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STUDY THE STABLE STRUCTURES OF $ScGe_6$ BY GA-DFT AND THE CO ADSORPTION ON $ScGe_6^-$ CLUSTER

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Abstract. The structures of $ScGe_6$ and $ScGe_6^-$ clusters were investigated by a combination of genetic algorithm with quantum chemical calculations (GA-DFT and DLPNO-CCSD(T)). Results show that the two most stable isomers of the $ScGe_6$ cluster have a pentagonal bipyramid structure with a Sc atom at the vertex and a Ge atom capping the face of tetragonal bipyramid with a Sc atom at the vertex with C_s symmetry. The pentagonal bipyramid with the scandium atom at the vertex with C_{5v} symmetry is the most stable $ScGe_6^-$ cluster. The CO adsorption on the most stable isomer of the anionic cluster was studied by PBE functional. The isomer A1 of $ScGe_6^-$ cluster can adsorb CO molecule as well. The most stable structure has CO along with the Sc-Ge bond. In two adsorption models at the Sc atom along the main axis, the Sc-CO adsorption model is more favorable than the Sc-OC model.

Keywords: $ScGe_6^{0/-}$ cluster, genetic algorithm, DFT, DLPNO-CCSD(T), CO adsorption

1. INTRODUCTION

Germanium clusters have been interested in widely application abilities in electronic, adsorption, catalyst, pharmacy field [1-4]. Clearly, germanium was used to produce LED, solar cell, lithium-ion battery with faster charge-discharge ability, stably through a large number of the cycle [3]. In addition, germanium can be used in pharmacy because of its non-toxic and high bio-compatibility [2]. The optic property, electronic property, stability of materials depends on their size [4, 5]. The small cluster can be a structural unit to build nanomaterials, bulky materials. Therefore, it is necessary to study the structure of small clusters to design new material which has high applications. The structures of germanium, scandium were studied as Ge_n (n=1-20) [6], Ge_n (n=2-6) [7, 8], Ge_n (n=2-13) [9], Ge_n (n=2-25) [10], Ge_n (n=3-7) [8], Ge_{27}^- [11], $Ge_{3\text{-}4}$ [12], $Ge_n^{0/+}$ (n= 8,9,10,11, 12,13,15,16) [13], $Sc_{2\text{-}3}$ [14], Sc_n^+ (n=2-13) [15], Sc_n^- (n=2-13) [16], Sc_n and Sc_nO (n=2-13) [17], $ScGe_n^-$ (n = 6-20) [18, 19]. These results indicated that the stability and property of transition metal-doped germanium are higher than pure germanium clusters [5, 20-23]. Because the 3*d* orbitals have near degeneration in energy, transition metal-doped germanium clusters can build many structures that have the same stability [6, 9, 18, 24].

In modern society, environmental pollutions have been interested. CO which is formed in burning fuels is one of the toxic pollutants. Many studies have been performed to find out the ways to remove CO. Scandium, germanium clusters are the good materials to adsorb CO. [16, 25-27] Three isomers of $ScGe_6^-$ cluster include isomer A, isomer B, isomer C [18]. The structure of isomer A is a pentagonal bipyramid with the scandium atom at one of the vertices. The structure of isomer B is two perpendicular rhomboid units that connect via a scandium atom. Isomer C‘s structure is also a pentagonal bipyramid with a scandium atom in its base. [18] The structure of the $ScGe_6$ cluster is still not reported.

To search for the global minimum structure, the genetic algorithm combines quantum chemistry calculation is one of useful methods. GA-DFT can find the global structure with high exact [28]. The density functional theory can optimize the structure cluster cheap and fast. The coupled-cluster CCSD(T) is the gold standard in quantum chemistry calculation. The CCSD(T) calculations require a strong computer with large memory and a long time to calculate. So, the CCSD(T) can be used for small size clusters. The DLPNO-CCSD(T) method in ORCA code can be used for larger size clusters than in CCSD(T) because of approximations. The DLPNO-CCSD(T) calculation can calculate 99% of the correlation energy of the CCSD(T) calculation. [29-31]

In this study, we use GA-DFT to search the stable structures of the $ScGe_6$ cluster. The anionic clusters' structures are optimized from neutral clusters' structures. Besides, we also build some local structures which were obtained from different references to compare [18]. Many stable structures of $ScGe_6^{0/-}$ clusters have been reported. The CO adsorption by anionic cluster $ScGe_6^-$ is studied on the most stable isomer to find the stable structures of CO adsorption.

2. CALCULATION METHODS

The structures of neutral cluster $ScGe_6$ were investigated by GA-DFT combined with the genetic algorithm and density functional theory [28-32]. The parameters of genetic algorithm were set up as 20 randomly initial structures, 15 structures in the next generations include 40% structures were kept from the previous generation, 20% mutation structures, 20% crossing structures, and 20% new random structures. A maximum generation of 10 was chosen. The stop condition of the process is 5 generations which have the energy error is not passed 0.01 eV or maximum generation have been done. GA process was performed by USPEX 10.3 code [33-35]. The energies of these processes were calculated by the pwscf code of the Quantum Espresso 6.0 package [36]. Besides, some local minimum structures were built from other references.

All obtained structures were reoptimized by PBE functional [37]. To save calculation time, the geometrical structure was optimized by a small basis set def2-SVP. Then, re-optimization was done by larger basis set def2-TZVPP. The relative energy and frequency values of optimized structures were obtained. The relative energies were calculated as the different between the energy of every cluster and the minimum energy of energy values of isomers. All position frequencies of clusters indicate that this structure is at the minimize position on the potential surface. The get better correlation energy, the DLPNO-CCSD(T) method [38, 39] was chosen to perform the single-point calculation for optimized geometry of cluster. The aug-cc-pVTZ basis set was used in DLPNO-CCSD(T) calculations. The DFT and DLPNO-CCSD(T) calculations were performed by ORCA 4.2.1 code [40].

The CO adsorption processes were studied by PBE functional. The initial structures of adsorption were created by putting CO up many different positions around the surface of the $ScGe_6^-$ cluster. First, the optimization was performed not to constrain point group symmetry. Then, the near symmetry was chosen. The def2-TZVPP basis set is used for all elements. The frequency values of adsorption structures were also calculated to confirm the obtained structure at the minimize position on the potential surface.

3. RESULTS AND DISCUSSION

3.1. Structure, relative stability of $ScGe_6$ clusters

The geometrical structures, symmetry point group, relative energies (RE) of 10 isomers were presented in **Figure 1** and **Table 1**. These isomers' structures of the $ScGe_6$ cluster are still not searched in the other references. As following results of relative energies by DLPNO-CCSD(T), the N1 isomer whose structure has C_s symmetry is the most stable isomer. The other isomers as N2, N3, N4, N5, N6, N7, N8, N9, N10 is less stable than N1 by 0.05, 0.16, 0.20, 0.24, 0.55, 0.66, 0.68, 0.78, 1.21 eV eV. As initial prediction by 3d orbital, many structures have the equivalent energy. The N2 isomer is near generated about energy with N1 isomer by 0.05 eV of relative energy. Three isomers N3, N4, N5 have equivalent stability. The relative energies of three isomers are respectively 0.16, 0.20, 0.24 eV from the DLPNO-CCSD(T) calculations. Four isomers of N6, N7, N8, N9 are small differences in energy.

The order of stability of N1, N2, N3, N4, N5 isomers by PBE functional are different from DLPNO-CCSD(T) calculation. The values of relative energies of these five clusters at PBE functional are N3 (0.00 eV) < N1 (0.02 eV) < N2 (0.07 eV) < N5 (0.23 eV) < N4 (0.28 eV). This difference can be explained by the different calculation abilities of correlation energy by different calculation methods [41]. The DLPNO-CCSD(T) can calculate about 99% of correlation energy than the gold standard CCSD(T) [30, 31]. Therefore, correlation energy plays important role to compare the stability of isomers, especially with transition metal-doped clusters because of energy degeneration.

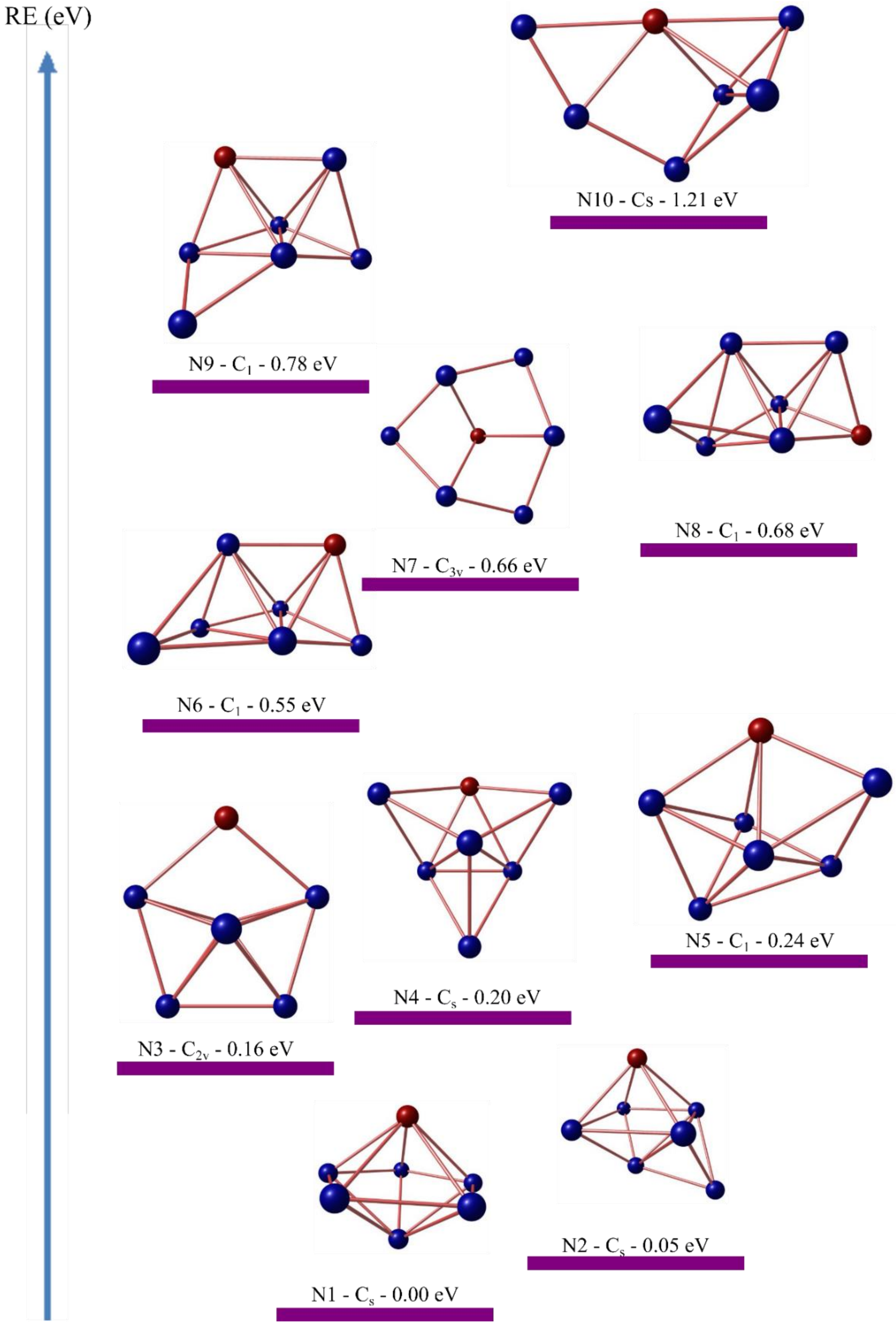
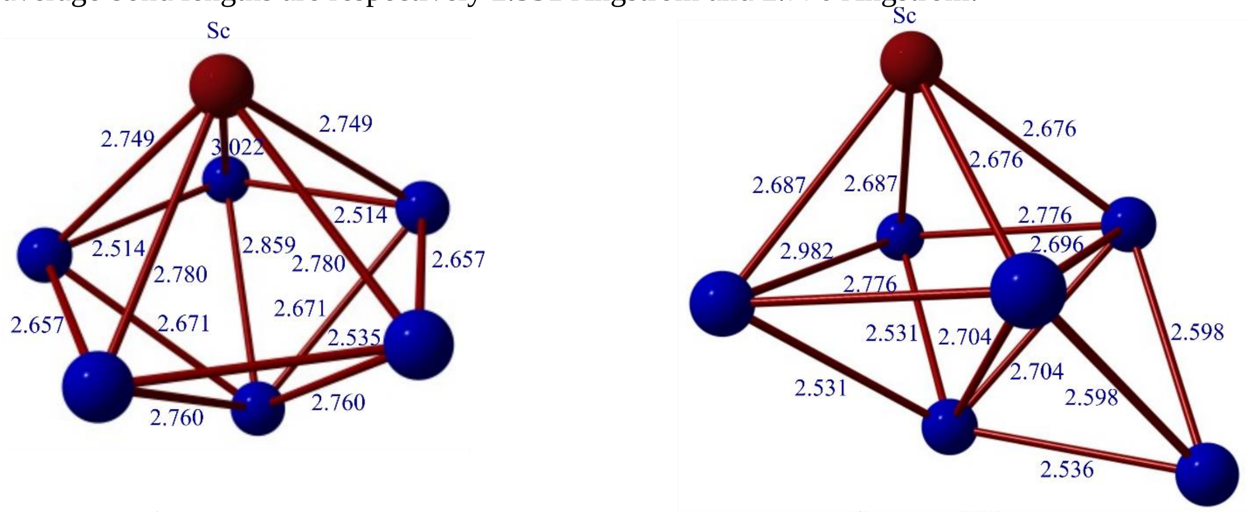


Figure 1. The geometrical, symmetry point group, relative energies of isomers of $ScGe_6$ cluster

Table 1. Symmetry point group, relative energies of isomers of $ScGe_6$ cluster by PBE functional and DLPNO-CCSD(T) method

Isomers	Symmetry	Relative energies (RE)	
		PBE	DLPNO-CCSD(T)
N1	C_s	0.02	0.00
N2	C_s	0.07	0.05
N3	C_s	0.00	0.16
N4	C_s	0.28	0.20
N5	C_1	0.23	0.24
N6	C_1	0.48	0.55
N7	C_{3v}	0.49	0.66
N8	C_1	0.51	0.68
N9	C_1	0.68	0.78
N10	C_s	1.08	1.21

The geometrical structures, bond lengths of two isomers of N1 and N2 of $ScGe_6$ cluster were displayed in **Figure 2**. Isomer N1 has a pentagonal bipyramid structure with a Sc atom at the vertex. Point group symmetry of N1 is C_s symmetry. The bond lengths of the Sc atom to the Ge atom on the base are from 2.749 Angstrom to 3.021 Angstrom. The bond lengths of Ge – Ge in isomer N1 structure are from 2.513 Angstrom of Ge-Ge bond on the base to 2.859 Angstrom of bond from a Ge atom on the base to a Ge atom at the vertex. Isomer N2 has a face-capped tetragonal bipyramidal structure with Cs symmetry. The bond lengths of Sc-Ge are from 2.676 Angstrom to 2.687 Angstrom. The shortest and largest Ge-Ge average bond lengths are respectively 2.531 Angstrom and 2.776 Angstrom.



isomer N1 isomer N2

Figure 2. The bond lengths of two stable isomers of $ScGe_6$ clusters

3.2. Structure, relative stability of $ScGe_6^-$ clusters

The geometrical structures, symmetry point group, relative energies of 8 isomers of anionic cluster $ScGe_6^-$ are presented in **Figure 3** and **Table 2**. The order stability of isomers of $ScGe_6^-$ cluster is good fitness between two methods of PBE functional and DLPNO-CCSD(T) calculations. Isomer A1 is the most stable isomer of the $ScGe_6^-$ cluster. This result is the same as the previous report [18]. The other isomers are less stable 0.77 eV (PBE) and 0.86 eV (DLPNO-CCSD(T)) than A1 isomer. Two isomers of A2 and A3 have equivalent stability with the near degeneration in energy of the 0.77 eV and 0.79 eV at PBE calculations and 0.86 eV and 0.88 eV at DLPNO-CCSD(T) calculations.

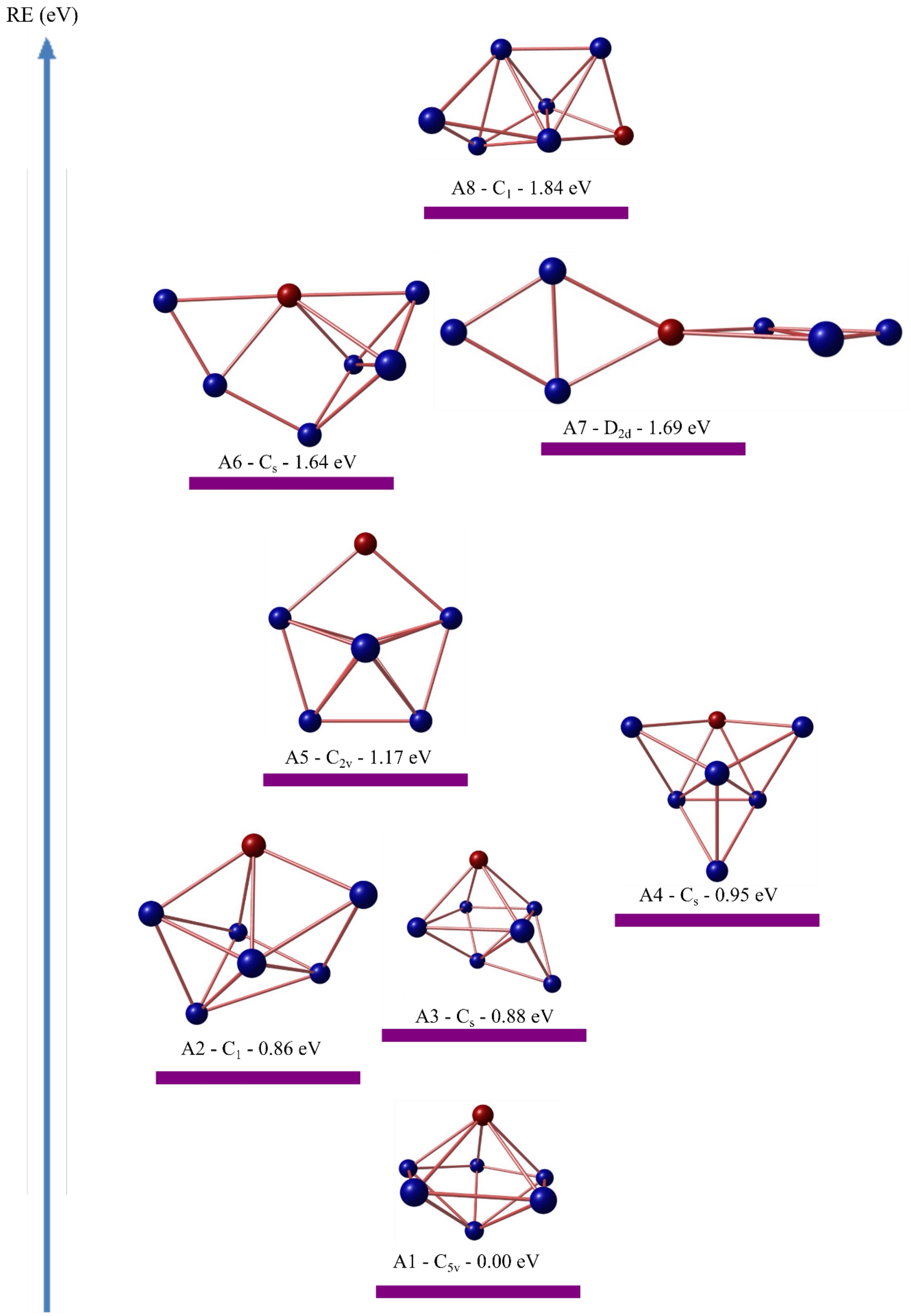


Figure 3. The geometrical structure, symmetry point group, relative energies of isomers of anionic cluster $ScGe_6^-$

Table 2. Symmetry point group, relative energies of isomers of $ScGe_6^-$ cluster by PBE functional and DLPNO-CCSD(T) method

Isomer	Symmetry	Relative energies (eV)	
		PBE	DLPNO-CCSD(T)
A1	C_{5v}	0.00	0.00
A2	C_1	0.77	0.86
A3	C_s	0.79	0.88
A4	C_s	0.89	0.95
A5	C_{2v}	1.32	1.17
A6	C_s	1.45	1.64
A7	D_{2d}	1.56	1.69
A8	C_1	1.54	1.84

The relative of A4, A5, A6, A7, A8 isomers are higher than the A1 isomer by 0.95, 1.17, 1.64, 1.69, 1.84 eV respectively at DLPNO-CCSD(T). These obtained values of relative energies by PBE functional are from 0.89 eV to 1.54 eV. In the previous report, three structures of the $ScGe_6^-$ cluster are respectively A, B, and C structures [18]. In this report, they are A1, A5 and A7, respectively. Besides, A2, A3, A4 isomers are more stable than A5 isomer. Two isomers of A6 and A8 are equivalent to A7 isomer.

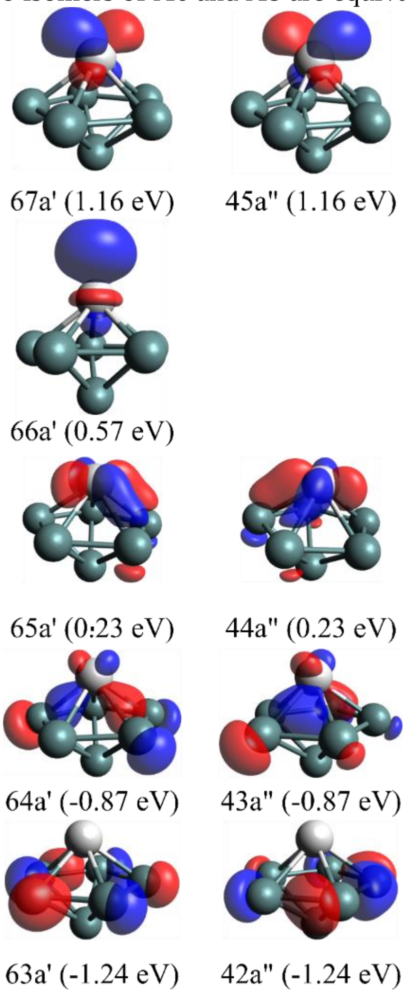
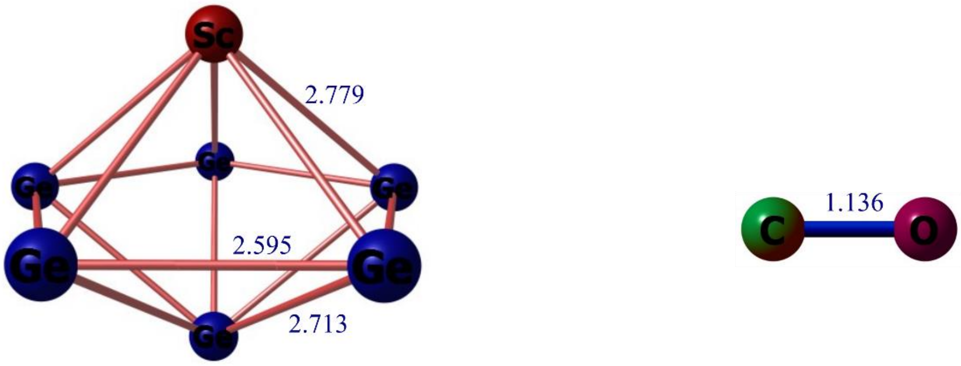

67a' (1.16 eV) 45a" (1.16 eV)
66a' (0.57 eV)
65a' (0:23 eV) 44a" (0.23 eV)
64a' (-0.87 eV) 43a" (-0.87 eV)
63a' (-1.24 eV) 42a" (-1.24 eV)

Figure 4. The molecular orbitals of $^1A'$ state of A1 isomer of $ScGe_6^-$ cluster obtained by PBE functional, def2-TZVPP basis set (with Sc atom at above of pyramid*)*

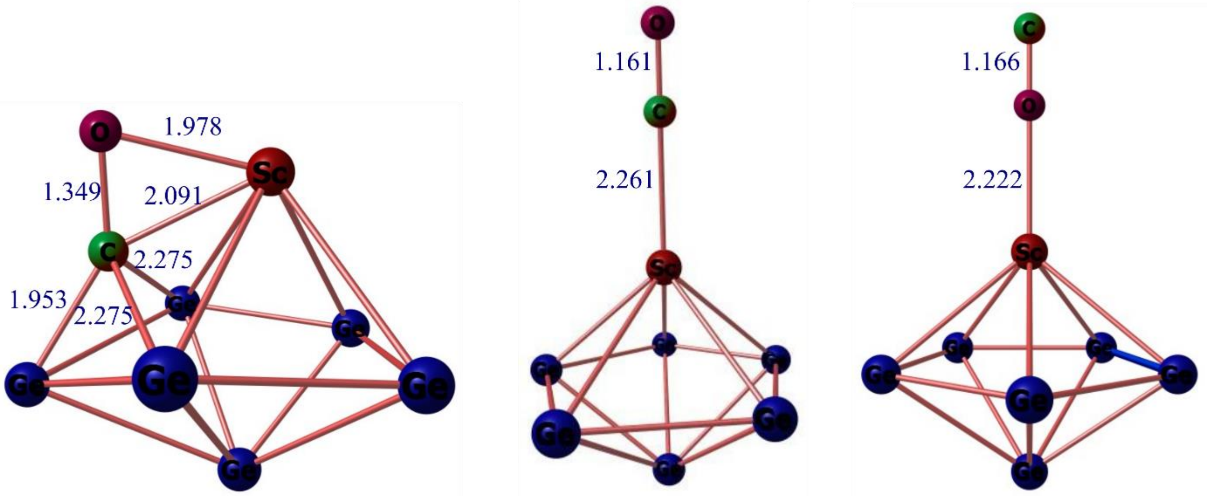
The most stable A1 isomer of $ScGe_6^-$ cluster has a C_{5v} symmetry point group. Because C_{5v} is not an Abelian point group, so the calculations were reduced to the C_s point group. The figure and energy values of molecular orbitals of ^{1}A' state of A1 isomer of ScGe$_6^-$ cluster as in Figure 4. The electronic structure of ^{1}A' state of A1 isomer of ScGe$_6^-$ cluster is $63a'^2 42a''^2 64a'^2 43a''^2 44a''^0 65a'^0 66a'^0$. The bond length of Sc-Ge bonds and Ge-Ge bonds which are optimized at PBE functional and def2-TZVPP basis set is displayed in Figure 5a. The bond lengths of Sc to Ge in the base, Ge-Ge in the base, Ge in the base to Ge at the bipyramid vertex are respectively 2.779, 2.595, 2.713 Angstrom. By B3LYP functional, these bond lengths are respectively 2.79, 2.6, 2.75 Angstrom [18]. The bond lengths of Sc to Ge in the base, Ge-Ge in the base, Ge in the base to Ge at the bipyramid vertex are respectively 2.779, 2.595, 2.713 Angstrom. By B3LYP functional, these bond lengths are respectively 2.79, 2.6, 2.75 Angstrom [18].

3.3 The CO adsorption of ScGe$_6^-$ cluster

The structure of the CO molecule was optimized at PBE functional, def2-TZVPP basic set as in Figure 5b. The bond length harmonic vibrational frequency of C-O is 1.136 Angstrom. This result is the same as the result of Feng, R., et al. [27]. The CO adsorption processes were performed by optimizing the random structure of the CO molecule on the surface of ScGe$_6^-$ cluster does not constrain symmetry. Then, the symmetry calculations were done to determine the point group symmetry of geometrical structures. The frequency values were also calculated to confirm the obtained structure at the minimum position on the potential surface. Three models and relative energies of CO adsorption on the A1 isomer of ScGe$_6^-$ cluster were displayed in **Figure 5c** and **Table 3**.



a) A1 isomer of ScGe$_6^-$ cluster b) CO



A - C_s - 0.00 eV **B** - C_s - 0.19 eV **C** - C_s - 0.72 eV

c) CO adsorption on A1 isomer of ScGe$_6^-$ cluster

Figure 5. The structures of A1 isomer of ScGe$_6^-$ cluster a), CO molecule b) CO adsorption by ScGe$_6^-$ cluster obtained by PBE functional, def2-TZVPP basis set

The A structure which is the most stable structure has the C_s symmetry point group. In this structure, the CO molecule was adsorbed at beside bond Sc-Ge. The B structure and C structure are also both at C_s point group symmetry with CO molecule at pyramid containing Sc. The B and C structures are less stable 0.19 eV and 0.72 eV, respectively. The model of Sc-CO is stable than the Sc-OC model as the relative energies at PBE functional, def2-TZVPP basis set. The Sc-CO model is the same as the CO adsorption on Sc_n (n=2-13) [17]. The A structure which is the most stable structure can be explained by the ability in creating many interactions between CO molecule with the Sc, Ge atoms on $ScGe_6^-$ cluster. In A structure, C of CO interacts with Sc and 3 Ge atoms; O of CO interacts with Sc. Because of multi-interactions, the C-O bond length on A structure is 1.35 Angstrom, which is longer than the C-O bond length in the CO molecule. The adsorption energy of A is 1.08 eV. In B or C structure, only one interacts between CO molecule and $ScGe_6^-$ cluster. The C-O bond length in B structure, C structure, and CO molecule is equivalent.

Table 3. Relative energies, C-O bond lengths, energies of adsorption processes by anion cluster

Structure	Relative energies (eV)	C-O bond length (Angstrom)	Adsorption energy (eV)
CO molecule		1.136	
A	0.00	1.349	1.08
B	0.19	1.161	0.89
C	0.72	1.171	0.36

4. CONCLUSION

The structures of the $ScGe_6$ cluster was investigated by GA-DFT calculations. Their relative energies of stable isomers of $ScGe_6$ cluster and $ScGe_6^-$ cluster were reported at PBE/def2-TZVPP level and DLPNO-CCSD(T)/aug-cc-pVTZ level. The most stable structures of $ScGe_6$ and $ScGe_6^-$ are the pentagonal bipyramid with the Sc atom at the vertex. The symmetry point group of the most stable neutral cluster and anionic cluster are respectively C_s and C_{5v}. Many isomers are near degenerate in energy. The stability of N2 is less stable than N1 by 0.05 eV. The isomer A1 of the $ScGe_6^-$ cluster can adsorb CO molecule as well. The most stable structure has CO along with the Sc-Ge bond. In two adsorption models at the Sc atom along the main axis, the Sc-CO adsorption model is more favorable than the Sc-OC model in adsorption energy.

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NGHIÊN CỨU CÁC CẤU TRÚC BỀN CỦA CÁC CLUSTER $ScGe_6$ BẰNG PHƯƠNG PHÁP GA-DFT VÀ SỰ HẤP PHỤ CO TRÊN CLUSTER $ScGe_6^-$

Tóm tắt. Cấu trúc của cluster $ScGe_6$ và $ScGe_6^-$ được nghiên cứu cứu bằng giải thuật di truyền kết hợp các phép tính hóa học lượng tử (GA-DFT và DLPNO-CCSD(T)). Kết quả cho thấy hai đồng phân bền nhất của cluster $ScGe_6$ có dạng lượng tháp ngũ giác với nguyên tử Sc ở đỉnh và cluster dạng lưỡng tháp tứ giác với Sc ở đỉnh với một nguyên tử Ge che ở mặt. Cấu trúc của hai đồng phân bền nhất của cluster trung hòa $ScGe_6$ có đối xứng C_s. Cluster $ScGe_6^-$ có cấu trúc lưỡng tháp ngũ giác với nguyên tử Sc ở đỉnh thuộc nhóm điểm đối xứng C_{5v}. Các cấu trúc hấp phụ CO của cluster $ScGe_6^-$ được nghiên cứu. Sự hấp phụ CO trên đồng phân bền nhất của cluster $ScGe_6^-$ được thực hiện với phiếm hàm PBE. Cấu trúc hấp phụ bền nhất có CO ở dọc theo cạnh liên kết Sc-Ge. Trong hai cấu trúc hấp phụ dọc theo trục chính tại nguyên tử Sc, kiểu hấp phụ Sc-CO bền hơn kiểu hấp phụ Sc-OC.

Từ khóa: cluster $ScGe_6^{0/-}$, giải thuật di truyền, DFT, DLPNO-CCSD(T), sự hấp phụ CO

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