Energy Storage by Beyond Lithium Batteries of Sodium and Potassium using Density Functional Theory Level

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Abstract: While lithium-ion batteries have their difficulties, the demand to improve beyond lithium batteries goes beyond sustainability and safety issues. With the pressure for renewable energy resources and the enchantingly digitalized current lifestyle, the need for batteries will augment. Therefore, this article has evaluated the promising alternative alkali metals of sodium-ion and potassium-ion batteries. A comprehensive investigation on hydrogen grabbing by Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] was carried out, including using DFT computations at the "CAM–B3LYP–D3/6-311+G (d,p)" level of theory. The hypothesis of the hydrogen adsorption phenomenon was confirmed by density distributions of CDD, TDOS, and ELF for nanoclusters of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂ or K[SiO–GeO]–2H₂. The fluctuation in charge density values demonstrates that the electronic densities were mainly located in the boundary of adsorbate/adsorbent atoms during the adsorption status. The advantages of lithium, sodium, or potassium instruments to operate at higher frequencies than Si/Ge instruments. Among these, sodium-ion batteries seem to show the most promise regarding initial capacity.

Keywords: sodium or potassium battery; density of states; charge distribution; materials modeling; hydrogen adsorption; energy storage.

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1. Introduction

Although lithium-ion batteries have become available in the current technology perspective through their high energy density, they face serious discussions in terms of safety and sustainability. With the increasing global demand for energy, there is an essential need for alternative, efficient energy storage systems. This is driving research into non-lithium battery systems. This paper presents comprehensive research on non-lithium battery technologies, specifically sodium-ion and potassium-ion batteries [1-6].

Along with the sodium ion, potassium ion is the prime chemistry replacement candidate for lithium-ion batteries. The potassium-ion has certain advantages over similar lithium-ion, such as the cell design being simple and the material and fabrication procedures being cheaper. The key advantage is the abundance and low cost of potassium compared to lithium, which makes potassium batteries a promising candidate for large-scale batteries such as household energy storage and electric vehicles. Another advantage of a potassium-ion battery over a lithium-ion battery is potentially faster charging [7–13].

Recently, Si-, Ge- or Sn-carbide nanostructures have been suggested as engaged Hgrabbing compounds [14–16]. Since the polarizability of silicon is more than that of carbon, it is supposed that Si–C/Si nanosheet might attach to compositions more strongly in comparison to the net carbon nano-surfaces [17–19].

In our previous works, the investigation of energy storage in fuel cells through hydrogen adsorption has been accomplished using DFT calculations through different nanomaterials consisting of silicon/germanium/tin/lead nano-carbides [20], magnesium - aluminum alloy [21] and aluminum/carbon/ silicon doping boron nitride nanocage [22].

Nanomaterials with remarkable specific structures indicate promising applications in the field of energy storage, electrocatalysis, and fuel cells. Currently, the present research aims to explore the possibility of using Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanoclusters for hydrogen storage by employing first-principles calculations. We have analyzed the structural and electronic properties of Li[SiO–GeO], Na[SiO–GeO] or K[SiO–GeO] nanoclusters and hydrogen-adsorbed nanoclusters of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂ or K[SiO–GeO]–2H₂. Using state-of-the-art computational techniques.

2. Materials and Methods

The aim of this study is to hydrogen adsorption by using alkali metals-based nanoclusters of Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] (Figure 1), which can increase the hydrogen storage in cell batteries, transistors or other semiconductors. In our research, the calculations have been done by CAM–B3LYP–D3 /EPR–3 level of theory.



(a)

Figure 1. Adding Li, Na, K to (a) [SiO–GeO] nanocluster and formation of (b) Li[SiO–GeO]; (c) Na[SiO–GeO]; (d) K[SiO–GeO] towards hydrogen adsorption and energy storage in novel batteries of (b') Li[SiO–GeO]–2H₂; (d') Na[SiO–GeO]–2H₂; (d') K[SiO–GeO]–2H₂.

Figure 1 shows the process of hydrogen adsorption by Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanoclusters and hydrogen-adsorbed nanoclusters of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂ or K[SiO–GeO]–2H₂. The Bader charge analysis [23] was discussed during the trapping of hydrogen atoms by Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanoclusters (Figure 1). The rigid potential energy surface using density functional theory [24–26] was performed due to the Gaussian 16 revision C.01 program package [27] and GaussView 6.1 [28]. The coordination input for hydrogen grabbing by Li[SiO–GeO], Na[SiO–GeO], and K[SiO–GeO] has lanl2dz and applied 6-311+G (d,p) basis sets.

3. Results and Discussion

3.1. Charge density differences analysis.

The amounts of charge density differences (CDD) are measured by considering isolated atoms or noninteracting ones.



Figure 2. CDD graphs for (a) Li[SiO–GeO]; (a') Li[SiO–GeO]–2H₂; (b) Na[SiO–GeO]; (b') Na[SiO–GeO]–2H₂; (c) K[SiO–GeO]; (c') K[SiO–GeO]–2H₂ nanoclusters.

The mentioned approximation can be the lightest to use because the superposition value may be received from the primary status of the self-consistency cycle in the code that carries out the density functional theory (Figure 2a–c, a'–c') [29].

In Figure 2a, the Li[SiO–GeO] cluster with the fluctuation in the region around -12 to +6 Bohr forms the nanocluster of Li[SiO–GeO]–2H₂ (Figure 2a') in the area around -12 to +3 Bohr. Furthermore, the atoms of O2, O3, O7–O12, O14, O15, O17, O18, O22–O27, O29, and O30 from Na[SiO–GeO] (Figure 2b) have shown a fluctuation around -12 to +4 Bohr towards the formation of Na[SiO–GeO]–2H₂ through hydrogen adsorption (Figure 2b'). In addition, the K[SiO–GeO] cluster with the fluctuation in the region around -12 to +4 Bohr (Figure 2c) forms the nanocluster of K[SiO–GeO]–2H₂ during hydrogen grabbing (Figure 2c') in the same range of area around -12 to +4 Bohr. The atomic charge was discussed during the trapping of hydrogens by Li[SiO–GeO], Na[SiO–GeO] or K[SiO–GeO] nanoclusters towards the formation of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂ or K[SiO–GeO]–2H₂, respectively (Table1).

Table 1. The atomic charge (Q/coulomb) for The atomic charge (Q/coulomb) for Li[SiO–GeO], Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂, K[SiO–GeO]nanoclusters, and K[SiO–GeO]–2H₂ nanoclusters.

Li[SiO-GeO]		Li[SiO-GeO]-2H ₂		Na[SiO-GeO]		Na[SiO-GeO]-2H ₂		K[SiO-GeO]		K[SiO-GeO]-2H ₂	
Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
Si1	1.4586	Si1	1.4565	Si1	1.4601	Si1	1.4585	Si1	1.4710	Si1	1.4709
O2	-0.6856	O2	-0.6559	O2	-0.6561	O2	-0.6875	O2	-0.6289	O2	-0.6290
O3	-0.8317	03	-0.8358	03	-0.8359	03	-0.8320	O3	-0.8318	O3	-0.8319
Si4	1.4365	Si4	1.4303	Si4	1.4184	Si4	1.4282	Si4	1.4174	Si4	1.4184
Si5	1.4612	Si5	1.4458	Si5	1.4531	Si5	1.4656	Si5	1.4487	Si5	1.4481
Si6	1.4613	Si6	1.4638	Si6	1.4554	Si6	1.4561	Si6	1.4700	Si6	1.4709
07	-0.6525	07	-0.6830	07	-0.6815	07	-0.6534	07	-0.7146	07	-0.7147
08	-0.8377	08	-0.8434	08	-0.8442	08	-0.8385	08	-0.8347	08	-0.8348
O9	-0.7899	09	-0.7870	09	-0.7889	09	-0.7911	O9	-0.7864	O9	-0.7864
O10	-1.0109	O10	-1.0019	O10	-0.9953	O10	-0.9970	O10	-1.0538	O10	-1.0543
011	-0.8020	011	-0.8024	011	-0.8070	011	-0.8067	011	-0.8086	011	-0.8085
O12	-0.9454	012	-0.9524	012	-0.9671	O12	-0.9570	O12	-0.9919	O12	-0.9916
Si13	1.6312	Si13	1.6329	Si13	1.6261	Si13	1.6351	Si13	1.5744	Si13	1.5739
O14	-0.7005	014	-0.7301	014	-0.7318	O14	-0.7084	O14	-0.7651	O14	-0.7672
O15	-0.7611	015	-0.7232	015	-0.7297	O15	-0.7669	O15	-0.7011	O15	-0.7018
Ge16	1.3977	Ge16	1.4175	Ge16	1.4172	Ge16	1.4025	Ge16	1.4046	Ge16	1.4053
O17	-0.6718	017	-0.6526	017	-0.6530	O17	-0.6715	O17	-0.6077	O17	-0.6075
O18	-0.7819	018	-0.7795	O18	-0.7796	O18	-0.7837	O18	-0.7826	O18	-0.7824
Ge19	1.3823	Ge19	1.3975	Ge19	1.4017	Ge19	1.3825	Ge19	1.3823	Ge19	1.3825
Ge20	1.3900	Ge20	1.3931	Ge20	1.3876	Ge20	1.3859	Ge20	1.3623	Ge20	1.3650
Ge21	1.3916	Ge21	1.4017	Ge21	1.4035	Ge21	1.3883	Ge21	1.4024	Ge21	1.4002
O22	-0.6229	O22	-0.6688	O22	-0.667	O22	-0.6235	O22	-0.6959	O22	-0.6964
O23	-0.7867	O23	-0.7833	O23	-0.7827	O23	-0.7863	O23	-0.7867	O23	-0.7866
O24	-0.9474	O24	-0.9440	O24	-0.9548	O24	-0.9516	O24	-0.9944	O24	-0.9944
O25	-0.7899	O25	-0.7749	O25	-0.7797	025	-0.7929	O25	-0.7850	O25	-0.7848
O26	-0.9187	O26	-0.9064	O26	-0.9315	O26	-0.9381	O26	-0.9694	O26	-0.9693
O27	-0.7748	O27	-0.7935	O27	-0.7889	O27	-0.7704	O27	-0.7819	O27	-0.7823

Li[SiO-GeO]		Li[SiO-GeO]-2H2		Na[SiO-GeO]		Na[SiO-GeO]-2H ₂		K[SiO–GeO]		K[SiO-GeO]-2H ₂	
Ge28	1.2474	Ge28	1.2558	Ge28	1.2887	Ge28	1.2880	Ge28	1.2213	Ge28	1.2212
O29	-0.6903	O29	-0.7345	O29	-0.7405	O29	-0.6994	O29	-0.7578	O29	-0.7603
O30	-0.7318	O30	-0.7221	O30	-0.7249	O30	-0.7380	O30	-0.6764	O30	-0.6782
Li31	0.7345	Li31	0.6437	Na31	0.8096	Na31	0.7180	K31	0.9096	K31	0.8790
Li32	0.7418	Li32	0.6386	Na32	0.7187	Na32	0.6409	K32	0.8911	K32	0.8709
		H33	-0.0264			H33	-0.0277			H33	-0.0609
		H34	-0.0074			H34	-0.0087			H34	-0.0399
		H35	0.1277			H35	0.1000			H35	0.0903
		H36	0.1036			H36	0.0818			H36	0.0666

The atomic charge of Si, Ge, O, and alkali metals of Li, Na, K, and hydrogen atoms absorbed on Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanoclusters have been measures. The values detect that with adding lithium, sodium and potassium, the negative atomic charge of oxygen atoms of O2, O3, O7–O12, O14, O15, O17, O18, O22–O27, O29, O30 in Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂ or K[SiO–GeO]–2H₂ nanoclusters augments. Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanoclusters have shown more efficiency than SiO–GeO clusters [30] for admitting the electron from electron donors of H33, H34, H35, and H36 (Table 1 and Figure3).



Figure 3. The fluctuation of atomic charge (Q/coulomb) for Li[SiO–GeO], Na[SiO–GeO] or K[SiO–GeO] nanoclusters. (Note: X=Li, Na, K)

The changes of charge density analysis in the adsorption process have illustrated that Li[SiO–GeO] has shown the "Bader charge" of -1.631 coulomb before hydrogen adsorption and -1.633 coulomb after hydrogen adsorption. Moreover, the changes of charge density analysis for Na[SiO–GeO] have shown the "Bader charge" of -1.626 coulomb before hydrogen adsorption and -1.635 coulomb after hydrogen adsorption. However, K[SiO–GeO] has shown the "Bader charge" of -1.626 coulomb before hydrogen adsorption and -1.635 coulomb after hydrogen adsorption. However, K[SiO–GeO] has shown the "Bader charge" of -1.574 coulombs before and after hydrogen adsorption. The differences of charge density for these structures are measured as: $\Delta Q_{\text{Li}[SiO-GeO]} = -0.002$, $\Delta Q_{\text{Na}}[SiO–GeO] = -0.009$ and $\Delta Q_{\text{K}}[SiO–GeO] = -0.00$. Therefore, the results have shown that the cluster of Na[SiO–GeO] and Li[SiO–GeO] may have the most tensity for electron accepting owing to hydrogen grabbing.

3.2. TDOS analysis.

Squirming the molecular orbital data owing to Gaussian graphs of unit altitude and entire width at "half maximum (FWHM)" of 0.3 eV by "GaussSum 3.0.2" [31] have computed https://biointerfaceresearch.com/

total density of states (TDOS) diagrams. Regarding the adsorption behavior of hydrogen by Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanoclusters, TDOS has been measured. This parameter can indicate the existence of important chemical interactions often on the convex side (Figure 4a–c, a'-c').



Figure 4. TDOS graphs of (a) Li[SiO–GeO], (a') Li[SiO–GeO]–2H₂; (b) Na[SiO–GeO]; (b') Na[SiO–GeO]–2H₂; (c) K[SiO–GeO]; (c') K[SiO–GeO]–2H₂ nanoclusters.

During the formation of the Li[SiO–GeO] cluster, Figure 4a showed sharp and sophisticated peaks of around -0.3, -0.45, and -0.60 a.u. Due to the covalent bond between two atoms of Li with SiO–GeO cluster. Moreover, Li[SiO–GeO]–2H₂ has indicated a duplicate peak around -0.45 to -0.5 a.u. During hydrogen adsorption (Figure 4a'). After H-grabbing by Na[SiO–GeO] cluster, pointed peaks around -0.3, -0.45, and -0.60 a.u. Due to a covalent bond between two atoms of Na with a SiO–GeO cluster (Figure 4b). Furthermore, Na[SiO–GeO]–2H₂ has indicated a duplicate peak around -0.45 to -0.5 a.u. During hydrogen adsorption (Figure 4b'). However, the maximum energy of TDOS for K[SiO–GeO] (Figure4c) with several peaks around -0.35, -0.45, -0.6, and -0.75 a.u. with a maximum density of state of ≈ 23 around -0.35 a.u. has been shown. Moreover, similar amounts of TDOS for K[SiO–GeO]–2H₂ (Figure 4c') through some fluctuations in the behavior of the graphs have been observed.

3.3. ELF analysis.

A type of scalar field called electron localization function (ELF) may demonstrate a broad span of bonding samples. Nevertheless, the distinction between deduced/raised electron

delocalization/localization into cyclic π -conjugated sets stays encouraging for ELF [32]. The grosser the electron localization is in an area, the more likely the electron movement is restricted. Therefore, they might be discerned from the ones away if electrons are totally centralized. As Bader investigated, the zones with large electron localization possess extensive magnitudes of Fermi hole integration [33]. However, with a six-dimensional function for the Fermi hole, it seems hard to study directly. Then, Becke and Edgecombe remarked that spherically averaged spin conditional pair probability possesses a direct correlation with the Fermi hole and proposed the parameter of ELF in the Multiwfn program [34,35] and popularized for the spin-polarized procedure [36]:

$$ELF(\mathbf{r}) = \frac{1}{1 + [D(\mathbf{r})/D_0(\mathbf{r})]}$$
(1)
where
$$D(\mathbf{r}) = \frac{1}{2} \sum_i \eta_i |\nabla \varphi_i(\mathbf{r})|^2 - \frac{1}{8} \left[\frac{|\nabla \rho_\alpha(\mathbf{r})|^2}{\rho_\alpha(\mathbf{r})} + \frac{|\nabla \rho_\beta(\mathbf{r})|^2}{\rho_\beta(\mathbf{r})} \right]$$
(2)
and

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

For close-shell system, since $\rho_{\alpha} = \rho_{\beta} = (1/2)\rho$, *D*, and *D*₀ terms can be simplified as:

$$D(\mathbf{r}) = \frac{1}{2} \sum_{i} \eta_{i} |\nabla \varphi_{i}(\mathbf{r})|^{2} - \frac{1}{8} \frac{|\nabla \rho(\mathbf{r})|^{2}}{\rho(\mathbf{r})}$$
(4)
$$D_{0}(\mathbf{r}) = (3/10)(3\pi^{2})^{2/3} \rho(\mathbf{r})^{5/3}$$
(5)

Regarding kinetic energy, ELF was rechecked to be more punctual for both Kohn-Sham DFT and post-HF wavefunctions [37]. In fact, the excess kinetic energy density caused by Pauli repulsion was unfolded by D(r), and D₀(r) may be inspected as Thomas-Fermi kinetic energy density. Because D₀(r) is brought forward the ELF as the origin, what the ELF shows is an affiliate localization. Trapping of hydrogens by Li[SiO–GeO], Na[SiO–GeO] or K[SiO–GeO] nanoclusters towards formation of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂ or K[SiO–GeO]–2H₂ can be defined by ELF graphs owing to exploring their delocalization/localization characterizations of electrons and chemical bonds (Figure 5a–c, a'–c') [38–41].





Figure 5. The graphs of ELF for (a) Li[SiO–GeO]; (a') Li[SiO–GeO]–2H₂; (b) Na[SiO–GeO]; (b') Na[SiO–GeO]–2H₂; (c) K[SiO–GeO]; (c') K[SiO–GeO]–2H₂ nanoclusters. (Counter line map on the right and shaded surface map with projection on the left).

Table 2. LUMO, HOMO, energy gap (ΔE), Ring perimeter (Å), Total ring area (Å²) for Li[SiO–GeO], Na[SiO–GeO], K[SiO–GeO] through hydrogen grabbing and formation of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂, K[SiO–GeO]–2H₂ heteroclusters.

Heteroclusters	Еномо (eV)	Elumo (eV)	$\Delta E = E_{LUMO} - E_{HOMO}$ (eV)	Ring perimeter (Å)	Total ring area (Å ²)	
Li[SiO-GeO]	-6.0781	-5.1750	0.9031	9.3332	5.1566	
Na[SiO–GeO]	-5.7812	-5.2378	0.5434	9.9122	6.6754	
K[SiO–GeO]	-6.0005	-5.0738	0.9267	9.9122	6.6754	
Li[SiO-GeO]-2H ₂	-5.7793	-5.2402	0.5390	9.9121	6.6752	
Na[SiO-GeO]-2H ₂	-5.9990	-5.1021	0.8963	9.9121	6.6752	
K[SiO-GeO]-2H ₂	-5.9990	-5.0760	0.9230	9.9121	6.6752	

A vaster jointed area engaged by an isosurface map has shown the electron delocalization in Li[SiO–GeO] (Figure5a), Li[SiO–GeO] –2H₂ (Figure5a'), Na[SiO–GeO] (Figure5b), Na[SiO–GeO] –2H₂ (Figure5b'), K[SiO–GeO] (Figure5c), and K[SiO–GeO] –2H₂ (Figure5c') through labeling atoms of O12, Si13, O26, Ge28, X31(X=Li, Na or K) and H35. The counter map of ELF can confirm that Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] nanocluster may increase the efficiency during hydrogen adsorption towards the formation of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂, or K[SiO–GeO]–2H₂ nanocluster.

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 H₂ molecules and heteroclusters of Li[SiO–GeO], Na[SiO–GeO] or K[SiO–GeO]. The applied wavefunction level is CAM–B3LYP–D3/6–311+G (d, p), which corresponds to HOMO and LUMO, respectively (Table 2).

The amount of "Mayer bond order" [42] is generally according to empirical bond order for the single bond is near 1.0. "Mulliken bond order" [43], in small accord with empirical bond order, is not appropriate for quantifying bonding strength, for which Mayer bond order always performs better. However, the "Mulliken bond order" is a good qualitative indicator for the "positive amount" of bonding and the "negative amount" of antibonding, which are evacuated and localized (Table 3).

a i			Bond order						
Compound	Bond type	Mayer	Wiberg	Mulliken	Laplacian	Fuzzy			
	O12-Si13	0.4808	0.6182	0.1665	0.2221	0.9710			
L'10'0 C 01	O12-Li31	0.1394	0.2026	0.1313	0.2376	0.1312			
L1[S10-Ge0]	O26–Ge28	0.4768	0.5818	0.2292	0.2465	1.0523			
	O26-Li31	0.2166	0.2763	0.1890	0.1645	0.1805			
	O12-Si13	0.4901	0.6129	0.1856	0.1967	0.9749			
	O12-Na31	0.1016	0.1560	0.1078	0.1402	0.3085			
Na[SiO-GeO]	O26–Ge28	0.4635	0.5751	0.2348	0.2198	0.9938			
	O26-Na31	0.1618	0.2016	0.1549	0.1438	0.3832			
	O12-Si13	0.4989	0.611	0.1963	0.1849	0.9632			
	O12–K31	0.2375	0.1403	0.0730	0.1863	0.3697			
K[SiO-GeO]	O26–Ge28	0.4990	0.5784	0.2610	0.2038	0.9878			
	O26-K31	0.1057	0.1846	0.1444	0.1391	0.4507			
	O12-Si13	0.4766	0.6110	0.1564	0.2119	1.0140			
	O12–Li31	0.1439	0.2034	0.1390	0.1956	0.1328			
Li[SiO-GeO]-2H2	O26–Ge28	0.4616	0.5722	0.2138	0.2404	1.0421			
	O26-Li31	0.2138	0.2699	0.1910	0.2985	0.1772			
	Li31–H33	0.1028	0.1796	0.0984	0.0856	0.2085			
	O12-Si13	0.4857	0.6181	0.1818	0.2073	0.9791			
	O12-Na31	0.1064	0.1558	0.1114	0.1376	0.3042			
Na[SiO-GeO]-2H ₂	O26–Ge28	0.4723	0.5841	0.2399	0.2223	1.0033			
	O26-Na31	0.1723	0.2029	0.1656	0.1640	0.3820			
	Na31–H33	0.0749	0.1613	0.0705	0.0648	0.2048			
	012–Si13	0.4963	0.6107	0.1906	0.1848	0.9630			
	O12–K31	0.1684	0.1393	0.0673	0.1045	0.3683			
K[SiO-GeO]-2H2	026–Ge28	0.4970	0.5780	0.2578	0.2040	0.9875			
	O26-K31	0.1092	0.1821	0.1390	0.1024	0.4489			
	K31–H33	0.0557	0.1706	0.0538	0.0429	0.2042			

Table 3. The bond order of Mayer, Wiberg, Mulliken, Laplacian, and Fuzzy from mixed alpha and beta density matrix for Li[SiO–GeO], Na[SiO–GeO], K[SiO–GeO] through hydrogen grabbing and formation of Li[SiO–GeO]–2H₂, Na[SiO–GeO]–2H₂, K[SiO–GeO]–2H₂ heteroclusters.

As is seen in Table 3, "Laplacian bond order" [44] has a straight cohesion with bond polarity, bond dissociation energy, and bond vibrational frequency. The low value of the Laplacian bond order might demonstrate that it is insensitive to the calculation degree applied for producing electron density [45–51]. Generally, the value of the "Fuzzy bond order" is near the Mayer bond order, especially for low-polar bonds, but much more stable with respect to the change in the basis set. Computation of "Fuzzy bond order" demands running "Becke's DFT" numerical integration, owing to which the calculation value is larger than an assessment of "Mayer bond order," and it can concede more precisely [52].

4. Conclusions

In summary, H-grabbing by the nanoclusters of Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] was investigated by first-principles computations of the DFT method. The alterations of charge density illustrated a remarkable charge transfer towards Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO]. The fluctuation in charge density values demonstrates that the electronic densities were in the boundary of adsorbate/adsorbent atoms during the adsorption status. Besides, thermodynamic parameters describing H-grabbing by alkali metals-based nanoclusters of Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] have been investigated, including the internal process of the adsorbent–adsorbate system.

It is well established that adding Li, Na, or K to cell batteries may increase their energy storage. In this work, we explore the effect of Li, Na, or K on SiO–GeO heterocluster. Moreover, hydrogen bond (H-bond) accepting sites by Li[SiO–GeO], Na[SiO–GeO], or K[SiO–GeO] can alleviate parasitic hydrogen evolution in aqueous electrolytes in lithium, sodium, or potassium-ion batteries. Today, it is crucial to distinguish the potential of hydrogen technologies and bring up all perspectives of their performance, from technological progress to economic and social effects. The authors intend to pursue research on sustainability and clean energy subjects to find new solutions for reducing the global dependency on fossil fuels.

Author Contributions

Conceptualization, F.M.; methodology, F.M.; software, —; validation, —; formal analysis, F.M.; investigation, F.M.; data curation, F.M.; writing—original draft preparation, F.M.; writing—review and editing, F.M.; The author has read and agreed to the published version of the manuscript.

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Conflict of Interest

The author declares no conflict of interest. https://biointerfaceresearch.com/

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