First Principles Study on SiₙO (n=14-18) and Si₁₀⁻mOm (m=1-8)

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Abstract

Combining the full-potential linear–muffin–tin–orbital molecular-dynamics (FP-LMTO-MD) and the Amsterdam Density Functional (ADF) with TZ2P basis set in conjunction with self-consistent-field (SCF), we have studied the geometric features and stabilities of the SiₙO (n=14-18) clusters. The total binding energy Eₑ, gap of HOMO (highest-occupied molecular orbital)-LUMO (lowest-unoccupied molecular orbital) Eᵥ, dipole moment μ and total constant volume heat capacity Cᵥ(tot) were also calculated. The results show that the one dopant oxygen atom tends to occupy the edge or the surface position in the middle size silicon clusters (Siₙ, n=14-18). To further understanding the evolutionary tendency of the physical characteristics for the Si-O clusters with different composition, the Siₙ⁻mOm (m=1-8) clusters were also studied using the same methods. It was found that the structures of the Siₙ⁻mOm (m=1-8) clusters evolve from compact three dimensions to chain-like with increasing of the O proportion. The binding energy curve of Si₁₀⁻mOₘ clusters with different m shows a dip at m=6, which suggests that an optimal proportion of O and Si atoms may exist in the Si₁₀⁻mOₘ (m=1-8) clusters.

Keywords: Si-O clusters; Stable structure; Bonding energy

Introduction

Silicon and its oxides are important materials because of their wide application potential, such as light-emitting materia, [1-3] solar energy [4] and catalyst [5]. With the deeply understanding of the physical properties of the silicon oxide materials, more new application fields have been developed [6,7]. For example, the SiO₂-based resistive switching behavior provides a new use for traditional SiO₂ materials [8]. In addition, the Si-O compounds are found to be very abundant in most dusty media in space, and thus important in astrophysical processes such as star and planet formation [9]. All these (potential) applications are closely related to the structures of these compounds, therefore a systematical study would be of great importance.

In recent years, the oxide silicon was investigated in both experiment [1,4,5,10-13] and theory [10-21] for its broad prospect in the application. Desjardin and co-workers [1] studied oxidation of Si (111)-(7×7) surface by STM. They found that the low coverage O₂ molecules absorbed on the surface could form more stable structures at room temperature. Very recently, Kinahan et al. [4] revealed the quantitative relationship between the coverage of site-specific oxygen and a decrease of the Si (111)-(7×7) surface stress in tensile by the same method. Wang et al. [5] studied the SiO₂ clusters using anion photoelectron spectroscopy and ab initio calculation. They presented that the SiO₂ may be a model structure for oxygen defect sites in bulk SiO₂.

On the other hand, the features of the Si-O clusters are the key points in the study of the Si-O systems. Kinds of Si-O clusters such as SimOn (m, n=1-8)[10,11], SimOn (n=3-5) [12], Si₃O₅ (m=1-5, n=1, 2m+1)[14], Si₅O₊ (n=3)[17], Si₆O₇ (n=1-12)[19], Si₇O₉ (n=1-14) [20] and Si₈O₉ (1≤n≤6) [21] were studied by first principle calculations. Many new possible structures of these clusters were drawn and numerous unfamiliar features of them were investigated. Based on the quantum-mechanical calculations, Zhang et al. [10] studied the O-ratio-dependent features of the SiₙOₘ (m,n=1-8) clusters. They found that energetically the most favorable small Si-O clusters have O atomic ratios at about 0.6. James [12] found that the structure of the ground state Si₃O₅ cluster is planar and the lowest energy structures of Si₅O₇ and Si₆O₉ are non-planar rings. Lu and coworkers [17] obtained the results that the binding energies of SiₙOₘ (m=1-5, n=1, 2m+1) clusters increase with the number of oxygen atoms, and the dissociation energies of these clusters are strong relative to the O and Si atoms ratio in one cluster. In addition, some researches focused on the (SiOₙ)ₙ, nanoclusters [15,16,18]. A number of ringed, tube-like, cage shape, columnar and disk-like nanostructures based on SiO₂ unit were illustrated in detail.

We studied oxygen molecule and one O atom adsorption on Siₙ (n=1-13) clusters by the FP-LMTO-MD method [22-25] and ADF program [26] and the lowest energy structures for these clusters were given [13,27]. The calculated results show that there is a potential barrier of dissociative chemisorption of O₂ when the Si clusters have more than four atoms. Moreover, it is found that the edge or the surface of the host Si clusters is the favorable adsorption sites for one O atom.

In this work, we investigated one oxygen atom adsorption on the middle size silicon clusters (Siₙ, n=14-18) and the Si₁₀⁻mOm (m=1-8) clusters using combination of the FP-LMTO-MD and ADF program. Our main purpose is to find the lowest energy structures of these clusters, and to explore the geometry and physical properties in the evolutionary procedure of the Si-O clusters with various compositions. Some new the lowest energy structures for these Si-O clusters were found. The total binding energy for Si₁₀⁻mOₘ (m=1-8) clusters decrease, and then increase with the increasing of the ratio of Si:O.

Methods

The initial structures of the SiₙO (n=14-18) clusters are constructed through an oxygen atom being absorbed on the positions of the lowest energy silicon clusters [28] which are given by previous studies.

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Received February 26, 2014; Accepted May 05, 2014; Published May 14, 2014

Citation: Y. H. Zhu, B.X. Li (2014) First Principles Study on SiₙO (n=14-18) and Si₁₀⁻mOm (m=1-8) Clusters. J Theor Comput Sci 1: 113. doi: 10.4172/jtco.1000113

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Geometrical optimization algorithm is performed on the initial structures without any symmetry constraints by the FP-LMTO-MD method. For the Si$_{10-m}$O$_{m}$ (m=1-8) clusters, a huge number of initial atomic conformations are randomly sampled within a real three-dimensional box, or cage, or ball structure. Moreover, several chain-like initial structures of the Si$_{10-m}$O$_{m}$ (m=1-8) clusters are also prepared.

After that, we choose the three lowest energy structures of each Si-O clusters in two types as candidates and re-optimize these selected structures by using the ADF program [26] version (2007.01) with TZ2P [29] basis set in conjunction with self-consistent-field (SCF). The TZ2P basis using in ADF is an all-electron basis with triple-zeta quality for valence region. The frozen-core approximation for the inner-core electrons is used. The orbitals up to 2p for silicon and 1s for oxygen are kept frozen. An accessional STOs (Slater Type Orbitals) basis set including s, p, d, f, and g-type is used to fit the molecular density and hence to present the Coulomb and exchange potentials more accurate. The combined self-consistent-field (SCF) is converged to a value of 10$^{-6}$. For both two types’ clusters, the frequencies of them are kept frozen. An accessional STOs (Slater Type Orbitals) basis set in conjunction with self-consistent-field (SCF). The structures by using the ADF program [26] version (2007.01) with TZ2P basis using in ADF is an all-electron basis with triple-zeta quality.

The three lowest energy structures for the Si$_{n}$O (n=14-18) clusters are both C$_{2}$, while for third one is C$_{3}$. The most stable structure for neutral Si$_{n}$O (n=14-18) cluster are listed in Table 1, which represents the neutral, cationic and anionic clusters respectively. The letters 0 and the sign +, - in parentheses indicate that the labeled structures are the neutral, cationic and anionic clusters, respectively. The number 0, a, b, c have C$_{1}$, Cs, and C$_{3}$ symmetries. The energy difference between them is only 0.01eV. Our calculated result shows that the largest energy difference between the adsorption structures with the same host Si structure can be up to 0.8 eV.

For the Si$_{15}$O cluster, their isomers are formed by an O atom being adsorbed to different sites of the ground state Si$_{15}$ cluster [6,28]. The Si$_{15}$O(O) structure with Cs symmetry lies 0.23eV energetically below the Si$_{15}$O(0) structure. Both of the structures Si$_{15}$O(0)b and the Si$_{15}$O(0)c have C$_{3}$ symmetries. The energy difference between them is only 0.01eV. Our calculated result shows that the largest energy difference between the adsorption structures with the same host Si structure can be up to 0.8 eV.

For Si$_{14}$O isomers, the symmetries of the lowest two binding energy Si$_{14}$O clusters are both C$_{2}$, while for third one is C$_{3}$. The most and second stable structures of them are formed by the second lowest energy structure of pure Si$_{14}$ cluster [28] absorbing an impurity oxygen atom at the different edge sites for a Si triangular pyramid unit. While, for the third stable Si$_{14}$O cluster, the O atom connects three Si atoms to form a triangular pyramid and lays on the apex site of the pyramid, as shown in Figure 1. The similar absorbed sites of O atom also can be found in other Si$_{n}$O (n=14-18) clusters (shown in the Figure 1 and 2).

Results and Discussions

Existing imaginary frequencies indicate that the given molecular structure is unstable. Our calculated results show that there are no imaginary frequencies in the energy minima structures for both two types’ Si-O clusters. It suggests that our obtained the lowest energy structures are stable.

Si$_{n}$O (n=14-18) clusters

The three lowest energy structures for the Si$_{n}$O (n=14-18) clusters are shown in Figure 1. The number 0 and the sign +, - in parentheses represent the neutral, cationic and anionic clusters respectively. The three isomers are labeled as a, b and c in order of decreasing stability. For example, (0,-) a indicates that the labeled structures are the most stable structure for neutral and anionic clusters. The calculated results for each neutral Si$_{n}$O (n=14-18) cluster are listed in Table 1, which include the total binding energy (E$_{tot}$, in eV), electron affinity (EA, in eV), ionization potential (IP, in eV), the gap of HOMO-LUMO (E$_{g}$, in eV), dipole moment (μ, in Debye), and total constant volume heat capacity (C$_{v,tot}$, in cal/mol·K).

For the Si$_{15}$O cluster, their isomers are formed by an O atom being adsorbed to different sites of the ground state Si$_{15}$ cluster [6,28]. The Si$_{15}$O(0)a structure with Cs symmetry lies 0.23eV energetically below the Si$_{15}$O(0)b structure. Both of the structures Si$_{15}$O(0)b and the Si$_{15}$O(0)c have C$_{3}$ symmetries. The energy difference between them is only 0.01eV. Our calculated result shows that the largest energy difference between the adsorption structures with the same host Si structure can be up to 0.8 eV.

For Si$_{14}$O isomers, the symmetries of the lowest two binding energy Si$_{14}$O clusters are both C$_{2}$, while for third one is C$_{3}$. The most and second stable structures of them are formed by the second lowest energy structure of pure Si$_{14}$ cluster [28] absorbing an impurity oxygen atom at the different edge sites for a Si triangular pyramid unit. While, for the third stable Si$_{14}$O cluster, the O atom connects three Si atoms to form a triangular pyramid and lays on the apex site of the pyramid, as shown in Figure 1. The similar absorbed sites of O atom also can be found in other Si$_{n}$O (n=14-18) clusters (shown in the Figure 1 and 2). The energy of the cluster Si$_{14}$O (0)a is about 0.73eV and 0.84eV more stable than Si$_{15}$O(0)b and Si$_{15}$O(0)c , respectively.

The three lowest binding energy structures of Si$_{15}$O cluster are C$_{2}$ symmetries. Comparison of the structures for the Si$_{15}$ [6, 28] and Si$_{16}$O...
cluster shows that the impure O atom will result in the compact pure cluster becoming loose. The distortion arising from the O atom doping is more significant for Si16O clusters than for other Si nO (n=14,15,17 and 18) clusters.

For the Si16O clusters shown in the Figure 1 are C₃ symmetric, which are formed by one O atom being absorbed to the lowest and the second stable structures is only 0.01 eV. For the third stable structure E₄ the absorbed O atom reduces the difference to less than 0.07 eV. Hence, the three structures of Si16O clusters can be regarded degenerate energetically.

Our calculated results reveal that the impurity oxygen atom is favorable to adsorb on the edge or surface site of the middle-size silicon clusters, the same phenomena also has been found in small-size SiO (n=1-13) clusters [27]. The Si atom with 3s²3p² electronic configurations, trends to through sp³ hybridization forming covalent bonds with other atoms. Meanwhile, the 2s²2p² O atom has lone electron pair of p orbital besides two p single electrons and probably forms two or three bonds with neighboring atoms in the mixed clusters. This is the main reason why the doped oxygen atom usually occupy the surface or edge site to form three or two bonds in the SiO clusters (the analyses in details see our previous study [13,27]).

For the adsorption structures with edge-capping O atom, O atom bridges two Si atoms by two bonds, in which the lengths are from 1.64 to 1.79 Å. The bond angles of the Si-O-Si are from 90.5 to 116.1 degree. For the surface adsorption, the O-Si bond lengths are around 1.83 Å and slightly longer than bonds in the edge-adsorption’s case. Compared with the Si (n=14-18) clusters [6,28], the structures of the SiO clusters become loose. We think the main reason is that the parts of charges transfer from the surrounding Si atoms to doped O atom and the covalent bonds are formed between them.

The calculated results indicate that the neutral and ionic clusters show similar geometrical configurations and different stability orders. It is found from observing the positions of all atoms for a given SiO cluster that the differences of coordinates for the ionic and neutral clusters are less than 0.2 Å. Such small difference is hardly to distinguish from the structural figures. So we use the same structure to describe the ionic and neutral cluster with similar motif. As shown in the Figure 1, the three lowest binding energy ionic and neutral Si16O clusters have same energetic orders. While, when n>14, the energetic orders of ionic and of neutral Si16O clusters are different. The energy gaps between HOMO and LUMO (Egs) of ionic and of neutral Si16O clusters are also different. For example, for example, for the three Si16O isomers at the lowest energy state, the Egs of the neutral clusters are 1.21 eV, 1.27 eV, and 1.08 eV, while 0.23 eV, 0.36 eV and 0.39 eV for cationic isomers and 0.44 eV, 0.31 eV and 0.32 eV for anionic ones, respectively. We speculate that the electronic redistributions due to add or reduce one electron may contribute to the energy order and Egs changes.

We have also investigated the magnetism properties of the neutral and ionic Si8O (n=14-18) clusters. It is found that the neutral clusters with even number of electrons have no magnetic moment because all the electrons are paired together in their respective molecular orbitals, whereas all the ionic clusters with odd number of electrons have the total magnetic moment of 1.0 μₜ, which is trivial, due to one unpaired electron. In addition, Mulliken population analyses imply that about 0.62 e to 0.66 e charge transfer from the silicon atoms to the oxygen atom.

### Table 1: The total binding energy (Eₐ, in eV), electron affinity (EA, in eV), ionization potential (IP, in eV), the gap of HOMO-LUMO (E₄, in eV), dipole moment (µ, in Debye), and total constant volume heat capacity (Cᵥ(tot), in cal/mol K), for the three lowest energy structures of SiₙO (n=14-18) clusters.

<table>
<thead>
<tr>
<th>Structure</th>
<th>Eₐ (eV)</th>
<th>EA (eV)</th>
<th>IP (eV)</th>
<th>E₄ (eV)</th>
<th>µ (Debye)</th>
<th>Cᵥ(tot) (cal/mol K)</th>
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<td>Si14oa</td>
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<td>2.61</td>
<td>6.76</td>
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<td>1.85</td>
<td>2.37</td>
<td>76.92</td>
</tr>
<tr>
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<td>7.11</td>
<td>1.56</td>
<td>0.42</td>
<td>76.51</td>
</tr>
<tr>
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<td>0.84</td>
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<tr>
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<td>0.92</td>
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and one $\text{Si}_2\text{O}_2$ rhombus buckled-chain structure. The computation of frequencies shows that the structure $\text{Si}_2\text{O}_4$ is stable because no imaginary frequencies exist. We also calculated the $\text{Si}_2\text{O}_6$ clusters. The structures are unstable, therefore, the dissociated $\text{SiO}_9$ cluster does not be listed.

The $\text{Si}_2\text{O}_6$ cluster is the most stable in all the $\text{Si}_{10-m}\text{O}_m$ ($m=1-8$) clusters. The chain-like $\text{Si}_2\text{O}_6$ cluster with $D_2$ symmetry is formed by three $\text{Si}_2\text{O}_2$-rhombuses sharing with two Si atoms. The lengths of Si-O bonds in the cluster are different. The lengths of Si-O bonds connecting the two ends Si atoms are 1.73 Å, which are longer than the other –bonds’ lengths (about 1.68 Å). Mulliken population analyses imply that the some charge transfer from silicon atoms to oxygen atoms. For neutral $\text{Si}_{10-m}\text{O}_m$ cluster, the dipole moment is zero due to symmetrical structure.

Figure 3 plots the total binding energies $E_{\text{tot}} (\text{Si}_{10-m}\text{O}_m)$ versus the number of oxygen atoms. As opposed to the linear curve of the nitrogen atom and aluminum atom doped to Si clusters [31,32], the curve for the Si-O mixed cluster shows a valley. With the number O atom increasing, the $E_{\text{tot}} (\text{Si}_{10-m}\text{O}_m)$ decreases linearly when $1\leq m \leq 6$, and then goes up when $m > 6$. This is to say that the lowest binding energy structure for $\text{Si}_{10-m}\text{O}_m$ cluster with the ratio of 0.6 for O component, which is similar to the findings by Zhang’s in the $\text{Si}_{10-n}\text{O}_n$ ($m,n=1-8$) clusters [14]. On the one hand, comparing the $\text{Si}_{10-m}\text{O}_m$ clusters, there is a tendency that the structures of the $\text{Si}_{10-m}\text{O}_m$ clusters evolve from compact three dimensions to chain-like with increasing of the proportions for O components. On the other hand, the symmetries of these clusters increase with O when $m=6$. Therefore, the energetic valley may suggest that the stability of the mixed Si-O clusters depends on the cooperation of the composition and structural properties.

The second different energy $\Delta^2 E$ (eV) is a sensitive quantity to reflect the stability of clusters. It is defined as $\Delta^2 E (\text{Si}_{10-m}\text{O}_m) = E_{\text{tot}} (\text{Si}_{10-(m-1)}\text{O}_{m-1}) + E_{\text{tot}} (\text{Si}_{10-(m+1)}\text{O}_{m+1}) - 2 E_{\text{tot}} (\text{Si}_{10-m}\text{O}_m)$. The $\Delta^2 E$ have the largest value at $m=6$, also indicates that the $\text{Si}_4\text{O}_6$ cluster is more stable than their neighboring clusters (Figure 4). In addition, the $\Delta^2 E$ also displays an even/odd alternating pattern as a function of cluster size. The clusters with even oxygen atoms present higher stability.

The energy gaps $E_g$ between the highest-occupied molecular orbital (HOMO) and the lowest-unoccupied molecular orbital (LUMO) are showed in Figure 5. The highest peak occurs again at the $\text{Si}_4\text{O}_6$ cluster. The energy gaps also display a certain even/odd alternating pattern as a function of cluster size. All the evidences mentioned above suggest that the ratio 4:6 is the optimal proportion for the stability of the $\text{Si}_{10-m}\text{O}_m$ ($m=1-8$) clusters. Chu et al. found that when O ratio reaches to about 60% in a small Si-O clusters, the energy gaps of the clusters present the biggest value [11]. Such result is a convincing evidence to support our conclusion.
Furthermore, it is found that the rhombus Si\textsubscript{2}O\textsubscript{2} unit is a basic structure of ground Si-O clusters \cite{5,11,33,34}. Two rhombus Si\textsubscript{2}O\textsubscript{2} units will buckle with each other by sharing a central Si atom to form a stable chain-like configuration. Such structural patterns are usually found in ground state Si-O clusters \cite{5,11,13,19,20}. In other word, to form the stable buckled rhombus Si-O chain, for each added Si atom needs two O atoms more. This may be the reason why the Si-O clusters with even oxygen atoms possess lower binding energy.

The heat capacities of the clusters are computed based on the ideal gas approximation omitting the electronic contribution. The heat capacity \( C_V \) is related to the number of degrees of freedom (DoF) of the cluster system. In ideal gas model, the nonlinear cluster with \( n \) atoms

**Figure 4:** The second different energies of the Si\textsubscript{10-m}O\textsubscript{m} (m=1-8) clusters \( \Delta_2 E \) (eV) versus the atom number of O atom m.

**Figure 5:** The energy gaps \( E_{gs} \) (eV) between the highest-occupied molecular orbital (HOMO) and the lowest-unoccupied molecular orbital (LUMO) of Si\textsubscript{10-m}O\textsubscript{m} (m=1-8) clusters.
The Si\textsubscript{n}O\textsubscript{(n=14-18)} and Si\textsubscript{10-m}O\textsubscript{m}(m=1-8) clusters are investigated systematically by using the FP-LMTO-MD and the ADF with TZ2P basis set in conjunction with SCF. The calculated results suggest that the edge and surface adsorption structures are the favorable structures for the middle size silicon clusters doped an oxygen atom. For Si\textsubscript{10-m}O\textsubscript{m} (m=1-8) clusters, their structures evolve from compact three dimensions to chain-like with increasing of the proportion of O. The Si\textsubscript{10}O\textsubscript{3} cluster has the lowest bonding energy and the largest ΔE. It suggests that the conclusion which the small silicon-oxygen clusters have the optimal ratio of 0.6 for O component [14] is still correct in the Si\textsubscript{10-m}O\textsubscript{m} (m=1-8) clusters. Whether the bigger Si-O clusters still have such optimal O ratio needs further study.

Acknowledgment

The Natural Science Foundation of Zhejiang Province (Grant No. Y6100098) the Science Foundation of Zhejiang Province Department of Education (Grant No. Y201003280) and the Science Foundation of Hangzhou Normal University (Grant No. 2010QN03) supported this work.

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