investigated lithium borocarbide as an anode material for Li^+ batteries. Till date, the search for suitable anode material for Li-ion battery continues. Hence in the present study, we have investigated Pure and Silicon doped BC_3 for Li and Na-ion battery applications using density functional theory (DFT). The atomic and molecular properties are studied and the obtained results are discussed.

II. METHODOLOGY

In the present study, we have chosen BC_3 monolayer (4 × 3 monolayer). It consists of 28 carbon and 8 boron atoms. Further, the hydrogen atoms are introduced as corner atoms to avoid terminal effect. The geometry optimization and energy calculations for the Pure and Silicon doped BC_3 monolayer are performed using M06-2X [24] with 6-31+G* basis. All the calculations are performed using GAMESS-US software [25]. Vibrational frequencies analysis is done to identify the stable minimum energy structure. The adsorption of Li/Li^+ and Na/Na^+ on BC_3monolayer can be understand by calculating adsorption energy,

$$E_{ad} = E(BC_3) + E(atom/ion) – E(atom/ion...BC_3)$$

where E is the total energy of the system. The Density of States (DOS) is calculated using Multiwfn programme [26].

The internal energy is calculated using,

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$$I.E = [(E(atom) + E(ion\text{-}BC_3) - (E(atom\text{-}BC_3) + E(ion)]$$

The cell voltage of Pure and Silicon doped $BC_3$is calculated using,

$$E_{cell} = -(E_{internal})/(ZF)$$

where, Z is the charge on the ion Z=1 and F is Faraday's constant 96500 c/mol.

The specific capacity value can be calculated by,

$$C_p = F/W$$

where, F is Faraday's constant, its value is 96500 c/mol. W is the molecular mass of the alkali metals adsorbed Pure and Silicon doped BC_3 monolayer.

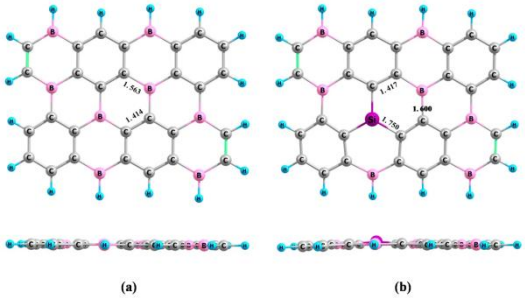

Fig. 1. Top and side views of optimized structures of (a) Pure and (b) Si-doped BC_3 at M06-2X/6-31+G* method.

III. RESULTS AND DISCUSSION

The geometry optimization and energy calculations of pure and Silicon doped BC_3 monolayers are done with M06-2X/6-31+G*. The obtained results are discussed in the order of Structures of Pure and Silicon doped BC_3 monolayers, Adsorption of Li/Li^+ on Pure and Silicon doped BC_3 monolayers, Adsorption of Na/Na^+ on Pure and Silicon doped BC_3 monolayers, Internal Energy and Cell Voltage and Specific Capacity.

Table- I: Energies of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and HOMO-LUMO gap energies of Pure and Si-doped BC_3 sheet. (Energies are given in eV)

Complex	HOMO	LUMO	HOMO-LUMO Gap
Pure BC_3	-7.92	-2.68	5.24
Si-doped BC_3	-5.35	-2.82	2.53

A. *Structures of Pure and Silicon doped BC_3 monolayers*

Fig 1(a) and 1 (b) show the optimized structures of pure and Silicon doped BC_3. In Pure BC_3, C-C and B-C bonds are present. The C-C and B-C bond length values are 1.414 Å and 1.563 Å respectively. This coincides well with the previous literatures on BC_3 [27]. In the case of Silicon doped BC_3, one boron atom is replaced with one Si atom. In this case C-C, B-C and Si-C bonds are present which has the bond length of 1.417 Å, 1.600 Å and 1.750 Å respectively. From the above, we understood that the structural properties of Pure BC_3 get altered while doping with Si atom. That is, the bonds are elongated while doping the Si atom into pure BC_3 monolayer.

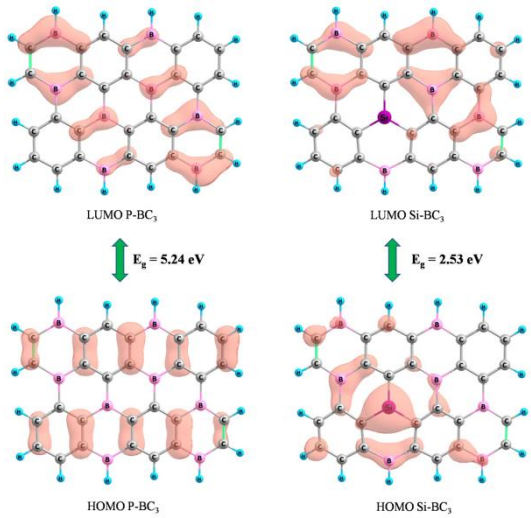

Fig. 2. The HOMO and LUMO diagrams of Pure and Si-doped BC_3 at M06-2X/6-31+G* method.

The HOMO and LUMO of pure and Silicon doped BC_3 and energy gap values are shown in Fig. 2. The energy gap of Pure BC_3 (i.e.) the difference between HOMO (-7.92 eV) and LUMO (-2.68 eV) is 5.24 eV. The energy gap values of Pure and Silicon doped BC_3 are shown in Table 1. While doping with Si atom, the energy gap (H-L gap) is reduced to 2.53 eV which has the HOMO value of -5.35 eV and LUMO value of -2.82 eV respectively. Thus, the Pure BC_3 monolayer becomes semiconducting like material while doping with Si atom.

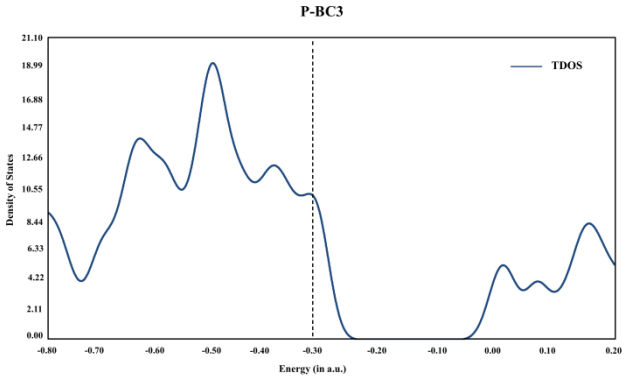

Fig. 3. (a) The density of states (DOS) diagram plotted for Pure BC_3 at M06-2X/6-31+G* method.

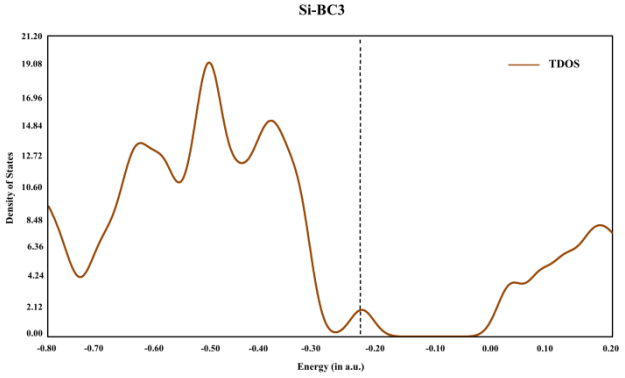

Fig. 3. (b) The density of states (DOS) diagram plotted for Si-doped BC_3 at M06-2X/6-31+G* method.

In order to understand the conduction and valence band of

selected structures, the density of states (DOS) diagram has been plotted. Figure 3 (a) and (b) shows the DOS diagram for Pure and Silicon doped BC_3 monolayers. From the DOS diagram, we can find that the Fermi energy level of Pure BC_3 is -8.71 eV is increased to -6.53 eV while doping with Si atom.

B. *Adsorption of Li/Li$^+$ on Pure and Silicon doped BC_3 monolayers*

The optimized structures of Li atom/ion adsorbed Pure and Silicon doped BC_3 monolayers are shown in Fig. 4. In Pure and Silicon doped BC_3 monolayer, the adsorption of Li atom and Li^+ is positioned above the hollow site. This site reported to be the most suitable position than the top and bridge sites [28], [29]. The distance between Li atom/ion and Pure and distance between Li atom/ion and Silicon doped BC_3 monolayers are listed in Table 2. Further, the distance between Li and Pure BC_3 monolayer is 2.260 Å. Similarly, the distance between Li and Silicon doped BC_3 monolayer is 2.428 Å. Similarly, the distance between Li^+ and Pure BC_3 monolayer is 2.348 Å and the distance between Li^+ and Silicon doped BC_3 monolayer is 2.465 Å.

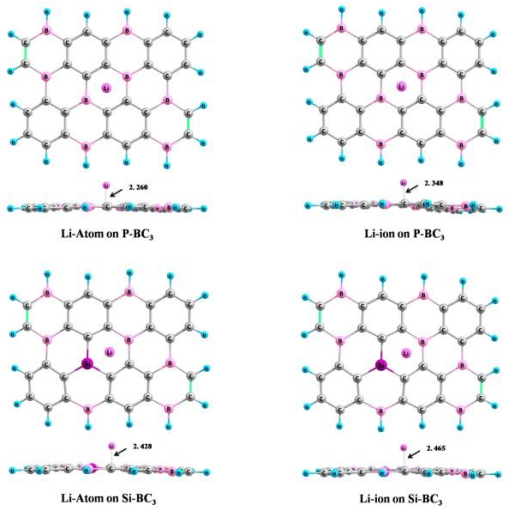

Fig. 4. Top and side views for the optimized structures of Li-atom and Li-ion on Pure and Si-doped BC_3 at M06-2X/6-31+G* method.

From the above values, we understood that the distance between Li atom adsorbed on Pure and Silicon doped BC_3 monolayer is less compared to the distance between Li^+ adsorbed on Pure and Silicon doped BC_3 monolayer. This is because of small amount of charge transfer (Q_t) and the values are listed in Table 2. In the case of Li atom adsorbed on Pure and Silicon doped BC_3 monolayer, the Q_t value is around 0.80. But in the case of Li^+ adsorbed on Pure and Silicon doped BC_3 monolayer, the Q_t value is only 0.61, -0.69 respectively. Earlier, Sangavi et al. have studied the adsorption of Li ions on Pure and defected graphene monolayers [28]. They calculated the distance between Li^+ and Pure graphene monolayer as 2.27 Å with the adsorption energy value of -2.4 eV.

In our case, the calculated adsorption energy values are given in Table 2. It can be noted that the charge transfer between Li^+ and BC_3 monolayer is very small when compared to charge transfer between Li atom and BC_3 monolayers, which further influences the adsorption energy values (Table 2). The adsorption energy value for Li adsorbed on Pure and Silicon doped BC_3 are -2.29 eV and -2.10 eV respectively. Similarly, the adsorption energy value for Li^+ on Pure and Silicon doped BC_3 are -1.87 eV and -1.85 eV respectively.

Table- II: Adsorption energy (E_{ads}), Distance (D_0) between atom/ion adsorbed on Pure and Si-doped bc_3 sheet (in Å) and Charge transfer (Qt) between atom/ion adsorbed on BC_3 sheet. (Energies are given in eV)

Complex	E_{ads}	D_0	Q_t
Pure BC_3			
Li atom..P- BC_3	-2.29	2.260	0.79
Li ion..P- BC_3	-1.87	2.348	0.61
Na atom..P- BC_3	-1.72	2.572	0.57
Na ion..P- BC_3	-1.36	2.638	0.46
Si-doped BC_3			
Li atom..Si- BC_3	-2.10	2.428	0.82
Li ion..Si- BC_3	-1.85	2.465	0.69
Na atom..Si-BC_3	-1.48	2.736	0.57
Na ion..Si- BC_3	-1.34	2.818	0.47

From the above values, we can observe that the Silicon doped BC_3 does not improve the results of Pure BC_3 in the adsorption energy values of Li atom/Ion. Figure 5 (a) and (b) shows the DOS diagram for Li^+ on Pure and Silicon doped BC_3 monolayers..

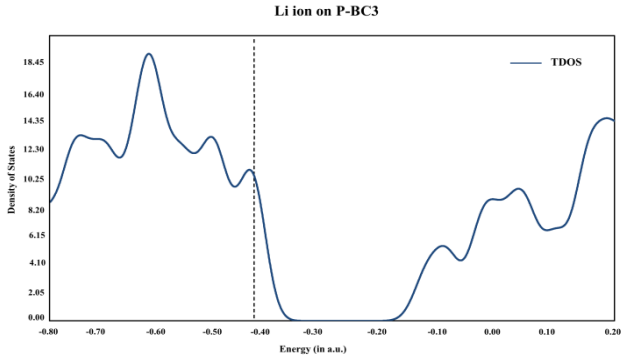

Fig. 5. (a) The density of states (DOS) diagram plotted for Li-ion adsorbed on Pure BC_3 at M06-2X/6-31+G* method.

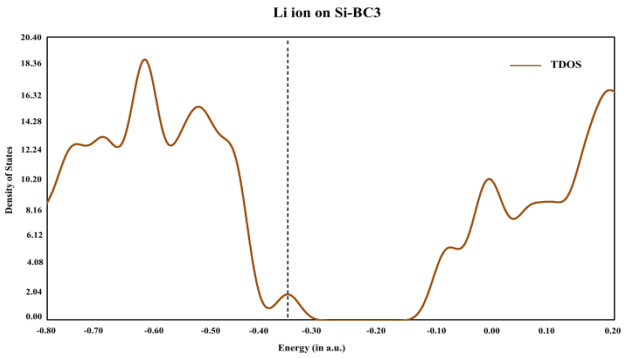

Fig. 5. (b) The density of states (DOS) diagram plotted for Li-ion adsorbed on Si-doped BC_3 at M06-2X/6-31+G* method.

The DOS for the Li^+ on Pure and Silicon doped BC_3 is in between -0.70 and -0.42 a.u and -0.20 and 0.15 a.u. This indicates that the significant changes in the

conduction and valence bands due to Li^+ on Pure and on Silicon doped BC_3.

C. *Adsorption of Na/Na$^+$ on Pure and Silicon doped BC_3 monolayers*

The optimized structures of Na atom/ion adsorbed on Pure and Na atom/ion adsorbed on Silicon doped BC_3 monolayers are shown in Fig. 6. The distance between Na atom/ion and Pure and distance between Na atom/ion and Silicon doped BC_3 are listed in Table 2. The distance between Na and Pure BC_3 monolayer is 2.572 Å. Similarly, the distance between Na and Silicon doped BC_3 monolayer is 2.736 Å. Further, the distance between Na^+ and Pure BC_3 monolayer is 2.638 Å and the distance between Na^+ and Silicon doped BC_3 monolayer is 2.818 Å.

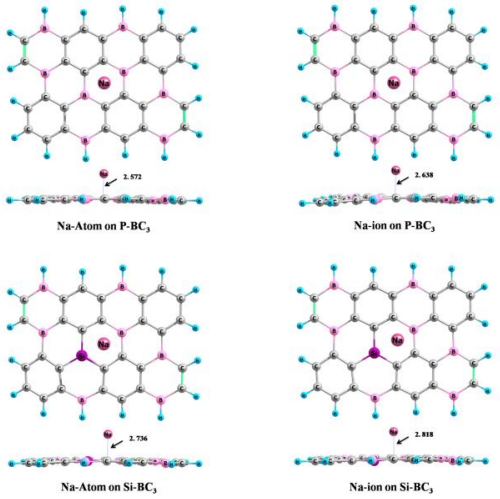

Fig. 6. Top and side views for the optimized structures of Na-atom and Na-ion on Pure and Si-doped BC_3 at M06-2X/6-31+G* method.

From the above values, it is observed that the distance between Na atom adsorbed on Pure and Silicon doped BC_3 monolayer is less compared to the distance between Na^+ adsorbed on Pure and Silicon doped BC_3 monolayer. It is noticed that by comparing the obtained bond length results, the bond length of Li atom/ion adsorbed on BC_3 monolayer is smaller than Na atom/ion adsorbed on BC_3 monolayer. This is because of Li atom/ion having the smaller ionic radius than Na atom/ion [28].

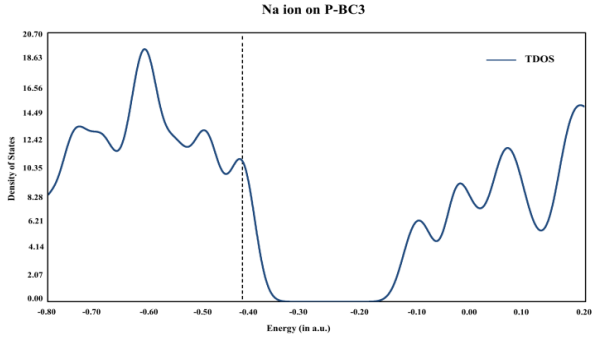

Fig. 7. (a) The density of states (DOS) diagram plotted for Na-ion adsorbed on Pure BC_3 at M06-2X/6-31+G* method.

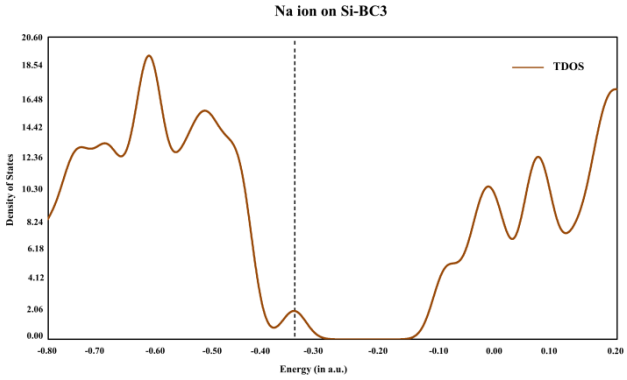

Fig. 7. (b) The density of states (DOS) diagram plotted for Na-ion adsorbed on Si-doped BC_3 at M06-2X/6-31+G* method.

In the case of Na atom adsorbed on Pure and Silicon doped BC_3 monolayer, the Q_t value is around 0.57. But in the case of Na^+ adsorbed on Pure and Silicon doped BC_3 monolayer, the Q_t value is only 0.47. Earlier, Sangavi et al. have studied the adsorption of Na on Pure and defected graphene sheets [28]. They calculated the distance between Na^+ and Pure graphene is 2.66 Å and the adsorption energy is -1.7 eV. In our case, the calculated adsorption energy values are given in Table 2. It can be noted that small amount of charge transfer between Na^+ and BC_3 monolayers compared to charge transfer between Na atom and BC_3 monolayers further influences the adsorption energy values (Table 2).

The adsorption energy value for Na atom adsorbed on Pure and Silicon doped BC_3 are -1.72 eV and -1.48 eV respectively. Similarly, adsorption energy value for Na^+ adsorbed on Pure and Silicon doped BC_3 are -1.36 eV and -1.34 eV respectively. From the above values, we can find that the Silicon doped BC_3 does not improve the results of Pure BC_3 in the adsorption energy values of Li atom/Ion. Figure 7 (a) and (b) shows the DOS diagram for Na^+ adsorbed on Pure and Silicon doped BC_3. The DOS for Na^+ adsorbed on the Pure and on the Silicon doped BC_3 monolayer is in between -0.70 and -0.42 a.u and around -0.20 and 0.15 a. This indicates that the significant changes in the conduction and valence bands due to the adsorption of Na^+ on Pure and on Silicon doped BC_3.

D. *Internal Energy and Cell Voltage*

In our calculations, the calculated internal energy and cell voltage values are given in Table 3. The internal energy values for the Li^+ with Pure and Silicon doped BC_3 are -40.22 kJ/mol and -23.50 kJ/mol respectively. The internal energy values for the Na^+ with Pure and Silicon doped BC_3 are -34.40 kJ/mol and -13.26 kJ/mol respectively. The corresponding cell voltage values of Li^+ with Pure and Silicon doped BC_3 are 0.47 eV and 0.24 eV respectively. For Na^+, cell voltage values are 0.36 eV and 0.14 eV for Pure and Silicon doped BC_3. From the above values, it is found that the Silicon doped BC_3 does not improve the results of Pure BC_3 monolayers. Earlier, Bhauriyal et al. have studied the BC_3 as electrode for Al-ion battery and observed a cell voltage of 2.41 eV [21].

Table- III: The internal energy (in kJ/mol), cell voltage (in Volts) and specific capacity (in

mAh/g) values of Pure and Si-doped BC_3 sheets.

Complex	Internal Energy	Cell Voltage	Specific Capacity
Pure BC_3			
Li Ion..P- BC_3	-40.22	0.47	215.77
Na Ion..P- BC_3	-34.40	0.36	208.34
Si-doped BC_3			
Li Ion..Si- BC_3	-23.50	0.24	207.89
Na Ion..Si- BC_3	-13.26	0.14	200.98

E. *Specific Capacity*

In our study, the calculated specific capacity for Pure and Silicon doped BC_3 monolayers is given in Table 3. The specific capacity values determine the charge storage capacity of the selected BC_3 material. The specific capacity for Li^+ adsorbed on Pure and Silicon doped BC_3 monolayers are 215.77 mAh/g and 207.89 mAh/g. The specific capacity value for Na^+ adsorbed on Pure and Silicon doped BC_3 monolayers are 208.34 mAh/g and 200.98 mAh/g respectively. Earlier, Sangavi et al. have obtained the specific capacity of 81–84 mAh/g for Li^+ and Na^+ adsorbed on defected graphene [28]. Similarly, Bhauriyal et al. have obtained the specific capacity of 74 mAh/g for BC_3 based Al-ion battery [21]. In our case, the specific capacity value for Pure BC_3 is higher than Silicon doped BC_3 monolayers. Further, Li^+ adsorbed on BC_3 monolayer have high Cp value than Na^+ adsorbed on BC_3 monolayer. This indicates that Li^+ is suitable for charge storage application than Na^+.

IV. CONCLUSION

In our present work, we have studied the Pure and Silicon doped boron carbide (BC_3) as electrode material for Li and Na-ion batteries. From the structural property analysis, it can be noted that the C-C and B-C bonds are elongated while doping the Si atom into Pure BC_3 monolayer. The energy gap for Pure BC_3 is calculated to be 5.24 eV. While doping with Si atom, the energy gap is reduce to 2.53 eV. Thus, Pure BC_3 monolayer becomes semiconducting like material while doping with Si atom. Our calculations show that the Li/Na atom adsorbed on Pure and Silicon doped BC_3 having high adsorption energy than Li/Na ion adsorbed on Pure and Silicon doped BC_3. This is because of smaller charge transfer in Li/Na ion adsorbed on monolayer compared to Li/Na atom adsorbed on monolayer. From the specific capacity value, it is found that Li^+ adsorbed on BC_3 monolayer having high C_p values than Na^+ adsorbed on BC_3 monolayer. This indicates that Li^+ is suitable for charge storage application than Na^+.

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