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Exploring Efficiency of Silicon Carbide for Next Generation of Alkali & Alkaline Earth Metals-Ion Batteries Using Quantum Mechanic Method

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ABSTRACT: Delving alternative high-performance anodes for lithium-ion batteries have always attracted scientist attention. A wide-bandgap semiconductor with excellent mechanical properties, “silicon carbide (SiC)”, has been introduced as the anode electrode. Two-dimensional SiC has special hybridization which can build it as an appropriate substitution for graphene. Energy storage technologies are keys in the extension and function of electric devices. To keep up with steady innovations in saving energy technologies, it is essential to progress corresponding practical strategies. In this research article, SiC has been designed and characterized as an anode electrode for lithium (Li), sodium (Na), beryllium (Be), and magnesium (Mg) ion batteries, forming SiLi_2C , SiNa_2C , SiBe_2C , and SiMg_2C nanoclusters. A comprehensive study of energy-saving by SiLi_2C , SiNa_2C , SiBe_2C , and SiMg_2C complexes was conducted using computational methods, accompanied by analysis of charge density differences (CDD), total density of states (TDOS), and localized orbital locator (LOL) for hybrid clusters of SiLi_2C , SiNa_2C , SiBe_2C , and SiMg_2C . Functionalizing lithium, sodium, beryllium, and magnesium can shift the negative charge distribution of carbon toward electron-acceptor states in SiLi_2C , SiNa_2C , SiBe_2C , and SiMg_2C nanoclusters. Higher Si/C content can increase battery capacity via SiLi_2C , SiNa_2C , SiBe_2C , and SiMg_2C nanoclusters during the energy storage process and improve rate performance by enhancing electrical conductivity. Besides, silicon carbide anode material may improve cycling consistency by mitigating electrode degradation, and it augments capacity owing to higher surface capacitance.

KEYWORDS: Novel hybrid-ion batteries; silicon carbide; alkali/alkaline earth metals; DFT

1 Introduction

Seeking alternative high-performance anodes for lithium-ion batteries was emphasized. A wide-bandgap semiconductor with excellent mechanical properties, “silicon carbide”, has been pursued as the anode electrode. A significant volume change during charge-discharge of Si-based nanostructures as anode electrodes for high-energy lithium-ion batteries has been considered the most serious obstacle to their commercial use [1–4].

In addition to the low diffusion barrier, moderate open-circuit voltage, and excellent electronic conductivity during sodiation, the researchers proposed that the SiC structure is a promising anode material for Na-ion batteries. More importantly, they found that the intercalation strength of Na ions into C-based multilayer materials could be enhanced by increasing the number of covalent bonds of “Na–C”, which could be realized via doping by atoms (Li, Be, B, Al, Si or P) with lower electronegativity than that of the C atom [5–9].



The novel structure of a SiC monolayer was investigated for sodium and potassium storage using DFT. It was revealed that SiC exhibits negative adsorption energies for K/Na adsorption on its surface. Furthermore, the SiC monolayer can efficiently achieve a high content of Na/K loading on both sides of its surface. Additionally, it is demonstrated that the semiconducting SiC monolayer transforms into a metallic state with excellent conductivity upon Na/K adsorption. These findings underscore the potential of the SiC monolayer as a promising anode candidate for both sodium- and potassium-ion batteries [10].

Anode materials based on silicon carbide and III-nitride nanosheets are investigated for magnesium-ion batteries (MIBs) as a possible alternative to lithium- and sodium-ion batteries. The results from density functional theory calculations reveal higher values of the internal energy change and cell voltage for MIBs with silicon carbide, boron nitride, aluminum nitride, and gallium nitride anode materials than for previously reported carbon nanomaterials [11].

Whereas the polarizability of the Si atom is more than that of the C atom, it is assumed that the Si-C/C/Si nanosurface may contribute more intensely to the compositions in the hybrid to the pure C-nanostructures [12–14]. The previous investigations of energy-saving devices through H-adsorption have been tailored owing to DFT calculations with a semiconductor group of Si/Ge/Sn/Pb nano-carbides [15], Mg-Al nanoalloy [16] and Al/C/Si doping of BN nanocomposite [17]. Nanomaterials with distinctive structures are being investigated for their potential in electrocatalysis, fuel cells, and energy-saving applications [18].

Recently, investigations have been done by outlining the electrochemical reaction mechanisms and challenges associated with Si-based anodes in alkali metal-ion batteries, and then they have presented various approaches, including the architectural engineering of Si, the surface engineering of Si-based materials, and the construction of Si-based composites to improve the battery performance. Therefore, the anticipated challenges and opportunities in developing silicon-based anode materials for alkali-metal-ion batteries can be explored [19].

In another study, Dong et al. used titanium silicon carbide (Ti_3SiC_2 , TSC) to prepare the Si-based anode composite (Si/TSC) to improve the performance of the LIB. TSC was used as a mechanical strengthening and highly conductive matrix for the Si-based anode [20]. Following in-depth characterization, samples were measured to assess, for the first time, their performance correlated with chemical composition variations in Li-, Na-, Be-, or Mg-batteries.

2 Theoretical Backgrounds, Materials and Methods

Development of the applied Density Functional Theory (DFT) methodology only became notable after Kohn and Sham released their reputable series of equations which are introduced as Kohn-Sham (KS) equations [21,22]:

$$\hat{H}_s = - \sum_i^M \frac{1}{2} \nabla_i^2 + \sum_i^M v_s(\vec{r}_i) = \sum_i^M \hat{h}_s \quad (1)$$

$$\hat{h}_s = - \frac{1}{2} \nabla_i^2 + v_s(\vec{r}_i) \quad (2)$$

By representing the single particle orbitals ψ_i , all electronic densities physically acceptable for the system of “non-interacting” electrons are written in the Eq. (3):

$$\rho(\vec{r}) = \sum_i^M |\psi_i(\vec{r})|^2 \quad (3)$$

Finally, the total energy could be measured by the KS method due to the Eq. (4):

$$E[\rho] = \sum_i^M n_i \left\langle \psi_i \left| -\frac{1}{2} \nabla^2 + v_{ext}(\vec{r}) + \frac{1}{2} \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d\vec{r}' \right| \psi_i \right\rangle + E_{xc}[\rho] + \frac{1}{2} \sum_{\beta}^N \sum_{\alpha \neq \beta}^N \frac{Z_{\alpha} Z_{\beta}}{|\vec{R}_{\alpha} - \vec{R}_{\beta}|} \quad (4)$$

Therefore, the precise exchange energy functional is described by the Kohn–Sham orbitals in lieu of the density which is cited as the indirect density functional. This research has employed the penetration of the hybrid functional of three-parameter basis set of “B3LYP (Becke, Lee, Yang, Parr)” within the conception of DFT upon theoretical computations [23,24]. The popular B3LYP (Becke, three-parameter, Lee–Yang–Parr) and the exchange–correlation functional become as Eq. (5) [23–25]:

$$E_{XC}^{B3LYP} = (1 - \alpha) E_x^{LSDA} + \alpha E_x^{HF} + b \Delta E_x^B + (1 - c) E_c^{LSDA} + c E_c^{LYP} \quad (5)$$

Calculations with spin polarization were performed within DFT [26]. The exchange correlation potentials were treated by the “Perdew–Burke–Ernzerhof (PBE)” parameterization within the “general gradient approximation (GGA)” [27,28]. Fig. 1a–d has shown alkali metals and alkaline earth metals-based nanoclusters of SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C.

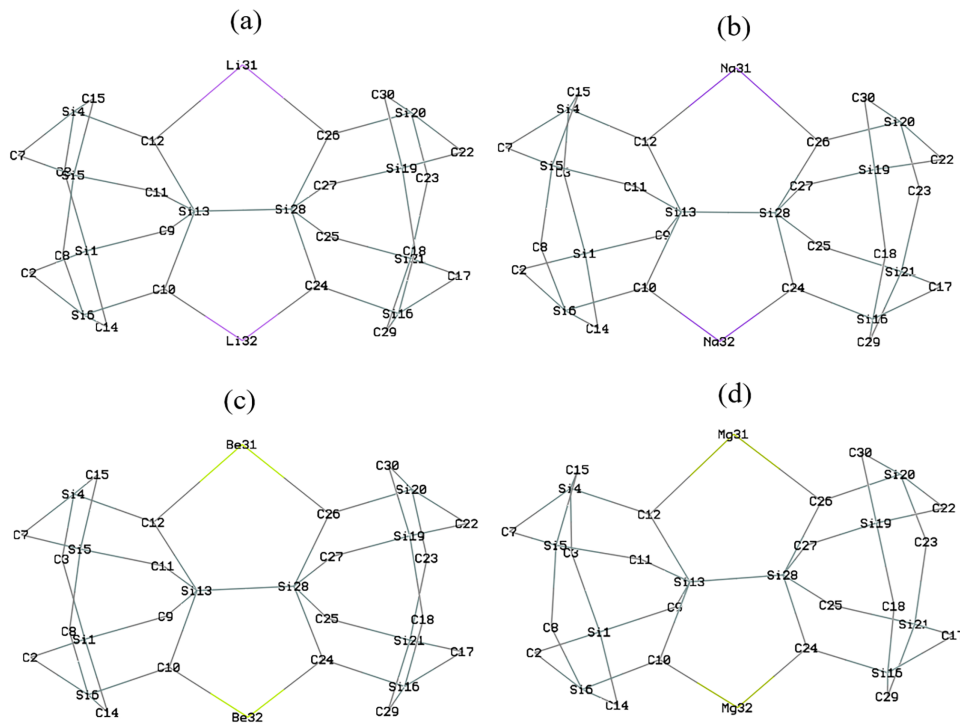


Figure 1: Adding Li, Na, Be, Mg to SiC nanocluster and formation of (a) SiLi₂C, (b) SiNa₂C, (c) SiBe₂C and (d) SiMg₂C complexes towards saving energy in novel batteries

The analysis of Bader charge parameter [29] has been illustrated for energy storage by hybrid clusters of SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C (Fig. 1a–d) accompanying the Gaussian 16 revision C.01 computational software [30] and the GaussView 6.1 graphical program [31].

One of the most significant advantages of applying SiC nanocluster as the anode material in Li-, Na-, Be- or Mg-batteries is increasing energy storage utility due to enhancing the electrical conductivity between Si/C and surface area. In this investigation, homogeneously distributed silicon or carbon elements can be

immobilized in the SiC matrix, which prevents their tendency to form the agglomeration under battery cycling. The Li/Na/Be/Mg insertion might also result the cleavage of some C–Li, C–Na, C–Be or C–Mg bonds in the SiC anode material and the expansion of favorable sites for the subsequent ion insertion in the network (Fig. 1a–d).

3 Results and Discussion

3.1 Charge Density Differences Analysis

In Fig. 2a–d, charge density differences (CDD) [32] have been shown for SiLi_2C , SiNa_2C , SiBe_2C and SiMg_2C nanoclusters with the vibration in the district about -12 to $+9$ Bohr through co-interaction between alkali metals of Li(31)–Li(32), Na(31)–Na(32) and alkaline earth metals of Be(31)–Be(32), Mg(31)–Mg(32).

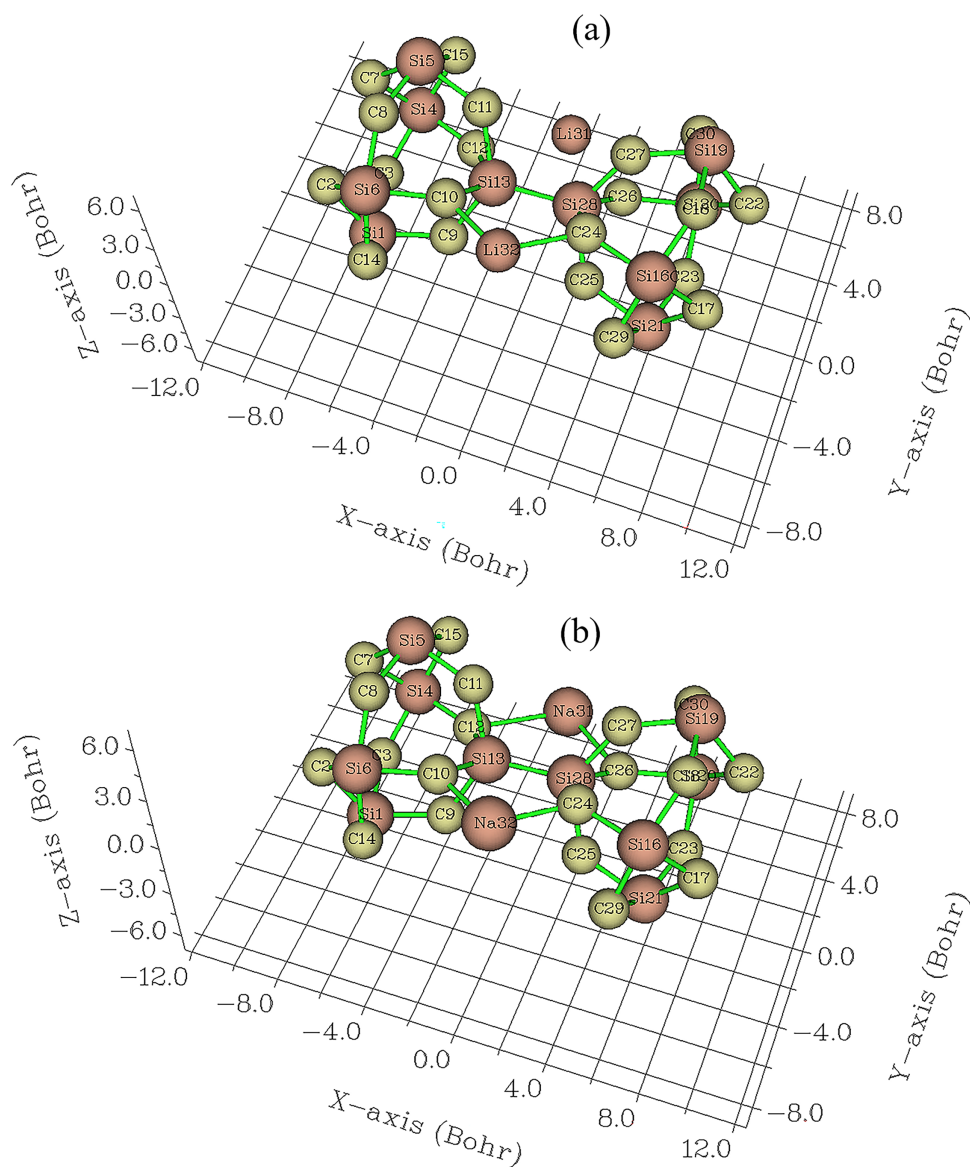


Figure 2: (Continued)

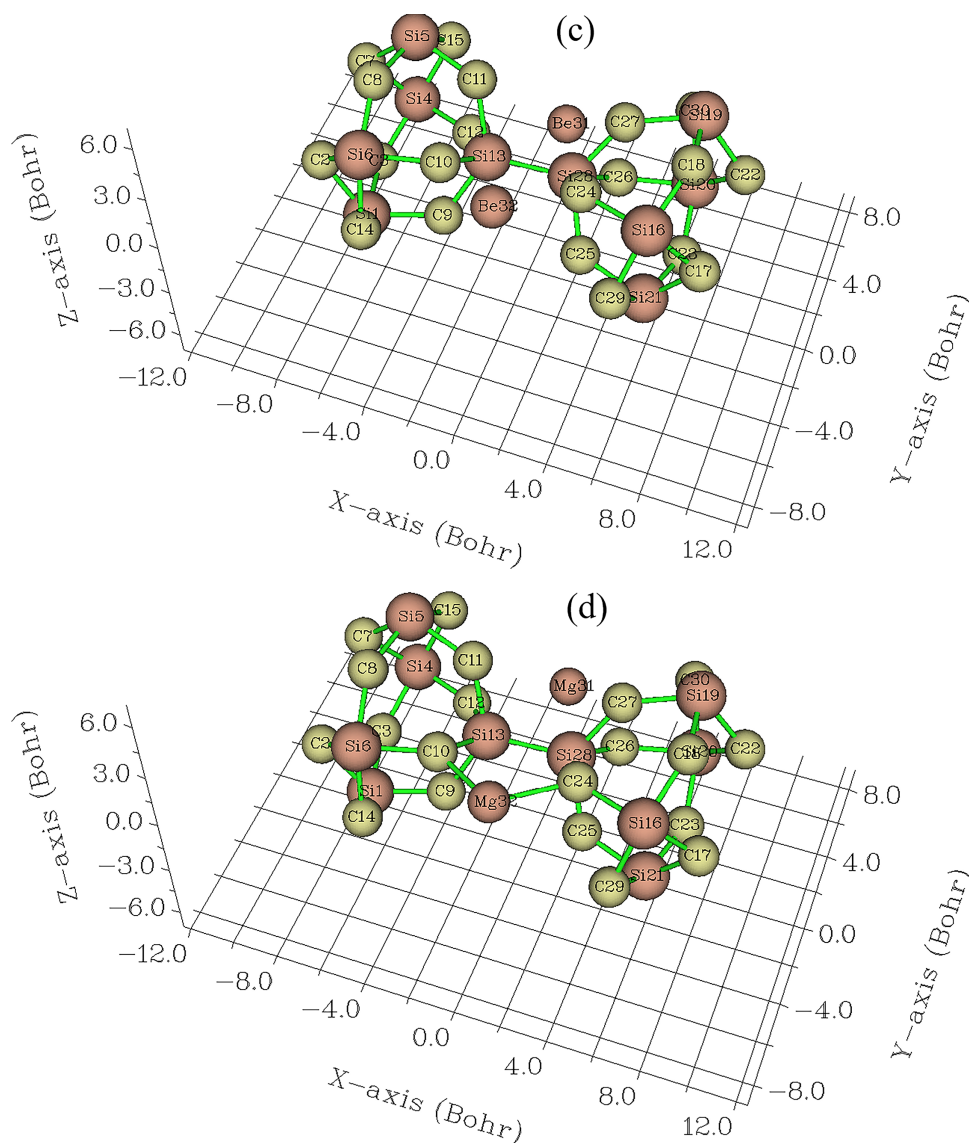


Figure 2: The CDD graphs for (a) SiLi_2C , (b) SiNa_2C , (c) SiBe_2C and (d) SiMg_2C nanoclusters

Moreover, the elements of C(2), C(3), C(7)–C(12), C(14), C(15), C(17), C(18), C(22)–C(27), C(29), C(30) from SiLi_2C , SiNa_2C , SiBe_2C and SiMg_2C nanoclusters have displayed the vibration about -12 to $+9$ Bohr (Table 1 and Fig. 2a,d).

The charge distribution has been illustrated during alkali and alkaline earth metals captured by SiC nanostructure towards formation of SiLi_2C , SiNa_2C , SiBe_2C and SiMg_2C nanoclusters, respectively (Table 1). Functionalizing of Li, Na, Be, Mg atoms can augment the negative atomic charge of C(2), C(3), C(7)–C(12), C(14), C(15), C(17), C(18), C(22)–C(27), C(29), C(30) as electron acceptors in SiLi_2C , SiNa_2C , SiBe_2C and SiMg_2C nanoclusters (Fig. 3a–d).

Table 1: The atomic charge (Q/coulomb) for SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C nanoclusters

SiLi ₂ C		SiNa ₂ C		SiBe ₂ C		SiMg ₂ C	
Atom	Q	Atom	Q	Atom	Q	Atom	Q
Si(1)	0.76	Si(1)	0.74	Si(1)	0.74	Si(1)	0.73
C(2)	-0.42	C(2)	-0.42	C(2)	-0.43	C(2)	-0.43
C(3)	-0.34	C(3)	-0.37	C(3)	-0.36	C(3)	-0.34
Si(4)	0.73	Si(4)	0.73	Si(4)	0.74	Si(4)	0.72
Si(5)	0.73	Si(5)	0.74	Si(5)	0.72	Si(5)	0.71
Si(6)	0.79	Si(6)	0.85	Si(6)	0.82	Si(6)	0.81
C(7)	-0.38	C(7)	-0.40	C(7)	-0.39	C(7)	-0.39
C(8)	-0.36	C(8)	-0.37	C(8)	-0.34	C(8)	-0.34
C(9)	-0.38	C(9)	-0.37	C(9)	-0.38	C(9)	-0.35
C(10)	-0.81	C(10)	-0.70	C(10)	-0.83	C(10)	-1.07
C(11)	-0.37	C(11)	-0.35	C(11)	-0.38	C(11)	-0.37
C(12)	-0.92	C(12)	-0.82	C(12)	-0.89	C(12)	-1.10
Si(13)	1.11	Si(13)	0.96	Si(13)	1.05	Si(13)	1.09
C(14)	-0.37	C(14)	-0.37	C(14)	-0.36	C(14)	-0.38
C(15)	-0.38	C(15)	-0.38	C(15)	-0.34	C(15)	-0.38
Si(16)	0.81	Si(16)	0.86	Si(16)	0.83	Si(16)	0.83
C(17)	-0.41	C(17)	-0.42	C(17)	-0.41	C(17)	-0.42
C(18)	-0.35	C(18)	-0.37	C(18)	-0.34	C(18)	-0.34
Si(19)	0.71	Si(19)	0.71	Si(19)	0.70	Si(19)	0.69
Si(20)	0.75	Si(20)	0.77	Si(20)	0.75	Si(20)	0.75
Si(21)	0.76	Si(21)	0.75	Si(21)	0.74	Si(21)	0.73
C(22)	-0.38	C(22)	-0.40	C(22)	-0.39	C(22)	-0.39
C(23)	-0.34	C(23)	-0.38	C(23)	-0.36	C(23)	-0.35
C(24)	-0.78	C(24)	-0.69	C(24)	-0.86	C(24)	-1.05
C(25)	-0.34	C(25)	-0.34	C(25)	-0.35	C(25)	-0.32
C(26)	-0.85	C(26)	-0.75	C(26)	-0.82	C(26)	-1.06
C(27)	-0.51	C(27)	-0.47	C(27)	-0.49	C(27)	-0.48
Si(28)	1.07	Si(28)	1.01	Si(28)	1.05	Si(28)	1.08
C(29)	-0.40	C(29)	-0.39	C(29)	-0.37	C(29)	-0.42
C(30)	-0.37	C(30)	-0.39	C(30)	-0.34	C(30)	-0.37
Li(31)	0.75	Na(31)	0.68	Be(31)	0.65	Mg(31)	1.15
Li(32)	0.50	Na(32)	0.37	Be(32)	0.67	Mg(32)	1.09

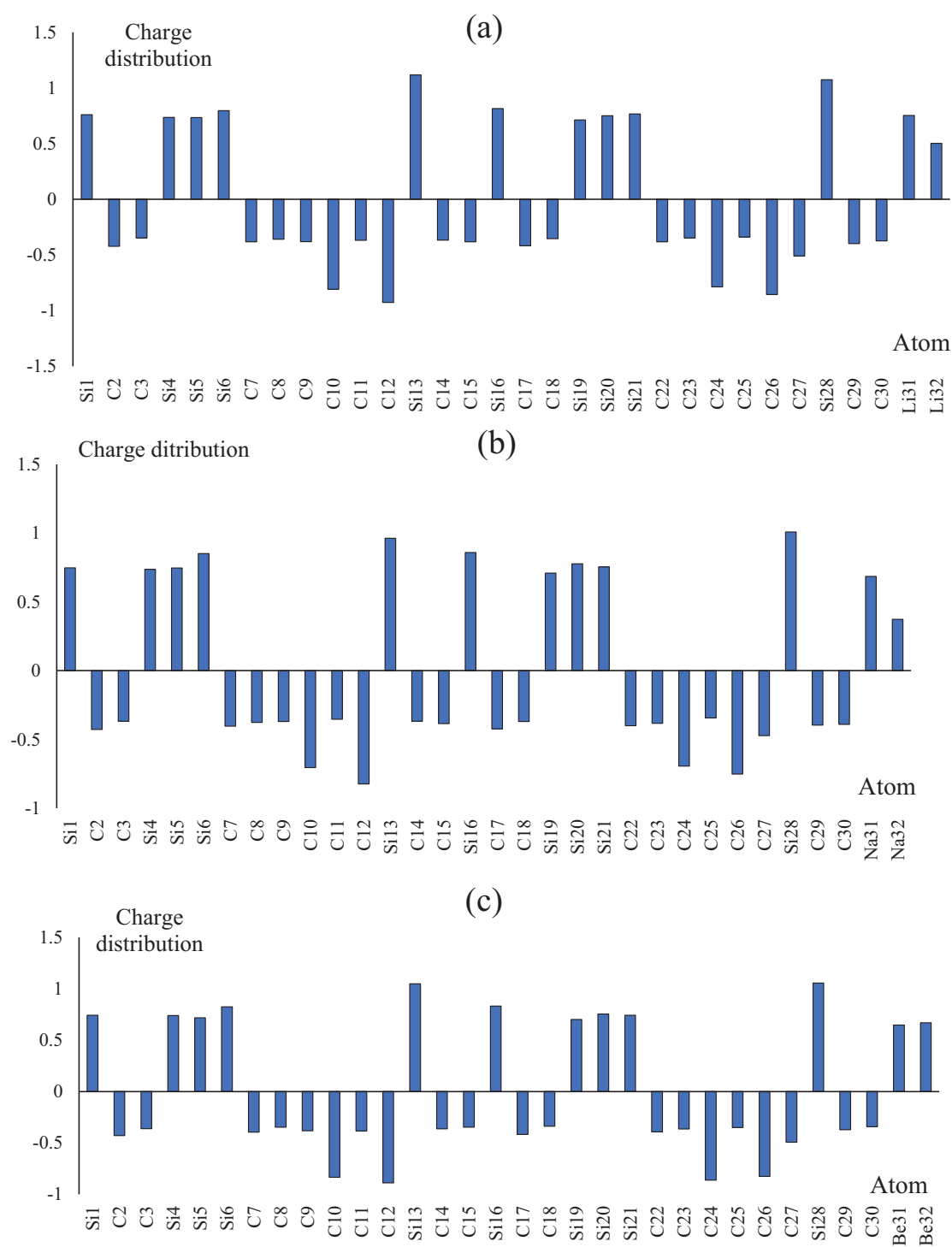


Figure 3: (Continued)

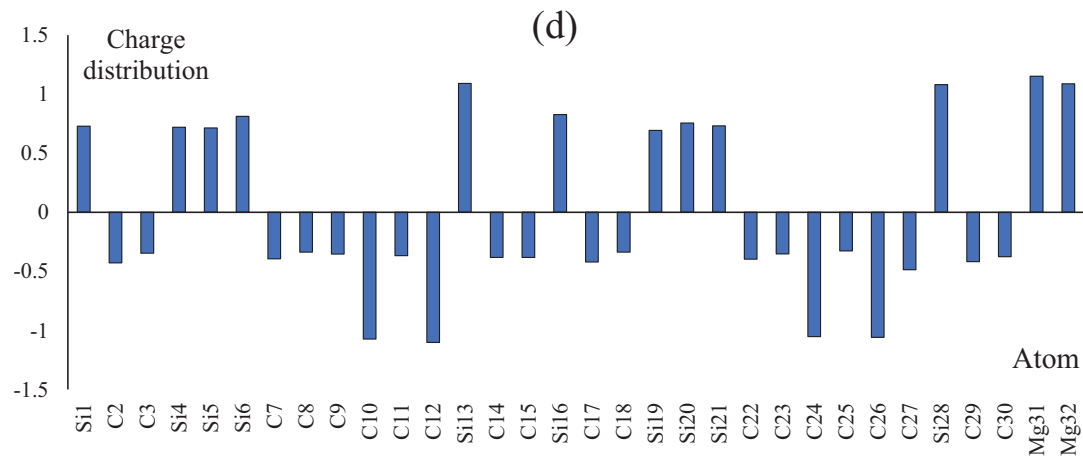


Figure 3: The changes of charge distribution for (a) SiLi₂C, (b) SiNa₂C, (c) SiBe₂C and (d) SiMg₂C nanoclusters

3.2 Total Density of States

In isolated system (such as molecule), the energy levels are discrete, the concept of “density of states (*DOS*)” is supposed to be completely valueless in this situation. Therefore, the “original total *DOS* (*TDOS*)” of an isolated system can be written as [33]:

$$TDOS(E) = \sum_i \delta(E - \epsilon_i) \quad (6)$$

The normalized Gaussian function is defined as:

$$G(x) = \frac{1}{c\sqrt{2\pi}} e^{-\frac{x^2}{2c^2}}, \text{ where } c = \frac{\text{FWHM}}{2\sqrt{2\ln 2}} \quad (7)$$

“FWHM (full width at half maximum)” is an adjustable parameter in “Multiwfn” [34,35]. Furthermore, the curve map of “broadened partial *DOS* (*PDOS*)” and “overlap *DOS* (*OPDOS*)” are valuable for visualizing the orbital composition analysis, that “*PDOS* function of fragment *A*” is defined as:

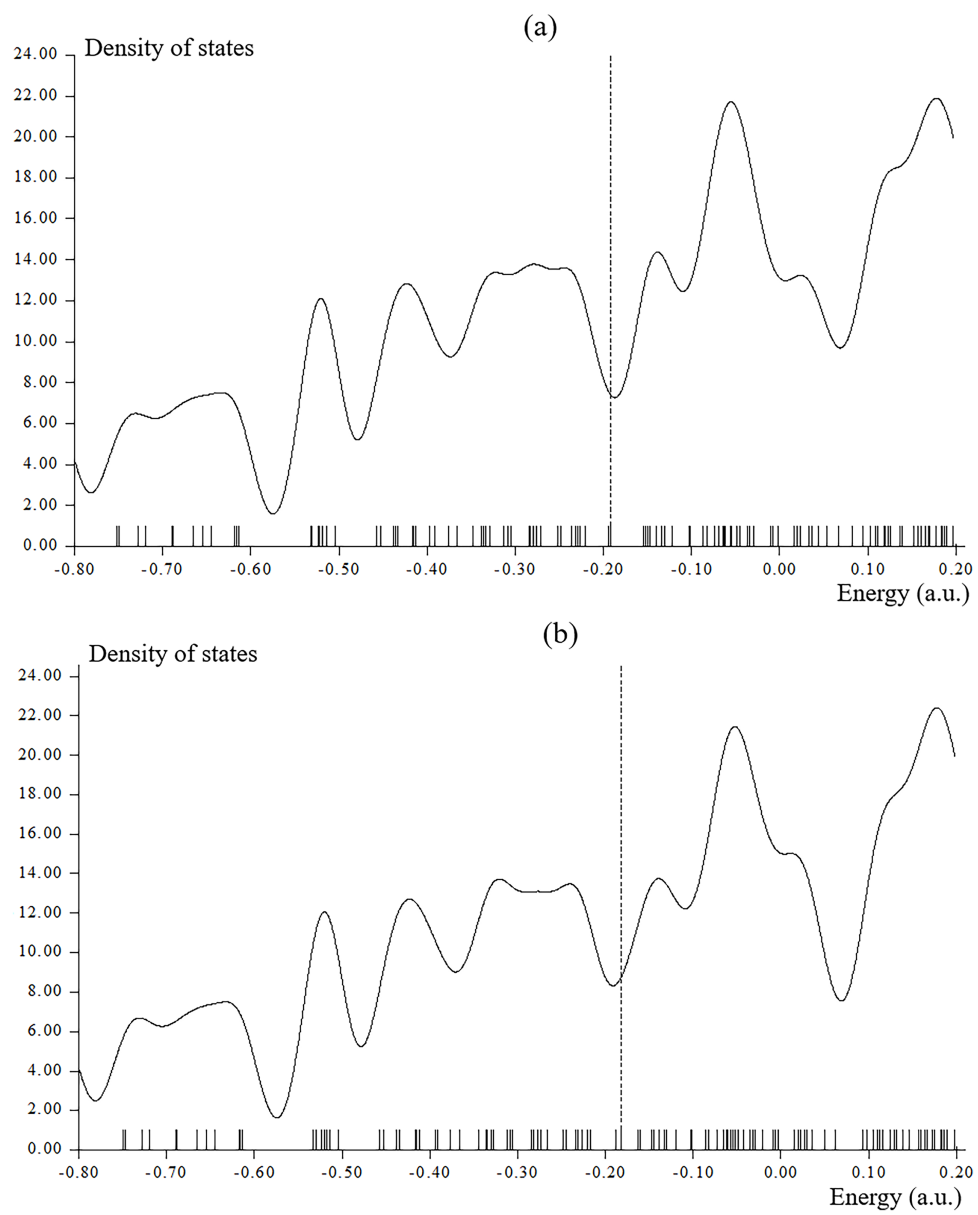
$$PDOS_A(E) = \sum_i \Xi_{i,A} F(E - \epsilon_i) \quad (8)$$

where “ $\Xi_{i,A}$ is the composition of fragment *A* in orbital *i*”. The “*OPDOS* between fragment *A* and *B*” is defined as:

$$OPDOS_{A,B}(E) = \sum_i X_{A,B}^i F(E - \epsilon_i) \quad (9)$$

where “ $X_{A,B}^i$ is the composition of total cross term between fragment *A* and *B* in orbital *i*”.

Regarding energy storage by SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C nanoclusters, *TDOS* has been evaluated. This factor can demonstrate the existence of important chemical interactions on the “convex side” (Fig. 4a–d).

**Figure 4:** (Continued)

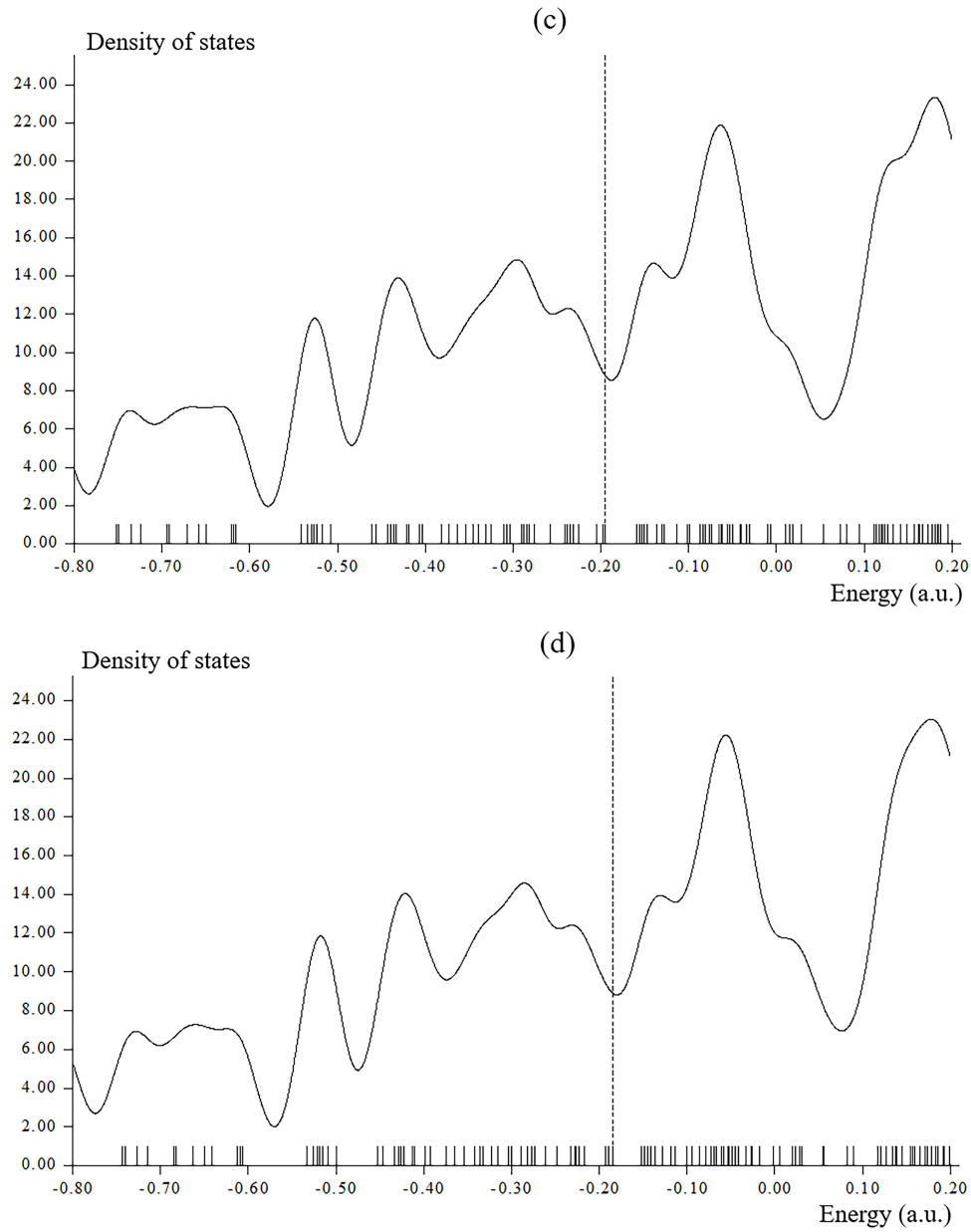


Figure 4: The TDOS graphs of (a) SiLi₂C, (b) SiNa₂C, (c) SiBe₂C and (d) SiMg₂C nanoclusters

3.3 Localized Orbital Locator Analysis

Localized orbital locator (LOL) has a similar expression compared to “electron localization function (ELF)” [36].

$$\text{LOL}(\mathbf{r}) = \frac{\tau(\mathbf{r})}{1 + \tau(\mathbf{r})}; \tau(\mathbf{r}) = \frac{D_0(\mathbf{r})}{\frac{1}{2} \sum_i \eta_i |\nabla \varphi_i(\mathbf{r})|^2} \quad (10)$$

$$D_0(\mathbf{r}) = \frac{3}{10} (6\pi^2)^{2/3} [\rho_\alpha(\mathbf{r})^{5/3} + \rho_\beta(\mathbf{r})^{5/3}] \quad (11)$$

“Multiwfn” [34,35] also supports the approximate version of “LOL” defined by “Tsirelson and Stash” [37,38], namely the actual kinetic energy term in “LOL” is replaced by “second-order gradient expansion like ELF” which may demonstrate a broad span of bonding samples. This “Tsirelson’s version of LOL” can be activated by setting “ELFLOL_type to 1. For special reason”, if “ELFLOL_type in settings.ini is changed from 0 to 2”, another formalism will be used:

$$\text{LOL}(\mathbf{r}) = \frac{1}{1 + \left[\frac{1}{\tau(\mathbf{r})} \right]^2} \quad (12)$$

If the parameter “ELFLOL_cut in settings.ini is set to x ”, then “LOL will be zero where LOL is less than x ”.

Trapping of Li, Na, Be, Mg atoms by SiC nanostructure (Fig. 5a–d) has concluded SiLi_2C , SiNa_2C , SiBe_2C and SiMg_2C nanoclusters (Fig. 5a–d).

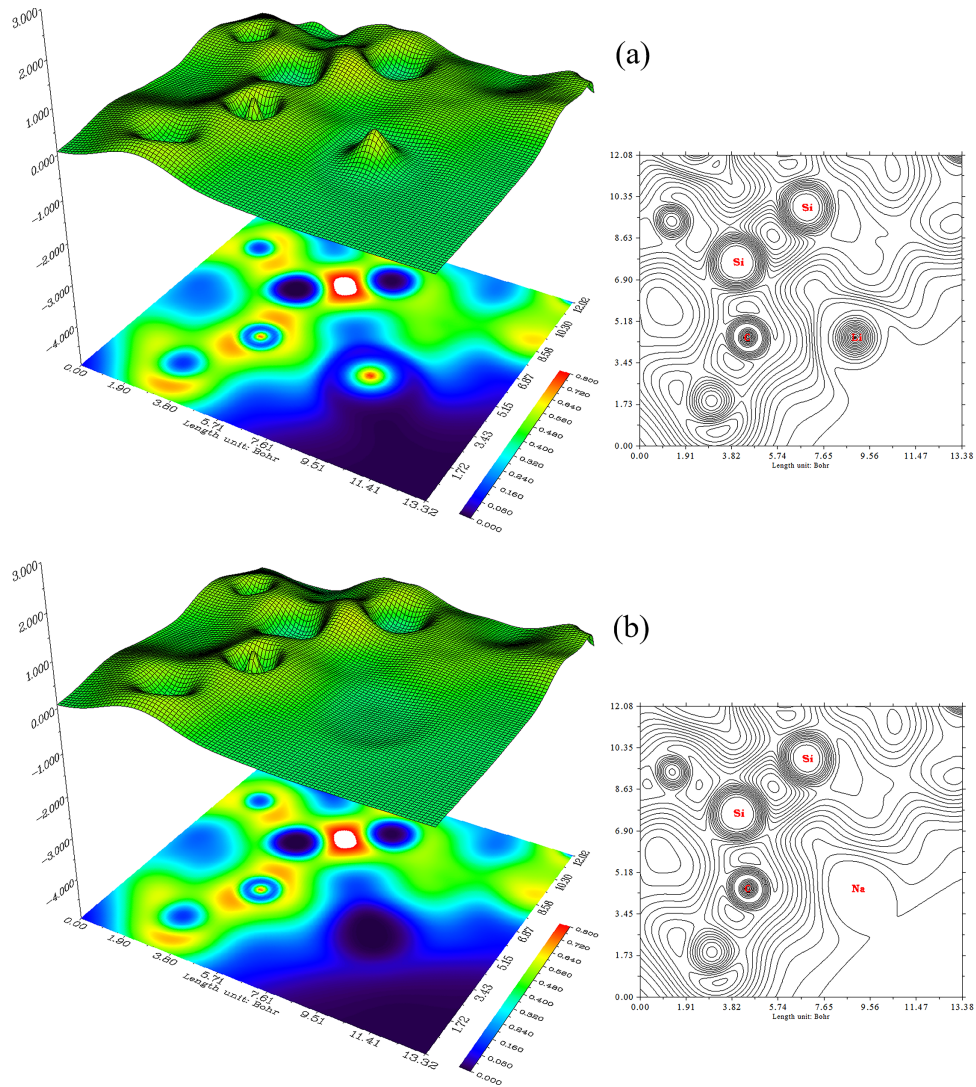


Figure 5: (Continued)

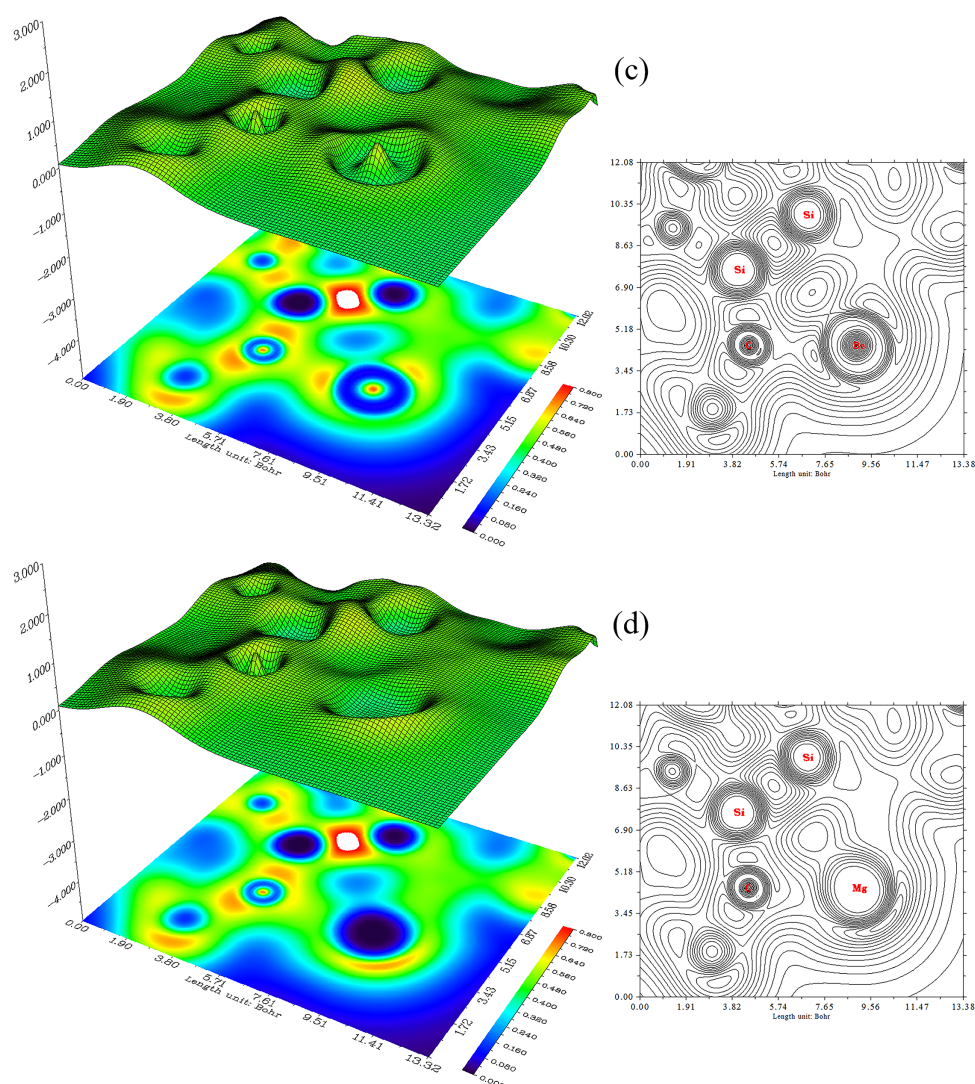


Figure 5: The counter (right side) and shaded (left side) maps of LOL graphs for (a) SiLi₂C, (b) SiNa₂C, (c) SiBe₂C and (d) SiMg₂C nanoclusters

SiLi₂C (Fig. 5a), SiNa₂C (Fig. 5b), SiBe₂C (Fig. 5c) and SiMg₂C (Fig. 5d) have demonstrated the electron delocalization through an isosurface map with labeling atoms of C(10), C(12), Si(13), C(24), C(26), Si(28), X(31)/X(32) (X = Li, Na, Be, Mg). In fact, the counter map of LOL can confirm that SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C nanoclusters may augment the efficiency of energy storage (Fig. 5a–d and Table 2).

Moreover, intermolecular orbital overlap integral is important in discussions of intermolecular charge transfer which can calculate HOMO-HOMO and LUMO-LUMO overlap integrals between the alkali/alkaline earth metals and silicon carbide (Table 2).

In addition, the amount of “Mayer bond order” [39] is generally according to empirical bond order for the single bond is nearly 1.0. “Mulliken bond order” [40] with a small accord with empirical bond order is not appropriate for quantifying bonding strength, for which Mayer bond order always performs better. However, “Mulliken bond order” is a good qualitative indicator for “positive amount” of bonding and “negative amount” of antibonding which are evacuated and localized, respectively (Table 3).

Table 2: The cell capacity (C, mAh g⁻¹), dipole moment (D/debye), HOMO (eV), LUMO (eV), energy gap ($\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}}$ /eV) and stability energy (E_s /kcal/mol) for SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C nanoclusters

Heteroclusters	C	D	E_{HOMO}	E_{LUMO}	ΔE	$E_s \times 10^{-3}$
SiLi ₂ C	100.20	1.25	-5.20	-4.20	1.00	-509.21
SiNa ₂ C	94.53	1.18	-4.96	-4.43	0.52	-499.96
SiBe ₂ C	198.86	1.09	-5.30	-4.33	0.97	-518.21
SiMg ₂ C	188.18	0.29	-5.06	-4.12	0.89	-500.80

Table 3: The bond order of Mayer, Wiberg, Mulliken, Laplacian and Fuzzy from mixed alpha and beta density matrix for SiLi₂C, SiNa₂C, SiBe₂C and SiMg₂C nanoclusters

Heteroclusters	Bond type	Bond order				
		Mayer	Wiberg	Mulliken	Laplacian	Fuzzy
SiLi ₂ C	Si(13)–Si(28)	0.73	0.67	0.56	2.11	0.90
	C(10)–Li(32)	0.40	0.42	0.48	0.43	0.36
	C(12)–Li(31)	0.16	0.26	0.27	0.27	0.18
	C(24)–Li(32)	0.36	0.41	0.44	0.42	0.34
	C(26)–Li(31)	0.20	0.31	0.31	0.40	0.22
SiNa ₂ C	Si(13)–Si(28)	0.69	0.66	0.42	0.47	0.87
	C(10)–Na(32)	0.41	0.27	0.59	0.59	0.53
	C(12)–Na(31)	0.16	0.20	0.32	0.31	0.33
	C(24)–Na(32)	0.41	0.27	0.56	0.53	0.51
	C(26)–Na(31)	0.22	0.23	0.37	0.36	0.39
SiBe ₂ C	Si(13)–Si(28)	0.81	0.69	0.60	0.66	0.91
	C(10)–Be(32)	0.82	0.80	0.83	0.85	0.66
	C(12)–Be(31)	0.47	0.50	0.42	0.46	0.39
	C(24)–Be(32)	0.78	0.77	0.82	0.83	0.63
	C(26)–Be(31)	0.59	0.62	0.50	0.52	0.49
SiMg ₂ C	Si(13)–Si(28)	0.89	0.69	0.68	0.63	0.88
	C(10)–Mg(32)	0.56	0.62	0.63	0.60	0.77
	C(12)–Mg(31)	0.33	0.44	0.40	0.44	0.51
	C(24)–Mg(32)	0.54	0.60	0.60	0.61	0.75
	C(26)–Mg(31)	0.41	0.52	0.45	0.47	0.60

As it is seen in Table 3, “Laplacian bond order” [41] has a straight cohesion with bond polarity, bond dissociation energy and bond vibrational frequency. The low value of Laplacian bond order might demonstrate that it is insensitive to the calculation degree applied for producing electron density. Generally, the value of “Fuzzy bond order” is near Mayer bond order, especially for low-polar bonds, but much more stable with respect to the change in basis-set. Computation of “Fuzzy bond order” demands running “Becke’s DFT” numerical integration, owing to which calculation value is larger than assessment of “Mayer bond order” and it can concede more precisely [42].

4 Conclusions

Alkali/Alkaline earth metals captured by silicon carbide towards the formation of SiLi_2C , SiNa_2C , SiBe_2C and SiMg_2C nanoclusters were studied by DFT computational methods. Changes in charge density indicate a notable charge transfer in the SiLi_2C , SiNa_2C , SiBe_2C , and SiMg_2C heteroclusters. Due to the semiconducting nature of SiC, it is usually composited with C for better ionic and electronic conductivities. It is well established that increasing Li, Na, Be, or Mg in cell batteries can enhance energy efficiency.

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Ethics Approval: Not applicable.

Conflicts of Interest: The authors declare no conflicts of interest to report regarding the present study.

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