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REGULAR ARTICLE

Study on structures and electron affinities of small potassium–silicon clusters Si_nK ($n = 2$–8) and their anions with Gaussian-3 theory

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Abstract The neutral Si_nK ($n = 2$–8) clusters and their anions have been systematically studied by means of the higher level of Gaussian-3 schemes. Equilibrium geometries and electron affinities have been calculated and are discussed for each considered size. For neutral Si_nK clusters, the ground state structure is found to be "attaching structure", in which the K atom is bound to Si_n clusters. The most stable isomer for their anions, however, is found to be "substitutional structures", which is derived from $Si_{(n+1)}$ by replacing the Si atom with a K. The dissociation energies of K atom from the lowest energy structures of Si_nK have also been estimated to examine relative stabilities.

Keywords Si_nK · Structures · Electron affinities · Dissociation energies · G3 theory

1 Introduction

Clusters of silicon and metal have received considerable attention in the past decade. Specially, alkali–silicon clusters possess scientific value because it has been known that they serve as promoters in catalysts, and can be used as power source material for spaceflight aero-crafts, emitters, and many other products [1–8]. Extensive experimental [9–13] and theoretical [14–22] studies on alkali metal–silicon clusters have recently been reported. For example, the electron affinities and ionization potentials of Si_nNa_m have been measured by means of photoelectron spectra [9–13]. Rabilloud et al. [14, 15] have performed investigation of structures and properties of neutral and positively charged $Si_nLi_p^+$ and $Si_nNa_p^+$ ($n \leq 6$, $p \leq 2$) clusters by means of B3LYP/6-31+G(d) method and concluded that the structures of the neutral (Si_nLi_p and Si_nNa_p) and their cations clusters keep the frame of the corresponding Si_n, Li, and Na species being adsorbed at the surface. We [7] have carried out G3 calculations for Si_nLi ($n = 2$–8) and their anions, and found that the ground state structures of neutral Si_nLi clusters are "attaching structure" and the most stable structures of Si_nLi^- anions are "substitutional structures".

The potassium–silicon clusters have been more sparsely studied than lithium– and sodium–silicon clusters. For neutrals of potassium–silicon clusters, the geometries, population analysis, and electric dipole moments of Si_nK_p ($n \leq 6$, $p \leq 2$) have only been reported by Rabilloud et al. [8, 16]. Compared with Si_nLi_p and Si_nNa_p, the most stable structures of Si_nA_p are found to be similar for A = Li, Na, and K [8, 16]. For anions of potassium–silicon clusters, Li et al. [21] have explored the ground state structures of Si_nK^- with $n \leq 10$. In this study, we have investigated the reliable electronic structures, electron affinities, and dissociation energies of small silicon–potassium clusters with the aim of understanding how their properties differ from those of bare silicon clusters. We found that the most stable isomer for negatively charged ion Si_nK^- is "substitutional structures". In addition, we found that the ground state

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structures of Si_nK^- with $n = 6, 7$, and 8 are different from those reported previously [21]. The ground state structures of Si_nK^- with $n = 6, 7$, and 8 presented in this paper are more stable than those reported previously [21].

2 Computational methods

All of calculations have been performed using the Gaussian-3 (G3) method [23, 24] and the Gaussian 03 package [25]. The G3 theory is a composite technique in which the geometry optimization is carried out at the MP2(full)/6-31G(d) level. The energy, a series of single-point energy calculation at the levels of QCISD(T)/6-31G(d), MP4/6-31G(d), MP4/6-31+G(d), MP4/6-31G(2*df*,*p*), and MP2(full)/G3large with the MP2(full)/6-31G(d) geometry is carried out. Then, this energy is modified by a series of corrections. Finally, the HF/6-31G(d) vibrational frequencies, scaled by 0.893, are applied for the zero-point vibrational energy (ZPVE) correction at 0 K. The combined G3 methods are the higher level of ab initio calculations of molecular energies of compounds containing first-, second-, and third-row atoms. The average absolute deviation from experiment for the electron affinities are only 0.99 kcal/mol for a set of 63 molecules [23, 24].

Two types of initial geometries for both neutral Si_nK ($n = 2$–8) and their anions are taken into account. One is the “substitutional structure”, which can be regarded as being derived from $Si_{(n+1)}$ by replacing a Si atom with a K atom. In addition, the other is the “attaching structure” in which the K atom is bound to Si_n geometry.[1] For the “attaching structure”, two types of structures are also taken into account. One is the bridge-site type and the other is the apex-site type, in which the potassium atom is bound to one of the silicon atoms. Nevertheless, the apex-site type is found to be either a saddle point or a local minimal point on the potential surface. An important fact is that the ground state structure of neutral Si_nK is “attaching structure” and the ground state structure of anion Si_nK^- is “substitutional structures”.

3 Result and discussion

The geometries optimized with MP2(full)/6-31G(d) level for Si_nK ($n = 2$–8) clusters and their anions are displayed in Fig. 1. Frequencies are calculated to verify that the structures are local minima on the potential energy surface and not transition states at MP2(full)/6-31G(d) level.

3.1 Si_2K and Si_2K^-

For neutral Si_2K, Rabilloud et al. [8, 16] have presented that its ground state structure is C_{2v} symmetry. Similarly to Si_2H [26], Si_2Li [6, 7], and Si_2Na [10, 22], neutral Si_2K has a $^2A_1$ ground state with a low-lying $^2B_1$ excited state. The latter state is only 0.05 eV higher in energy at the G3 level of theory. The bond distance of K–Si is predicted to be 3.325 Å at MP2(full)/6-31G(d) level, which is in excellent agreement with the value of 3.33 Å predicted by the B3LYP/6-31+G(d) scheme [8, 16].

For negatively charged ion Si_2K^-, the ground state structure displays C_{2v} symmetry with $^1A_1$ state. This result agrees with those reported by Li’s report [21]. The bond length of K–Si is predicted to be 3.118 Å at MP2(full)/6-31G(d) level, which agrees excellently with the value of 3.120 Å predicted by the MP2(full)/6-311+G(d) method. As can be seen from Fig. 1, the K–Si bond distance of anion Si_2K^- is shorter than that of neutral by 0.207 Å. The reason, similarly to Si_nNa system described by Kishi et al. [11], is that the additional electron going into the SOMO of the neutral Si_nK becomes doubly occupied in the anion, which localizes mainly on the Si_n framework. However, the electron back-donation from the Si_n framework to the K atom is induced and makes the bond between the Si_n and K atom strong.

3.2 Si_3K and Si_3K^-

The results of G3 calculation show that the geometries of the ground state structure of Si_3K display C_{2v} symmetry, which are the same as those reported by Rabilloud et al. [8, 16]. Similarly to Si_3H [27, 28], Si_3Li [6, 7], and Si_3Na [10], Si_3K has a $^2A_1$ ground state with a low-lying $^2B_2$ excited state. The latter state is only higher in energy by 0.16 eV at the G3 level. The K–Si bond lengths are calculated to be 3.209 and 3.240 Å for $^2A_1$ and $^2B_2$ electronic state, respectively. Rabilloud et al. [8, 16] presented a K–Si bond distances of 3.26 Å at B3LYP/6-31+G(d) level of theory.

For negatively charged ion Si_3K^-, the ground state structures possess C_{2v} symmetry with $^1A_1$ state. The K–Si bond lengths are calculated to be 3.162 Å, which are shorter than that of neutral with $^2A_1$ state by 0.047 Å. The reason is described earlier. At MP2(full)/6-311+G(d) level, the K–Si bond length of Si_3K^- is predicted to be 3.142 Å [21].

3.3 Si_4K and Si_4K^-

Three minima for Si_4K are shown in Fig. 1. Both Si_4K–I and Si_4K–II are “attaching structure” and display C_s

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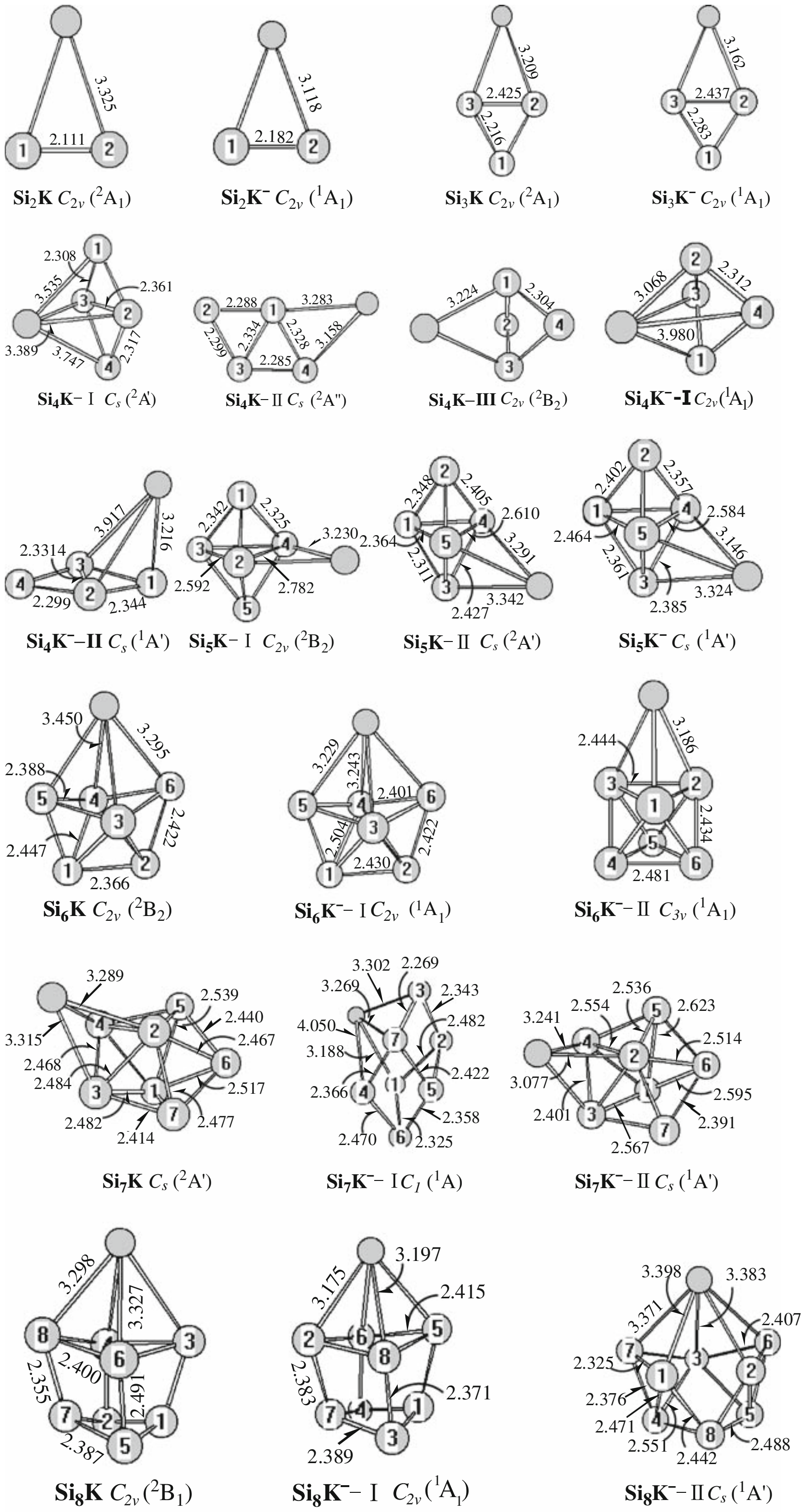
[1] The ground state structure are *isosceles triangle* for Si_3, *rhombus* for Si_4, *trigonal bipyramid* for Si_5, *tetragonal bipyramid* for Si_6, *pentagonal bipyramid* for Si_7, *distorted bicapped octahedron* for Si_8 and *bicapped pentagonal bipyramid* for Si_9. Also see Refs. [7, 30–32].



Si_2K C_{2v} ($^2A_1$) Si_2K^- C_{2v} ($^1A_1$) Si_3K C_{2v} ($^2A_1$) Si_3K^- C_{2v} ($^1A_1$)

Si_4K– I C_s ($^2A'$) Si_4K– II C_s ($^2A''$) Si_4K–III C_{2v} ($^2B_2$) Si_4K^--I C_{2v}($^1A_1$)

Si_4K^-–II C_s ($^1A'$) Si_5K– I C_{2v} ($^2B_2$) Si_5K– II C_s ($^2A'$) Si_5K^- C_s ($^1A'$)

Si_6K C_{2v} ($^2B_2$) Si_6K^-– I C_{2v} ($^1A_1$) Si_6K^-– II C_{3v} ($^1A_1$)

Si_7K C_s ($^2A'$) Si_7K^-– I C_1 (^1A) Si_7K^-– II C_s ($^1A'$)

Si_8K C_{2v} ($^2B_1$) Si_8K^-– I C_{2v} ($^1A_1$) Si_8K^-– II C_s ($^1A'$)

Fig. 1 The optimized geometries for neutral Si_nK ($n = 2$–8) and their anions in which only silicon atoms are numbered. The MP2(full)/6-31G(d) bond lengths are shown in Å

symmetry, whereas the former is $^2A'$ state, and the latter is $^2A''$ state. The $^2A''$ state is higher in energy than the $^2A'$ state by 0.13 eV at the G3 level. This result is different from those reported previously [8, 16]. We have also performed DFT calculations. At the B3LYP level with G3Large basis set [23, 24], the planar isomer of Si_4K-II is also higher in energy than that of the Si_4K-I structure by 0.06 eV. This case is different from Si_4Li. For Si_4Li, the planar isomer of the $^2A''$ state is slightly lower in energy than that of the $^2A'$ state at the B3LYP/G3Large level [7]. The ground state of Si_4A (A = Li, Na, K) is different from Si_4H. In fact, the H–Si bonds of ground state structures of Si_nH with the exception of Si_2H and Si_3H are stretched bounds [29]. However, the A–Si bonds for ground state geometries of Si_nA are bridged [6–16]. The C_{2v} symmetry of the $^2B_2$ Si_4K-III isomer is "substitutional structure". That is, it can be regarded as being derived from Si_5 by replacing a Si atom with a K atom. Energetically, it is higher in energy than the Si_4K-I by 0.47 eV. As can be seen from Fig. 1, the bond distances for the two equivalent K–Si bonds of Si_4K-I structure are predicted to be 3.389 Å at MP2(full)/6-31G(d) level.

For negatively charged ion Si_4K^-, two isomers are shown in Fig. 1. The Si_4K^--I, "substitutional structure", with C_{2v} symmetry and $^1A_1$ state is predicted to be the most stable. The Si_4K^--II displays C_s symmetry with $^1A'$ state and belongs to "attaching structure". That is, it can be regarded as being derived from Si_4 by attaching to a K atom. Energetically, it is higher in energy than the Si_4K^--I by 0.13 eV at the G3 level of theory. The geometries of Si_4K^--I are similar to that of structure predicted at MP2(full)/6-311+G(d) level of theory [21]. The shorter K–Si bond lengths for Si_4K^--I are calculated to be 3.068 Å.

3.4 Si_5K and Si_5K^-

Two minima for Si_5K are shown in Fig. 1. The Si_5K-I structure derived from Si_5 by edge capping with a K atom displays C_{2v} symmetry with $^2B_2$ state. The Si_5K-II isomer derived from Si_5 by face capping with a K atom displays C_s symmetry with $^2A'$ state. At B3LYP/6-31+G(d) level of theory, Rabilloud et al. reported that the Si_5K-II isomer was the ground state structure for Si_5K [8, 16]. However, the Si_5K-I structure is more stable than that of Si_5K-II isomer by 0.32 eV in energy at the G3 level of theory. The two equivalent K–Si bond lengths for Si_5K-I are calculated to be 3.230 Å.

For negatively charged ion Si_5K^-, the ground state structure is C_s symmetry with $^1A'$ state as can be seen from Fig. 1. This result is the same as the previous result predicted at MP2(full)/6-311+G(d) level of theory [21]. The geometry of ground state of Si_5K^- can be regarded as being derived from not only Si_5 by face capping with a K atom ("attaching structure") but also Si_6 by replacing a Si atom with a K atom ("substitutional structure"). The bond lengths of Si_5K^- are calculated to be 3.146 Å for the two equivalent K–Si bonds and 3.324 Å for K–Si3 bond. All of these K–Si bond lengths are shorter than those of corresponding neutral (Si_5K-II) by 0.145 and 0.018 Å, respectively. The reason is described earlier.

3.5 Si_6K and Si_6K^-

The geometry of the ground state of neutral Si_6K, "attaching structure", displays C_{2v} symmetry with $^2B_2$ state (see Fig. 1). This result agrees with the result predicted by B3LYP/6-31+G(d) scheme [8, 16]. The bond lengths are predicted to be 3.295 Å for the two equivalent $K-Si_5$ and $K-Si_6$ bonds and 3.450 Å for the another two equivalent $K-Si_3$ and $K-Si_4$ bonds, all of which are shorter than the B3LYP/6-31+G(d) K–Si bond lengths by 0.065 and 0.020 Å, respectively [8, 16].

For anion Si_6K^-, the lowest-energy structure, Si_6K^--I shown in Fig. 1, displays C_{2v} symmetry with $^1A_1$ state. This result is different from those reported previously [21]. Li et al. [21] presented that the ground state structure of Si_6K^- displayed C_{3v} symmetry as Si_6K^--II shown in Fig. 1. At the G3 level of theory, the Si_6K^--I structure is more stable than the Si_6K^--II by 0.07 eV in energy. In fact, the geometry of ground state of Si_6K^--I belongs to not only "attaching structure", but also "substitutional structure". As can be seen from Fig. 1, the K–Si bond distances of anion Si_6K^--I are again shorter than that of neutral Si_6K.

3.6 Si_7K and Si_7K^-

The geometry of the ground state of neutral Si_7K, "attaching structure", possesses C_s symmetry with $^2A'$ state (see Fig. 1). This result is different from the ground state structure of Si_7Li and Si_7Na [7, 10, 18], which are C_{2v} symmetry with $^2B_1$ state. For Si_7K, the geometry of C_{2v} symmetry with $^2B_1$ state is higher in energy than that of C_s symmetry with $^2A'$ state by 0.05 eV. The bond lengths of the ground state structure are predicted to be 3.315 Å for the two equivalent $K-Si_3$ and $K-Si_4$ bonds and 3.289 Å for $K-Si_2$ bonds.

Two minima for anion Si_7K^- are shown in Fig. 1. The Si_7K^--I is "substitutional structure" and displays C_1 symmetry. The Si_7K^--II is "attaching structure" and displays C_s symmetry with $^1A'$ state. Li et al. [21] presented that the ground state structure of Si_7K^- was Si_7K^--II isomer at MP2(full)/6-311+G* level. We also performed the MP2(full)/6-311+G* calculation. The results show that the Si_7K^--I structures are more stable than the Si_7K^--II isomers by 0.22 eV in energy at MP2(full)/6-311+G*. At the G3 level, both the Si_7K^--I and the Si_7K^--II isomers are nearly identical in energy (the Si_7K^--I structures are slightly lower than the Si_7K^--II isomers by −0.007 eV at the G3 level with ZPVE correction). Compared to the single-point energy at the levels of QCISD(T)/6-31G(d), MP4/6-31G(d), MP4/6-31+G(d), MP4/6-31G(2*df*,*p*), and MP2(full)/G3large with MP2(full)/6-31G(d) geometry, the results show that Si_7K^--I structures are more stable than the Si_7K^--II isomers by 0.12, 0.27, 0.33, 0.28, and 0.19 eV in energy, respectively. In this case, we assign the Si_7K^--I geometry to the ground state structure of anion Si_7K^-.

3.7 Si_8K and Si_8K^-

The geometry of the ground state of neutral Si_8K, “attaching structure”, has C_{2v} symmetry with $^2B_1$ state (shown in Fig. 1). The bond lengths are predicted to be 3.327 Å for the two equivalent K–Si_4 and K–Si_6 bonds, 3.298 Å for the equivalent K–Si_8 and K–Si_3 bonds.

For anion Si_8K^-, two isomers are shown in Fig. 1. The Si_8K^--I is not only “attaching structure”, but also “substitutional structure”, and displays C_{2v} symmetry with $^1A_1$ state. Compared with the neutral Si_8K, the K–Si bond distances of anion Si_8K^--I are again shorter by 0.130 and 0.123 Å, respectively. The Si_8K^--II isomer with C_s symmetry and $^1A'$ state is similar to the C_1 structure reported by Li et al. [21]. Energetically, the Si_8K^--II isomer is less stable than the Si_8K^--I structure by 0.74 eV in energy at the G3 level. At MP2(full)/6-311+G* level, the Si_8K^--II isomer is less stable than the Si_8K^--I structure by 0.63 eV.

It is interesting to note that the ground state structures of anion Si_nK^- can be regarded as being derived from $Si_{(n+1)}$ by replacing a Si atom with a K atom, that is, “substitutional structure”. Although the ground state structures of Si_nK^- ($n = 2, 3, 5, 6, 8$) can also be regarded as being derived from Si_n by attaching to a K atom, the ground state structures of Si_4K^- and Si_7K^- are conclusive evidence that the lowest-energy structures are “substitutional structures”. For neutral Si_nK, the most stable structure is “attaching structure” in which the K atom is bound to at least two silicon atoms. This result is the same as that of previous studies [8, 16].

3.8 Electron affinities

The adiabatic electron affinities (EA) (defined as the difference of total energies in the manner EA = E (optimized neutral) – E (optimized anion) of Si_nK clusters are calculated at the G3 level. The ZPVE corrected electron affinities of Si_nK are predicted to be 1.48 (1.48) eV for Si_2K, 1.49 (1.49) eV for Si_3K, 1.36 (1.36) eV for Si_4K, 2.19 (2.18) eV for Si_5K, 1.75 (1.76) eV for Si_6K, 1.62 (1.61) eV for Si_7K, and 2.69 (2.71) eV for Si_8K (presented in parentheses without ZPVE correction). Compared to Si_nLi and Si_n (see Fig. 2), it can be found that (1) the variation trend of the calculated EAs of Si_nK and Si_nLi clusters vary in parallel curves with local maxima around $n = 5$ and 8 and local minima at $n = 4$ and 7. As expected the EAs of Si_nK is always lower than that of Si_nLi cluster; and (2) the EA of Si_nK cluster is lower than that of the corresponding Si_n at the cluster size $n \leq 7$, whereas it is higher at $n \geq 8$. For Si_nLi clusters, the EA is lower than that of the corresponding Si_n at the cluster size $n \leq 4$, and it is higher at $n \geq 5$ [7]. The reason can be explained as follows. (1) When a alkali metal atom is adsorbed on Si_n clusters, the charge transfer from alkali metal atom to silicon clusters (in fact, alkali metal atom is positive charge and silicon cluster is negative charge in Si_nA) results in decrease of the electron affinities of Si_n cluster. However, with the increase of silicon cluster size, the average charge obtained by each silicon atom became less and less. That is, the effect of decrease of electron affinities becomes weak with the increase of silicon cluster size. (2) The change from closed-shell to open-shell (that is, the Si_n cluster is generally closed-shell and Si_nA cluster is open-shell) results in increase of the electron affinities. (3) The negative charge of Si_n clusters in Si_nK is more negative than that in Si_nLi because the ionization potential of lithium atom is larger than that of potassium (that is, the ability of capture electron for Si_nK is weaker than for Si_nLi). All of these lead to the results described above.

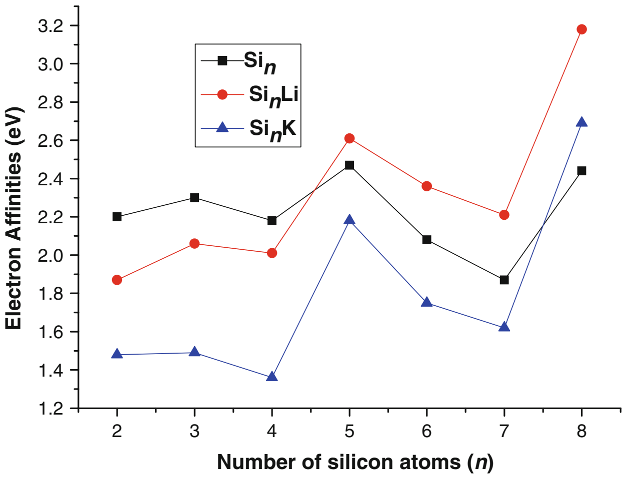


Fig. 2 The ZPVE corrected adiabatic electron affinities (EA) in eV for Si_n, Si_nLi, and Si_nK ($n = 2$–8) clusters versus the clusters size n. The EAs of Si_n and Si_nLi clusters are taken from Ref. [7]

3.9 Dissociation energies

The dissociation energy (D_e) (defined as the energy required in the reaction $Si_nK \rightarrow Si_n + K$) of Si_nK clusters are predicted with the G3 scheme to be 2.43 (2.45) eV for Si_2K, 2.20 (2.23) eV for Si_3K, 1.93 (1.94) eV for Si_4K, 2.27 (2.31) eV for Si_5K, 1.88 (1.91) eV for Si_6K, 1.36 (1.38) eV for Si_7K, and 2.09 (2.12) eV for Si_8K (presented in parentheses without ZPVE correction). From the D_e, the stability of bonding a K atom to silicon clusters can be found. The higher the values of these dissociation energies are, the more stable the clusters bonding of a K atom are. A better way of comparing the local relative stabilities of different size clusters is by means of the incremental

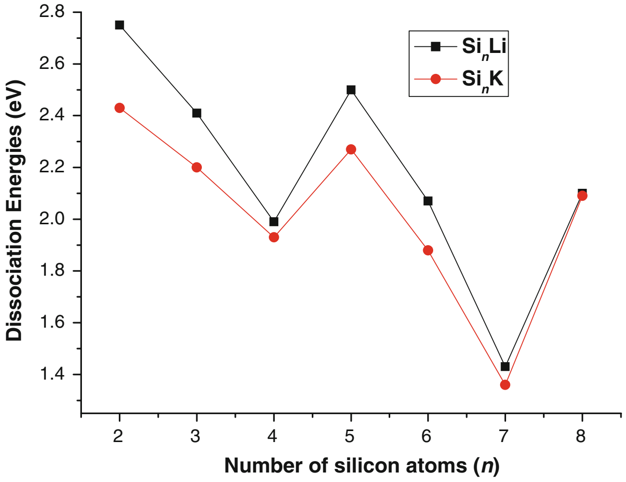


Fig. 3 The ZPVE corrected dissociation energies (D_e) in eV for Si$_n$Li and Si$_n$K ($n = 2$–8) clusters versus the clusters size n. The D_e of Si$_n$Li clusters are taken from Ref. [7]

binding energies [30]. The D_e of the Si$_n$K and Si$_n$Li [7] clusters as a function of the size of the clusters is shown in Fig. 3. As can be seen from Fig. 3, the two parallel oscillating curves, the top curve for Si$_n$Li and the lower curve for Si$_n$K, show that (1) the Si$_n$K (and Si$_n$Li) for $n = 4$ and 7 are less stable than for $n = 2$, 5, and 8 because the dissociation energies are local minima for $n = 4$ and 7 and local maxima for $n = 2$, 5, and 8. These also indicate that Si$_n$ for $n = 4$ and 7 are more stable and for $n = 2$, 5, and 8 are less stable. This result is consistent with previous result with respect to Si$_n$ [30–32]. And (2) as expected the dissociation energies of lithium atom are larger than that of potassium atom since the small size of Li atom results in a higher stability. That is, Li adsorption on surface of silicon clusters is more stable than K.

4 Conclusions

The equilibrium geometries and electronic structures of small Si$_n$K clusters ($n = 2$–8) and their anions have been systematically investigated by means of the higher level of the G3 scheme. Similarly, to Si$_n$Li, the ground-state structures of neutral Si$_n$K are predicted to be "attaching structure" in which the potassium atom is bound to Si$_n$ clusters. The ground-state structures of anion Si$_n$K$^-$, however, are "substitutional structures" which is derived from Si$_{(n+1)}$ by replacing a Si atom with a K$^-$. The adiabatic electron affinities of Si$_n$K have been calculated. The reliable adiabatic electron affinities are predicted to be 2.43 (2.45) eV for Si$_2$K, 2.20 (2.23) eV for Si$_3$K, 1.93 (1.94) eV for Si$_4$K, 2.27 (2.31) eV for Si$_5$K, 1.88 (1.91) eV for Si$_6$K, 1.36 (1.38) eV for Si$_7$K, and 2.09 (2.12) eV for Si$_8$K (presented in parentheses without ZPVE correction). The dissociation energies of K from the lowest energy structure of Si$_n$K clusters have been calculated and used to reveal relative stability. The dissociation energies are predicted to be 2.43 (2.45) eV for Si$_2$K, 2.20 (2.23) eV for Si$_3$K, 1.93 (1.94) eV for Si$_4$K, 2.27 (2.31) eV for Si$_5$K, 1.88 (1.91) eV for Si$_6$K, 1.36 (1.38) eV for Si$_7$K, and 2.09 (2.12) eV for Si$_8$K (presented in parentheses without ZPVE correction). As expected both the electron affinities and the dissociation energies of Si$_n$K are smaller than that of Si$_n$Li. To the best of our knowledge, there are no experimental data regarding the electron affinity and dissociation energy for Si$_n$K systems. Our results may thus provide a reference for further investigations.

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