C₃₂, Si₃₂ and B₁₆N₁₆ as anode electrodes of Li-, Na- and K-ion batteries: theoretical examination

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Abstract. In this study, the potential of C₃₂, Si₃₂ and B₁₆N₁₆ nanocages as anode electrodes of Li-, Na- and K-ion batteries via density functional theory was investigated. The effects of halogen-adoption of C₃₂, Si₃₂ and B₁₆N₁₆ on potentials of metal-ion batteries were examined. Results showed that B₁₆N₁₆ as an anode electrode in metal-ion batteries has higher potential than C₃₂ and Si₃₂. Results illustrated that (i) a K-ion battery has higher cell voltage and higher performance than Li- and Na-ion batteries; (ii) halogen-adoption of nanocages increased the cell voltage of studied metal-ion batteries and (iii) F-adopted metal-ion batteries have higher cell voltage than Cl- and Br-adopted metal-ion batteries. Finally, F-B₁₅N₁₆ as an anode electrode in K-ion batteries has the highest performance and it can be proposed as novel metal-ion batteries.

Keywords. Battery; nanocage; adoption; voltage; anode and halogen.

1. Introduction

A rechargeable battery is a kind of electronic battery that has many electro-chemical cells and it can be recharged several times. The rechargeable batteries have been used in starter of cars, consumer devices and battery reservoir centres [1–6]. In a lithium-ion battery (LIB), as performance kind of rechargeable cells, there are two processes: in the charging process the lithium ions transfer from the positive to negative electrode and in the discharge process the motion of lithium ions is the reverse of the charge process [7–12]. The LIBs are low in safety, have small lifetime and leakage of lithium is an important issue [13–18].

Due to low cost of other metals, it is predictable that LIBs can be exchanged by novel metal-ion batteries with high capacity, high performance and high rate in charge and discharge processes [18–25]. Graphite, due to its low cost, cyclic durability and high energy stability, has been used for anode electrodes, and also potential of some compounds such as germanium, transition metals and silicon for anode electrodes of metal-ion batteries have been examined [2,26–32].

In previous studies, the potential and capacity of nano-electrodes in metal-ion batteries have been investigated and results proved that nanotubes and nanocages have higher

valences and higher energy capacity than graphite [33–41]. Results confirmed that hydrogenation, adoption and functionalization of nanostructures increased their valences when they used as anode materials in metal-ion batteries [42–47]. Results also showed that adoption and functionalization of nanostructures improved their chemical and physical properties as anode electrodes in metal-ion batteries [48–54].

Datta *et al* [55] proposed h-BN for black-phosphorene (Pn) in anode material in both LIBs and sodium (Na)-ion batteries (NIBs). Their results showed that binding energy of Li/Na in the h-BN/black-Pn heterostructure is greatly enhanced vis-a-vis pristine Pn along with reduction in the barrier for movement of Li/Na within the layers. Their results proven that high capacity, small volume change and high mobility of Li/Na within the layers make h-BN-capped black-Pn an excellent anode material in LIBs/SIBs.

Karmakar *et al* [56] explored the feasibility of Pn analogues, i.e. group IV mono-chalcogenide monolayers, to serve as anode materials in LIBs by density functional theory (DFT). Their results showed that lithium binds efficiently to these monolayers, of which Li@SiS and Li@SiSe show appreciable stability comparable with Pn. They proposed monolayer SiS and SiSe as promising electrode materials in LIBs due to low diffusion barrier, moderate to high-specific

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capacity, low open-circuit voltage, small volume change and good electrical conductivity.

Luo *et al* [57] investigated recent development on anode materials for NIBs and they also expanded carbon-based and alloy based anodes and highlighted progress in metal-ion batteries. Results showed that strategies of minimizing the surface area of carbon anodes for improving the first-cycle coulombic efficiency were outlined, where graphene oxide was employed. Results also showed that electrochemical intercalation of Na ions into reduced graphene oxide was applied for fabricating transparent conductors, demonstrating the great feasibility of Na-ion intercalation for optical applications.

Tsuneda *et al* [58] compared the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies of typical molecules with the negative vertical ionization potentials and electron affinities, respectively. Their results showed that only long-range-corrected functionals give the orbital energies close to the minus ionization potentials and electron affinities and only long-range-corrected functionals were found to retain the orbital energies almost constant for fractional-occupied orbitals.

Hirao *et al* [59] confirmed that the long-range-corrected density functionals reproduce frontier-orbital energies and the HOMO and LUMO gaps better than other density functionals. They compared the negative of the HOMO and LUMO energies with the vertical ionization potentials and electron affinities, respectively, for 113 molecules, and their results showed that the LC functional satisfied Koopmans' theorem. Their results also showed that the LC functional includes more relaxation effect than Hartree–Fock and more correlation effect than the other density functionals without the LC scheme.

Hosseini *et al* [60] investigated the performance of BN nanocage, and its structurally manipulated forms as anode materials for LIBs by means of DFT calculations. They investigated the effects of hydrogenation of the BN nanocage and encapsulation of an anion inside the BN nanocage and potential of the BN nanocage as an anode material for LIBs. Their results showed that encapsulating a fluoride inside the BN nanocage significantly increased the electrochemical cell voltage (V_{cell}) of the BN nanocage.

Najafi *et al* [61] examined the applications of BN nanocages and nanotubes as anode materials for LIBs by DFT. Their results showed that V_{cell} of BNNT (8, 0) and BNNT (10, 0) were higher than that of $\text{B}_{30}\text{N}_{30}$ and $\text{B}_{36}\text{N}_{36}$. Their results also showed that functionalization of the studied BN-nanostructures improved the potential of anode materials of LIBs.

Nejati *et al* [62] investigated the potential of $\text{B}_{12}\text{N}_{12}$ nanocages as anode in NIBs by DFT. They proposed a strategy to increase the cell voltage and performance of NIBs. Their results showed that encapsulation of different halides ($\text{X} = \text{F}^-, \text{Cl}^-, \text{Br}^-$) into the BN nanocage increased the cell voltage. Their results also showed that by

increasing the atomic number of X, the cell voltage of the studied BN nanocage as an anode electrode of NIBs was increased.

Hosseini *et al* [63] investigated the potential of BN nanosheets in anode of NIBs by means of DFT. Their results showed that replacing three N atoms of the hexagonal ring with larger P atoms increased the performance of the BN nanosheet as an anode of a NIB but the replacement of B by Al decreased its performance.

In this study, in the first step the potential of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ nanocages as anode electrodes in LIBs *via* DFT was investigated. In the second step, the C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ nanocages were doped with halogen atoms and their abilities as anode electrodes in LIBs were examined. In the third step, a potential NIB and potassium-ion battery (KIB) was compared with an LIB. In the fourth step, novel metal-ion batteries with higher performance will be proposed.

2. Computational details

In this study, the geometries of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ nanocages were optimized *via* GAMESS software *via* DFT/M06-2X theory and the 6-311 + G(2d,2p) basis set [64–68]. The adoption of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ with halogen atoms ($\text{X} = \text{F}, \text{Cl}, \text{Br}$) was investigated and geometries of $\text{X}-\text{C}_{31}$, $\text{X}-\text{Si}_{31}$ and $\text{X}-\text{B}_{15}\text{N}_{16}$ complexes were optimized at mentioned computational levels. The adsorption of metal atoms (M) and metal-ion atoms (M^+) on the surfaces of C_{32} , Si_{32} , $\text{B}_{16}\text{N}_{16}$, $\text{X}-\text{C}_{31}$, $\text{X}-\text{Si}_{31}$ and $\text{X}-\text{B}_{15}\text{N}_{16}$ was investigated and geometries of $\text{M}-\text{C}_{32}$, $\text{M}-\text{Si}_{32}$, $\text{M}-\text{B}_{16}\text{N}_{16}$, $\text{M}-\text{X}-\text{C}_{31}$, $\text{M}-\text{X}-\text{Si}_{31}$ and $\text{M}-\text{X}-\text{B}_{15}\text{N}_{16}$ complexes were optimized at mentioned computational levels. In this study, the vibrational frequency calculations of all studied structures *via* DFT/M06-2X theory and the 6-311+G(2d,2p) basis set were done in order to evidence that all of the optimized geometries are factual local minima and also thermodynamic parameters of the studied reactions were calculated by using vibrational frequency analysis [64–68].

In this study, total Gibbs free energy of the studied species, G , at temperature T is estimated using equation (1) as follows:

$$G = E_0 + \text{ZPE} + \Delta H_{\text{trans}} + \Delta H_{\text{rot}} + \Delta H_{\text{vib}} + RT - TS \quad (1)$$

where E_0 is the calculated total electronic energy, ZPE stands for zero-point energy, ΔH_{trans} , ΔH_{rot} and ΔH_{vib} are the translational, rotational and vibrational contributions to the enthalpy, respectively. Finally, RT represents PV-work term and is added to convert the energy to enthalpy [69–72].

The Gibbs free energy of the process of adoption of halogen atoms ($\text{X} = \text{F}, \text{Cl}, \text{Br}$) in the studied nanostructures was calculated *via* equation (2) as follows:

$$G_{\text{ad}} = G(\text{X-nanostructure}) - G(\text{nanostructure}) - 0.5G(\text{X}_2) \quad (2)$$

where $G(\text{X-nanostructure})$ corresponds to the Gibbs free energy of complexes of nanostructure with halogen atoms, $G(\text{X}_2)$ is the Gibbs free energy of the halogen molecule and $G(\text{nanostructure})$ is the Gibbs free energy of the nanostructure [69–72]. The Gibbs free energy of adsorption of metal on the surfaces of studied nanostructure was calculated via equation (3) as follows:

$$G_{\text{ad}} = G(\text{M-nanostructure}) - G(\text{nanostructure}) - G(\text{M}) \quad (3)$$

where $G(\text{M-nanostructure})$ corresponds to the Gibbs free energy of complex of nanostructure with a metal, $G(\text{M})$ is the Gibbs free energy of the metal and $G(\text{nanostructure})$ is the Gibbs free energy of the nanostructure [69–72].

The E_{ad} of the studied complexes of nanostructures with metals were calculated via $E_{\text{ad}} = E(\text{M-nanostructure}) - E(\text{nanostructure}) - E(\text{M}) + E_{\text{BSSE}}$. In this study, the energies of the basis set superposition error (E_{BSSE}) for the studied interactions between the nanostructures and metals were calculated by using the counterpoise correction method and the obtained results are reported in supplementary table S1 [67,73,74].

By assuming the nanostructures such as C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ as anodes for metal-ion batteries, equations (4 and 5) as reactions in the anode and cathode can be defined, respectively as follows:

The complete reaction for the metal-ion batteries can be defined via equation (6) as follows:

The cell voltage (V_{cell}) for a cell via the Nernst equation can be defined via equation (7) as follows:

$$V_{\text{cell}} = -\Delta G_{\text{cell}}/zF, \quad (7)$$

where F is the Faraday constant ($96,500 \text{ C mol}^{-1}$) and z is the charge of Li^+ , Na^+ and K^+ (for cation in electrolyte, $z = 1$) and ΔG_{cell} is the change of Gibbs free energy of equation (6). In previous studies, V_{cell} values of LIBs, NIBs and KIBs via the DFT method were calculated and the used z values of Li^+ , Na^+ and K^+ in the Nernst equation for LIBs, NIBs and KIBs are 1 [43–50,55–57,60–63]. The energy difference between the HOMO and the LUMO of the studied nanostructures was defined as HOMO – LUMO gap (E_{HLG}) and it can be calculated via $E_{\text{HLG}} = E_{\text{LUMO}} - E_{\text{HOMO}}$; where E_{LUMO} and E_{HOMO} are the energies of the LUMO and HOMO of the studied nanostructures.

3. Results and discussion

3.1 C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ as anode electrodes in metal-ion batteries

In this section, the potential of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ as anode electrodes in metal-ion batteries (LIBs, NIBs and KIBs) via the DFT method was investigated and novel metal-ion batteries with higher performance were identified. The structures of complexes of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ with Li, Na and K are presented in figure 1. The bond lengths in Å of Li, Na and K with C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ are reported in supplementary table S2.

The calculated Gibbs free energy (G_{ad}) values for complexes of metals and metal ions with C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ are presented in table 1. Results showed that, all calculated G_{ad} values were negative and all the studied adsorptions were possible from thermodynamic view point.

Results showed that G_{ad} value of $\text{K-B}_{16}\text{N}_{16}$ is higher than G_{ad} values of K-Si_{32} and the G_{ad} value of K-Si_{32} is higher than G_{ad} value of K-C_{32} . Also, results showed that G_{ad} value of $\text{Li-B}_{16}\text{N}_{16}$ is higher than G_{ad} values of Li-Si_{32} and G_{ad} value of Li-Si_{32} is higher than G_{ad} value of Li-C_{32} . Results also showed that G_{ad} value of $\text{K-B}_{16}\text{N}_{16}$ is higher than G_{ad} values of $\text{Na-B}_{16}\text{N}_{16}$ and G_{ad} value of $\text{Na-B}_{16}\text{N}_{16}$ is higher than G_{ad} value of $\text{Li-B}_{16}\text{N}_{16}$. Also, results showed that G_{ad} value of K-C_{32} is higher than G_{ad} values of Na-C_{32} and the G_{ad} value of Na-C_{32} is higher than G_{ad} value of Li-C_{32} . Results also showed that G_{ad} values of Li, Na and K on the surface of $\text{B}_{16}\text{N}_{16}$ are higher than G_{ad} values of Li, Na and K on surfaces of C_{32} and Si_{32} . It can be concluded that $\text{K-B}_{16}\text{N}_{16}$ and Li-C_{32} have the highest and the lowest G_{ad} values, respectively.

Hosseini *et al* [63] calculated the E_{HLG} values of BN-nanosheets via the B3LYP functional and 6-31G(d) basis set and their results showed that E_{HLG} values of BN-nanosheet, Al-BN-nanosheet and P-BN-nanosheet were 5.88, 4.98 and 5.38 eV, respectively. Also they calculated the E_{HLG} values of complexes of nanosheets with Na atoms and their results showed that the E_{HLG} values of Na-BN-nanosheet, Na-Al-BN-nanosheet and Na-P-BN-nanosheet were 1.64, 2.09 and 1.17 eV, respectively.

Nejati *et al* [62] calculated the E_{HLG} value of the $\text{B}_{12}\text{N}_{12}$ cage via the B3LYP functional and 6-31G(d) basis set in GAMESS software and the results showed that E_{HLG} values of $\text{B}_{12}\text{N}_{12}$ and $\text{Na-B}_{12}\text{N}_{12}$ were 6.84 and 1.59 eV, respectively. They investigated the E_{HLG} values of complex of $\text{B}_{12}\text{N}_{12}$ with F, Cl and Br atoms and their results showed that the E_{HLG} values of $\text{F-B}_{12}\text{N}_{12}$, $\text{Cl-B}_{12}\text{N}_{12}$ and $\text{Br-B}_{12}\text{N}_{12}$ were 7.02, 5.41 and 4.56 eV, respectively. The E_{HLG} values of complexes of $\text{F-B}_{12}\text{N}_{12}$, $\text{Cl-B}_{12}\text{N}_{12}$ and $\text{Br-B}_{12}\text{N}_{12}$ with Na atoms and their results showed that the E_{HLG} values of $\text{Na-F-B}_{12}\text{N}_{12}$, $\text{Na-Cl-B}_{12}\text{N}_{12}$ and $\text{Na-Br-B}_{12}\text{N}_{12}$ were 1.67, 1.65 and 2.01 eV, respectively.

Hosseini *et al* [60] investigated the E_{HLG} values of $\text{B}_{12}\text{N}_{12}$ and $\text{H}_{12}\text{B}_{12}\text{N}_{12}$ via the B3LYP functional and 6-31G(d) basis

Figure 1. Structure of the studied complexes.

set and their results showed that E_{HLG} values of B₁₂N₁₂ and H₁₂B₁₂N₁₂ were 6.84 and 2.51 eV, respectively. Also they calculated the E_{HLG} values of complexes of B₁₂N₁₂ and H₁₂B₁₂N₁₂ with Li atoms and the results showed that the E_{HLG} values of Li-B₁₂N₁₂ and Li-H₁₂B₁₂N₁₂ were 6.10 and 2.38 eV, respectively.

In a previous study, the E_{HLG} value of BN nanosheet was ca. 5.81 eV which is close to the experimental band gap

(~5.50 eV) of the hexagonal BN sheets [75]. Bagheri *et al* [76] calculated the E_{HLG} values of C₂₄ and Li-C₂₄ via the M06-2X functional and 6-31G(d) basis set and the results showed that E_{HLG} values of C₂₄ and Li-C₂₄ were 3.87 and 3.34 eV, respectively [77].

The calculated E_{HOMO} , E_{LUMO} and E_{HLG} values of complexes of Li, Na and K with C₃₂, Si₃₂ and B₁₆N₁₆ are reported in table 2. Results showed that, E_{HOMO} value of

Table 1. The G_{ad} (kcal mol⁻¹) and V_{cell} (V) values of the studied complexes.

Complex	G_{ad}	V_{cell}	Complex	G_{ad}	V_{cell}	Complex	G_{ad}	V_{cell}
K-C ₃₂	-7.13	1.29	K-Si ₃₂	-7.48	1.35	K-B ₁₆ N ₁₆	-8.20	1.48
Na-C ₃₂	-6.36	1.15	Na-Si ₃₂	-6.68	1.21	Na-B ₁₆ N ₁₆	-7.32	1.32
Li-C ₃₂	-5.68	1.03	Li-Si ₃₂	-5.96	1.08	Li-B ₁₆ N ₁₆	-6.53	1.18
K-F-C ₃₁	-15.96	2.89	K-F-Si ₃₁	-16.75	3.03	K-F-B ₁₅ N ₁₆	-18.36	3.32
Na-F-C ₃₁	-14.25	2.58	Na-F-Si ₃₁	-14.96	2.71	Na-F-B ₁₅ N ₁₆	-16.39	2.97
Li-F-C ₃₁	-12.72	2.30	Li-F-Si ₃₁	-13.35	2.42	Li-F-B ₁₅ N ₁₆	-14.63	2.65
K-Cl-C ₃₁	-15.11	2.73	K-Cl-Si ₃₁	-15.85	2.87	K-Cl-B ₁₅ N ₁₆	-17.37	3.14
Na-Cl-C ₃₁	-13.49	2.44	Na-Cl-Si ₃₁	-14.16	2.56	Na-Cl-B ₁₅ N ₁₆	-15.51	2.81
Li-Cl-C ₃₁	-12.04	2.18	Li-Cl-Si ₃₁	-12.64	2.29	Li-Cl-B ₁₅ N ₁₆	-13.85	2.51
K-Br-C ₃₁	-14.25	2.58	K-Br-Si ₃₁	-14.96	2.71	K-Br-B ₁₅ N ₁₆	-16.39	2.97
Na-Br-C ₃₁	-12.72	2.30	Na-Br-Si ₃₁	-13.35	2.42	Na-Br-B ₁₅ N ₁₆	-14.63	2.65
Li-Br-C ₃₁	-11.36	2.06	Li-Br-Si ₃₁	-11.92	2.16	Li-Br-B ₁₅ N ₁₆	-13.07	2.36
K ⁺ -C ₃₂	-36.82		K ⁺ -Si ₃₂	-38.64		K ⁺ -B ₁₆ N ₁₆	-42.35	
Na ⁺ -C ₃₂	-32.87		Na ⁺ -Si ₃₂	-34.50		Na ⁺ -B ₁₆ N ₁₆	-37.81	
Li ⁺ -C ₃₂	-29.35		Li ⁺ -Si ₃₂	-30.80		Li ⁺ -B ₁₆ N ₁₆	-33.75	
K ⁺ -F-C ₃₁	-82.47		K ⁺ -F-Si ₃₁	-86.55		K ⁺ -F-B ₁₅ N ₁₆	-94.85	
Na ⁺ -F-C ₃₁	-73.63		Na ⁺ -F-Si ₃₁	-77.28		Na ⁺ -F-B ₁₅ N ₁₆	-84.68	
Li ⁺ -F-C ₃₁	-65.74		Li ⁺ -F-Si ₃₁	-68.99		Li ⁺ -F-B ₁₅ N ₁₆	-75.60	
K ⁺ -Cl-C ₃₁	-78.06		K ⁺ -Cl-Si ₃₁	-81.91		K ⁺ -Cl-B ₁₅ N ₁₆	-89.76	
Na ⁺ -Cl-C ₃₁	-69.69		Na ⁺ -Cl-Si ₃₁	-73.14		Na ⁺ -Cl-B ₁₅ N ₁₆	-80.14	
Li ⁺ -Cl-C ₃₁	-62.22		Li ⁺ -Cl-Si ₃₁	-65.30		Li ⁺ -Cl-B ₁₅ N ₁₆	-71.56	
K ⁺ -Br-C ₃₁	-73.63		K ⁺ -Br-Si ₃₁	-77.28		K ⁺ -Br-B ₁₅ N ₁₆	-84.68	
Na ⁺ -Br-C ₃₁	-65.74		Na ⁺ -Br-Si ₃₁	-68.99		Na ⁺ -Br-B ₁₅ N ₁₆	-75.60	
Li ⁺ -Br-C ₃₁	-58.70		Li ⁺ -Br-Si ₃₁	-61.60		Li ⁺ -Br-B ₁₅ N ₁₆	-67.51	

K-C₃₂ is lower than E_{HOMO} values of Li-C₃₂ and Na-C₃₂. Also, E_{HOMO} value of K-B₁₆N₁₆ is lower than E_{HOMO} values of Li-B₁₆N₁₆ and Na-B₁₆N₁₆. Results also showed that E_{HOMO} values of Li, Na and K on B₁₆N₁₆ are lower than E_{HOMO} values of Li, Na and K on the surfaces of C₃₂ and Si₃₂. Results showed that, E_{HLG} value of K-C₃₂ is lower than E_{HLG} values of Li-C₃₂ and Na-C₃₂. Also E_{HLG} value of K-B₁₆N₁₆ is lower than E_{HLG} values of Li-B₁₆N₁₆ and Na-B₁₆N₁₆. It can be concluded that K-B₁₆N₁₆ and Li-C₃₂ have the lowest and the highest E_{HLG} values, respectively.

The calculated V_{cell} (in V) of complexes of Li, Na and K with C₃₂ and B₁₆N₁₆ are reported in table 1. Results showed that V_{cell} value of K-B₁₆N₁₆ is higher than V_{cell} values of K-Si₃₂ and the V_{cell} value of K-Si₃₂ is higher than V_{cell} value of K-C₃₂. Also, results showed that V_{cell} value of Li-B₁₆N₁₆ is higher than V_{cell} values of Li-Si₃₂ and the V_{cell} value of Li-Si₃₂ is higher than V_{cell} value of Li-C₃₂. Results also showed that V_{cell} value of K-B₁₆N₁₆ is higher than V_{cell} values of Na-B₁₆N₁₆ and the V_{cell} value of Na-B₁₆N₁₆ is higher than V_{cell} value of Li-B₁₆N₁₆. Also, results showed that V_{cell} value of K-C₃₂ is higher than V_{cell} values of Na-C₃₂ and the V_{cell} value of Na-C₃₂ is higher than V_{cell} value of Li-C₃₂. Results showed that V_{cell} values of Li, Na and K on the surface B₁₆N₁₆ are higher than V_{cell} values of Li, Na and K on the surfaces of C₃₂ and Si₃₂. It can be concluded that K-B₁₆N₁₆ and Li-C₃₂ have the highest and the lowest V_{cell} values, respectively. Finally, in this section two important results can be concluded:

(1) the B₁₆N₁₆ as an anode in metal-ion batteries has higher potential than C₃₂ and Si₃₂ and (2) the KIB has higher V_{cell} and higher performance than the NIB and KIB.

3.2 Halogen-adoption of C₃₂, Si₃₂ and B₁₆N₁₆ nanocages

In this section, the effects of F, Cl and Br adoption of C₃₂, Si₃₂ and B₁₆N₁₆ on their performance as anode electrodes of metal-ion batteries *via* the DFT method were investigated. The calculated G_{ad} values of F-, Cl- and Br-doped C₃₂, Si₃₂ and B₁₆N₁₆ are presented in table 3. Results showed that, all calculated G_{ad} values were negative and therefore G_{ad} values confirmed that adoption of C₃₂, Si₃₂ and B₁₆N₁₆ with F, Cl and Br was possible from thermodynamic view point.

Results showed that G_{ad} value of F-C₃₁ are higher than G_{ad} values of Cl-C₃₁ and Br-C₃₁. Also G_{ad} value of F-B₁₅N₁₆ are higher than G_{ad} values of Cl-B₁₅N₁₆ and Br-B₁₅N₁₆. Results also showed that G_{ad} values of F-, Cl- and Br-doped B₁₅N₁₆ are higher than G_{ad} values of F-, Cl- and Br-doped C₃₁ and F-, Cl- and Br-doped Si₃₁. Results showed that, adoption of C₃₂, Si₃₂ and B₁₆N₁₆ with F atom is possible processes from thermodynamic view point and F-C₃₁, F-Si₃₁ and F-B₁₅N₁₆ can be suitable candidates as anode electrodes of metal-ion batteries.

In this section, the potential of F, Cl and Br-doped C₃₁, Si₃₂ and B₁₅N₁₆ as anodes in LIBs, NIBs and KIBs *via* the DFT method was investigated. The structures of complexes

Table 2. The E_{HOMO} , E_{LUMO} and E_{HLG} (eV) values of studied complexes.

Complex	E_{HOMO}	E_{LUMO}	E_{HLG}
K-C ₃₂	-4.62	-1.34	3.28
Na-C ₃₂	-4.75	-1.20	3.55
Li-C ₃₂	-4.88	-1.07	3.80
K-F-C ₃₁	-3.91	-3.03	0.88
Na-F-C ₃₁	-4.21	-2.70	1.51
Li-F-C ₃₁	-4.49	-2.40	2.09
K-Cl-C ₃₁	-4.07	-2.85	1.21
Na-Cl-C ₃₁	-4.34	-2.55	1.79
Li-Cl-C ₃₁	-4.61	-2.28	2.33
K-Br-C ₃₁	-4.21	-2.70	1.51
Na-Br-C ₃₁	-4.49	-2.40	2.09
Li-Br-C ₃₁	-4.73	-2.14	2.59
K-Si ₃₂	-4.57	-1.16	3.41
Na-Si ₃₂	-4.67	-1.05	3.62
Li-Si ₃₂	-4.78	-0.93	3.85
K-F-Si ₃₁	-4.07	-2.61	1.46
Na-F-Si ₃₁	-4.32	-2.34	1.98
Li-F-Si ₃₁	-4.55	-2.08	2.47
K-Cl-Si ₃₁	-4.19	-2.47	1.71
Na-Cl-Si ₃₁	-4.43	-2.20	2.23
Li-Cl-Si ₃₁	-4.64	-1.98	2.66
K-Br-Si ₃₁	-4.32	-2.34	1.98
Na-Br-Si ₃₁	-4.55	-2.08	2.47
Li-Br-Si ₃₁	-4.74	-1.86	2.88
K-B ₁₆ N ₁₆	-4.21	-1.53	2.68
Na-B ₁₆ N ₁₆	-4.34	-1.36	2.98
Li-B ₁₆ N ₁₆	-4.45	-1.21	3.24
K-F-B ₁₅ N ₁₆	-3.77	-3.19	0.57
Na-F-B ₁₅ N ₁₆	-3.84	-3.10	0.73
Li-F-B ₁₅ N ₁₆	-4.07	-2.76	1.31
K-Cl-B ₁₅ N ₁₆	-3.90	-3.06	0.84
Na-Cl-B ₁₅ N ₁₆	-3.96	-2.94	1.01
Li-Cl-B ₁₅ N ₁₆	-4.18	-2.61	1.57
K-Br-B ₁₅ N ₁₆	-3.96	-2.87	1.08
Na-Br-B ₁₅ N ₁₆	-4.07	-2.76	1.31
Li-Br-B ₁₅ N ₁₆	-4.29	-2.45	1.83

Table 3. The G_{ad} (kcal mol⁻¹) values of studied complexes.

Complex	G_{ad}	Complex	G_{ad}	Complex	G_{ad}
F-C ₃₁	-35.78	Cl-C ₃₁	-33.87	Br-C ₃₁	-31.95
F-Si ₃₁	-37.55	Cl-Si ₃₁	-35.54	Br-Si ₃₁	-33.53
F-B ₁₅ N ₁₆	-41.15	Cl-B ₁₅ N ₁₆	-38.95	Br-B ₁₅ N ₁₆	-36.74

of halogen-C₃₁, halogen-Si₃₁ and halogen-B₁₅N₁₆ with Li, Na and K are presented in figure 1. The bond lengths of Li, Na and K with halogen-C₃₁, halogen-Si₃₁ and halogen-B₁₅N₁₆ and also bond lengths of halogen atoms with bordering C, Si and N atoms are reported in supplementary table S2.

The calculated G_{ad} values of complexes of metals and metal ions with halogen-C₃₁, halogen-Si₃₁ and halogen-B₁₅N₁₆ are

presented in table 1. Results showed that, all calculated G_{ad} values were negative and studied adsorptions were possible from thermodynamic view point.

Results showed that G_{ad} value of K-halogen-B₁₅N₁₆ is higher than G_{ad} values of K-halogen-Si₃₁ and the G_{ad} value of K-halogen-Si₃₁ is higher than G_{ad} value of K-halogen-C₃₁. Also, results showed that G_{ad} value of Li-halogen-B₁₅N₁₆ is higher than G_{ad} values of Li-halogen-Si₃₁ and the G_{ad} value of Li-halogen-Si₃₁ is higher than G_{ad} value of Li-halogen-C₃₁. Results also showed that G_{ad} value of K-halogen-B₁₅N₁₆ is higher than G_{ad} values of Na-halogen-B₁₅N₁₆ and the G_{ad} value of Na-halogen-B₁₅N₁₆ is higher than G_{ad} value of Li-halogen-B₁₅N₁₆. Also, results showed that G_{ad} value of K-halogen-C₃₁ is higher than G_{ad} values of Na-halogen-C₃₁ and the G_{ad} value of Na-halogen-C₃₁ is higher than G_{ad} value of Li-halogen-C₃₁. Results also showed that G_{ad} values of Li, Na and K on the surface of halogen-B₁₅N₁₆ are higher than G_{ad} values of Li, Na and K on the surfaces of halogen-C₃₁ and halogen-Si₃₁. Results showed that G_{ad} values of metal-F-nanocage are higher than G_{ad} values of metal-Cl-nanocage and metal-Br-nanocage and also G_{ad} value of metal-halogen-nanocages are higher than G_{ad} values of metal-nanocage. Results also showed that G_{ad} values of Li, Na and K on halogen-B₁₅N₁₆ are higher than G_{ad} values on halogen-C₃₁ and halogen-Si₃₁. It can be concluded that K-F-B₁₅N₁₆ and Li-Br-C₃₁ have the highest and the lowest G_{ad} absolute values, respectively.

The calculated E_{HOMO} , E_{LUMO} and E_{HLG} values of complexes of Li, Na and K with halogen-C₃₁, halogen-Si₃₁ and halogen-B₁₅N₁₆ are reported in table 2. Results showed that, E_{HOMO} value of K-halogen-C₃₁ are lower than E_{HOMO} values of Li-halogen-C₃₁ and Na-halogen-C₃₁. Also E_{HOMO} value of K-halogen-B₁₅N₁₆ is lower than E_{HOMO} values of Li-halogen-B₁₅N₁₆ and Na-halogen-B₁₅N₁₆. Results also showed that E_{HOMO} values of Li, Na and K on halogen-B₁₅N₁₆ are lower than E_{HOMO} values of halogen-C₃₁ and halogen-Si₃₁.

Results showed that, E_{HLG} value of K-halogen-C₃₁ are lower than E_{HLG} values of Li-halogen-C₃₁ and Na-halogen-C₃₁. Also E_{HLG} value of K-halogen-B₁₅N₁₆ is lower than E_{HLG} values of Li-halogen-B₁₅N₁₆ and Na-halogen-B₁₅N₁₆. It can be concluded that K-F-B₁₅N₁₆ and Li-Br-C₃₁ have the lowest and the highest E_{HLG} values, respectively.

Hosseini *et al* [60] calculated the G_{cell} and V_{cell} values of B₁₂N₁₂ and F-B₁₂N₁₂ as anode electrodes of LIBs. Their results showed that the G_{cell} and V_{cell} values of B₁₂N₁₂ were -25.3 kcal mol⁻¹ and 1.09 V, respectively. The G_{cell} and V_{cell} values of F-B₁₂N₁₂ were -70.9 kcal mol⁻¹ and 3.07 V, respectively. Results showed that encapsulating a fluoride inside the B₁₂N₁₂ nanocage increased the V_{cell} from 1.09 to 3.07 V and so encapsulating a fluoride inside the BN nanocage can be considered a suitable strategy to improve the performance of the BN nanocage as an anode electrode of LIBs.

Nejati *et al* [62] calculated the G_{cell} and V_{cell} values of B₁₂N₁₂ as an anode electrode of NIBs. Their results

showed that the G_{cell} and V_{cell} values of $\text{B}_{12}\text{N}_{12}$ were $-21.2 \text{ kcal mol}^{-1}$ and 0.92 eV , respectively. They calculated the G_{cell} and V_{cell} values of encapsulated $\text{B}_{12}\text{N}_{12}$ with F, Cl and Br atoms as anode electrodes of NIBs. Their results showed that the G_{cell} values of $\text{F-B}_{12}\text{N}_{12}$, $\text{Cl-B}_{12}\text{N}_{12}$ and $\text{Br-B}_{12}\text{N}_{12}$ were -85.3 , -87.9 and $-90.5 \text{ kcal mol}^{-1}$, respectively. Their results also showed that the V_{cell} values of $\text{F-B}_{12}\text{N}_{12}$, $\text{Cl-B}_{12}\text{N}_{12}$ and $\text{Br-B}_{12}\text{N}_{12}$ were 3.70 , 3.81 and 3.93 eV , respectively.

A comparison of calculated V_{cell} values of $\text{B}_{12}\text{N}_{12}$ and F-encapsulated $\text{B}_{12}\text{N}_{12}$ as anode electrodes of Li and Na metal-ion batteries by Nejati [62] and Hosseini [60] showed that: (1) encapsulating fluoride inside the $\text{B}_{12}\text{N}_{12}$ improved the performance of $\text{B}_{12}\text{N}_{12}$ as an anode electrode of LIBs and NIBs; (2) the V_{cell} values of $\text{B}_{12}\text{N}_{12}$ as an anode electrode of LIBs are higher than V_{cell} values of $\text{B}_{12}\text{N}_{12}$ as an anode electrode of NIBs, ca. 0.17 V and (3) the V_{cell} values of F-encapsulated $\text{B}_{12}\text{N}_{12}$ as an anode electrode of LIBs are lower than V_{cell} values of F-encapsulated $\text{B}_{12}\text{N}_{12}$ as an anode electrode of NIBs, ca. 0.63 V .

The calculated V_{cell} values of complexes of Li, Na and K with halogen- C_{31} , halogen- Si_{31} and halogen- $\text{B}_{15}\text{N}_{16}$ are reported in table 1. Results showed that, V_{cell} value of K-halogen- C_{31} is higher than V_{cell} values of Li-halogen- C_{31} and Na-halogen- C_{31} . Also V_{cell} value of K-halogen- $\text{B}_{15}\text{N}_{16}$ is higher than V_{cell} values of Li-halogen- $\text{B}_{15}\text{N}_{16}$ and Na-halogen- $\text{B}_{15}\text{N}_{16}$. Results also showed that V_{cell} values of Li, Na and K on halogen- $\text{B}_{15}\text{N}_{16}$ are higher than V_{cell} values on halogen- C_{31} and halogen- Si_{31} . It can be concluded that K- $\text{F-B}_{15}\text{N}_{16}$ and Li- Br-C_{31} have the highest and the lowest V_{cell} values, respectively.

In the present paper, similar to works of Nejati [62] and Hosseini [60], results confirmed that F adoption of $\text{B}_{16}\text{N}_{16}$, C_{32} and Si_{32} increased their V_{cell} as anode electrodes of LIBs, NIBs and KIBs. In the present paper, similar to works of Nejati [62] and Hosseini [60], results confirmed that V_{cell} of $\text{F-B}_{15}\text{N}_{16}$, F-C_{31} and F-Si_{31} in KIBs and NIBs are higher than V_{cell} of $\text{F-B}_{15}\text{N}_{16}$, F-C_{31} and F-Si_{31} in LIBs.

According to the calculated potential of halogen-metal-ion batteries in this section, it can be concluded: (1) the halogen adoption of nanocages increased the V_{cell} of LIBs, NIBs and KIBs; (2) the F-doped nanocages as anode electrodes of metal-ion batteries have higher V_{cell} and higher performance than Cl- and Br-doped nanocages; (3) the KIBs have higher V_{cell} and higher performance than LIBs and NIBs and (4) K- $\text{F-B}_{15}\text{N}_{16}$ as anode electrodes of metal-ion batteries has the highest performance.

In the present paper, the dependencies between calculated G_{cell} and V_{cell} of the studied complexes and the corresponding E_{HOMO} and E_{HLG} values were investigated. The calculated G_{cell} of the studied complexes were correlated against the corresponding E_{HOMO} and E_{HLG} values and obtained equations (1 and 2) from these linear regressions were as follows:

$$G_{\text{cell}}(\text{kcal mol}^{-1}) = -15 \times E_{\text{HOMO}}(\text{eV}) - 72 \quad (8)$$

$$G_{\text{cell}}(\text{kcal mol}^{-1}) = 6 \times E_{\text{HLG}}(\text{eV}) - 21. \quad (9)$$

The correlation coefficients of equations (8 and 9) were 0.87 and 0.93 , respectively. The calculated V_{cell} of the studied complexes were correlated against the corresponding E_{HOMO} and E_{HLG} values and the obtained equations (10 and 11) from these linear regressions were as follows:

$$V_{\text{cell}}(\text{V}) = 3 \times E_{\text{HOMO}}(\text{eV}) + 16 \quad (10)$$

$$V_{\text{cell}}(\text{V}) = -1 \times E_{\text{HLG}}(\text{eV}) + 6. \quad (11)$$

The correlation coefficients of equations (10 and 11) were 0.88 and 0.94 , respectively.

According to equations (8–11), it can be concluded that there are linear dependencies between the G_{cell} and V_{cell} of the studied complexes and the corresponding E_{HOMO} and E_{HLG} values. Therefore, the obtained equations enable us to estimate the G_{cell} and V_{cell} of the studied complexes from structural parameters of the studied complexes such as E_{HOMO} and E_{HLG} values. Results showed that, nanostructure complexes as anodes of metal-ion batteries with lower E_{HLG} and $|E_{\text{HOMO}}|$ values have higher $|G_{\text{cell}}|$ and V_{cell} values and so they have higher performances. These linear dependencies between adsorption indexes (G_{cell} and V_{cell}) and structural parameters (E_{HOMO} and E_{HLG}) can be useful in the selection and propose the novel adopted nanostructures with enhanced potential as anode electrodes of metal-ion batteries.

4. Conclusion

In this study, the potential of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ as anode electrodes of LIBs, NIBs and KIBs *via* DFT was investigated. Also the effects of halogen adoption of C_{32} , Si_{32} and $\text{B}_{16}\text{N}_{16}$ on potential of a metal-ion battery were examined. Obtained results in the present paper are: (1) the $\text{B}_{16}\text{N}_{16}$ as an anode in metal-ion batteries has higher potential than C_{32} and Si_{32} ; (2) the KIB has higher V_{cell} and higher performance than NIBs and LIBs; (3) the halogen adoption can increase the V_{cell} of the studied metal-ion batteries; (4) the F-doped metal-ion batteries have higher V_{cell} and higher performance than Cl- and Br-doped metal-ion batteries and (5) K- $\text{F-B}_{15}\text{N}_{16}$ has the highest performance and it can be proposed as novel metal-ion batteries with high potential.

Supplementary information

Calculated E_{BSSE} and bond length values of studied complexes are presented in supplementary data.

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