Si$_n$C$_{13-n}$ ($n = 1 – 12$) Clusters: An All-electron DFT Investigation

Xingyu ZHOU[1], **Zhiqiang DING**[1], **Hao Zhang**[1], **Jin GUO**[1,2], **Hua NING**[1,2]*, **Ying LIU**[3]

[1] *Guangxi Key Laboratory of Processing for Non-ferrous Metallic and Featured Materials, College of Physics Science and Technology, Guangxi University, Nanning 530004, P.R. China*
[2] *Guangxi Collaborative Innovation Center of Structure and Property for New Energy and Materials, School of Material Science and Engineering, Guilin University of Electronic Technology, Guilin, 541004, P.R. China*
[3] *Department of Physics, Hebei Normal University, Shijiazhuang 050016, Hebei, China*

The geometrical and electronic structures of Si$_n$C$_{13-n}$ ($n = 1 – 12$) nanoclusters have been investigated using all-electron density functional theory (DFT) with the generalized gradient approximation (GGA). The binding energies, highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) gaps, and the vibrational frequencies have been computed. We note that the binary clusters have a number of isomeric structures with lower symmetries and the stability of the clusters increases as the number of carbon atoms increases. As the number of silicon atoms increases, the lowest-energy structures of the Si$_n$C$_{13-n}$ ($n = 1 – 12$) clusters transform from planar structures to three-dimensional structures. The HOMO-LUMO gaps of the lowest-energy structures indicate that with the exception of Si$_6$C$_7$ and Si$_{12}$C, the ground states are of high chemical stability and have the characteristics of semiconductors. In addition, the Mülliken populations show that there is significant charge transfer from the silicon atoms to the carbon atoms.
Keywords: SiC, clusters, ground state, stability.

1. INTRODUCTION

The structures and properties of mixed silicon-carbon clusters have been the subject of great scientific interest both theoretically and experimentally over the past decades. Although carbon and silicon are in the same column (Group IV) of the periodic table of elements, their chemical and bonding properties are rather different. Carbon exhibits huge flexibility by forming either single or multiple bonds, resulting in a variety of cluster geometries [1 – 3]; silicon prefers single bonds and generates compact three-dimensional (3D) structures. The study of mixed silicon-carbon clusters is therefore of interest not only for producing new materials for the nanoelectronics industry, but also for understanding the nature of these clusters from a fundamental perspective.

In the past two decades, a series of mixed silicon-carbon clusters has been studied [4 – 8]. By using the local density approximation (LDA) method and time-dependent density functional theory (DFT), the electronic and geometrical structures of small Si$_n$C$_m$ ($m + n \leq 5$) clusters were calculated [9, 10]. Next, the geometries, electronic states and energies of medium size Si$_n$C$_{m-n}$ ($2 \leq n \leq 6$; $m = 3 – 16$) and Si$_{n-1}$C, Si$_{n-2}$C$_2$ ($n = 3 – 8$) were predicted at B3LYP/6-311g* and MP2/6-311G(d) levels [11 – 13]. Following, the structures and stabilities of various isomers of (SiC)$_{12}$ cluster were systematically computed using the DFT at the level of BLYP [14]. Furthermore, the infrared radiation (IR) spectra calculated for their typical low-energy structures of (SiC)$_{12}$ cluster were presented. Subsequently, Li et al reported the carbon-rich structures of C$_9$Si$_n$ ($n = 1 – 5$) clusters using the DFT B3LYP/6-

311++G(2df) method [15]. They noted that the C atoms were found to form linear (n = 2), or single-ring (n = 1, 3) or double-rings (n = 4, 5) while the Si atoms preferred to attach to the carbon rings in the form of C$_2$Si units. Recently, the evolution of electronic structures, charge redistributions and structural properties of Si$_n$C$_m$ ($n + m = 10$) clusters were studied by using the DFT [16]. Nazrulla et al suggested that carbon atoms were the electron rich centres, while silicon atoms were electron deficient in every alloy cluster. For larger sizes of mixed Si-C clusters, Zhu et al [17] investigated the growth patterns and electronic property of Si$_{12}$C$_{12}$ cluster-assembled materials. In addition, by using the DFT and the coupled-cluster theory, some Si$_n$C$_m$ ($m, n \leq 12$) clusters ranging in size from SiC$_3$ to Si$_{12}$C$_{12}$ were predicted [18]. Most recently, silicon impacts on structure, stability and aromaticity of C$_{20-n}$Si$_n$ heterofullerenes ($n = 1 – 10$) were studied in a density functional perspective [19]. However, the studies of the Si-rich or C-rich mixed silicon-carbon clusters are still far from complete.

In the present article, we make a detailed study of the stability and structural properties of Si$_n$C$_{13-n}$ ($n = 1 – 12$) nanoclusters by using all-electron DFT. The rest of this article is arranged as follows. Section 2 presents the computational methods. In section 3, we discuss the optimized structures and electronic structures of Si$_n$C$_{13-n}$ ($n = 1 – 12$) clusters. A brief summary of our results is given in section 4.

2. COMPUTATIONAL METHODS

In the calculations, the electronic exchange-correlation energy was treated under the generalized gradient approximation (GGA) with the corrected-exchange potential of the Becker exchange functional and the Lee-

---

* Corresponding author. Tel.: +86-771-3237386.
E-mail address: *ninghua@gxu.edu.cn* (H. Ning)

Yang-Parr correlation functional (BLYP) [20, 21]. A double-numerical-polarized (DNP) basis set with unconstrained spin was chosen to carry out the electronic structure calculation. The convergence criteria of the optimization were 2×10^{-3} eV/Å and 5×10^{-3} Å for the energy gradient and atomic displacement, respectively. The charge density was required to converge to 1×10^{-6} e/Å^3, corresponding to a total energy convergence of 1×10^{-5} eV. All calculations were performed using the DMol^3 package [22, 23].

For the Si_nC_{13-n} $(n = 1 - 12)$ clusters, the initial structures were taken from pure Si_{13} clusters with some of silicon atoms replaced by carbon atoms [24]. A number of linear and annular structures and correlative structures reported in Ref. [12, 25] were also considered. Firstly, we performed symmetry-constrained geometry optimization to search for the low-lying metastable isomers among the abundant initial structures. Next, the lower-energy configurations were identified by continuing the optimization without any symmetry restrictions. Finally, frequency analyses were performed at the same theoretical level of approximation to check whether the optimum structures found are transition states or true minima on the potential energy surfaces of the corresponding cluster systems.

3. STRUCTURES AND DISCUSSION

For Si_nC_{13-n} $(n = 1 - 12)$ clusters, a great number of low-energy isomers with very little difference in structure are found. Geometric sketch figures of the ground states and metastable states are shown in Fig. 1. In the equilibrium geometries of the Si_nC_{13-n} $(n = 1 - 4)$ clusters, silicon atoms prefer to bond at one or both end(s) of a carbon chain or ring. The lowest-energy structures of Si_nC_{13-n} $(n = 5 - 10)$ clusters show that carbon atoms prefer forming kernels at the centre of configuration. In the case of $Si_{11}C_2$ and $Si_{12}C$, however, the carbon atoms are located at surface sites.

In Fig. 1, SiC_{12}(a) is a linear structure with the lowest binding energy being -79.109 eV. The metastable structure SiC_{12}(b) with C_{2v} symmetry is a ring, and its energy is 0.264 eV higher than that of SiC_{12}(a). For the Si_2C_{11} cluster, the most stable structure is Si_2C_{11}(a) with $D_{\infty h}$ symmetry in which the silicon atoms bond at the two ends of a carbon chain. This result is in good agreement with that of Ref. [12]. The energy of Si_2C_{11}(b), with C_{2v} symmetry, is 1.107 eV higher than that of Si_2C_{11}(a), and the carbon atoms favour forming a ring. For the Si_3C_{10} cluster, the planar structure, Si_3C_{10}(a) with C_s(I) symmetry, is the ground state, silicon atoms bond at the two ends. With all silicon atoms bonding at one end, the energies of Si_3C_{10}(b) and Si_3C_{10}(c) are 1.045 eV, 1.539 eV higher than that of Si_3C_{10}(a), respectively.

It can be noted that almost all the lowest-energy configurations of the Si_nC_{13-n} $(n = 4 - 12)$ clusters are 3D structures. We only list three 3D lowest-energy structures for each Si_nC_{13-n} $(n = 4 - 12)$ cluster.

The planar and linear structures are not list in Fig. 1 due to the fact that the structures have much higher energies than the 3D structures. For the Si_4C_9 cluster, the lowest energy structure is Si_4C_9(a) with C_s(I) symmetry,
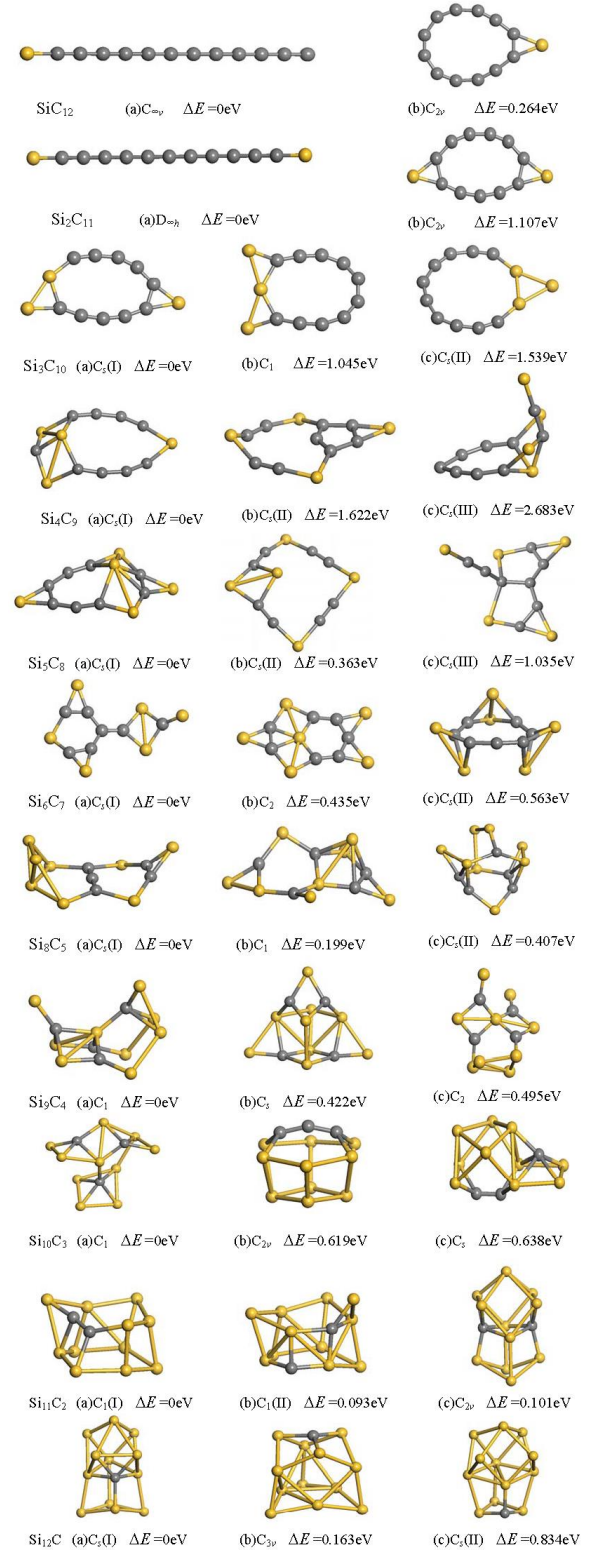
silicon atoms prefer to bond at the two ends.

Fig. 1. The lower-lying structures and corresponding symmetries of Si_nC_{13-n} $(n = 1 - 12)$ clusters are shown. Black balls and grey balls refer to carbon atoms and silicon atoms, respectively. The energy ΔE is calculated with respect to the energy of the most stable isomer

Si_4C_9(b) lies more than 1.0 eV above Si_4C_9(a) in energy. Another 3D structure, Si_4C_9(c) is 1.061 eV higher in energy than is Si_4C_9(b).

For the Si_5C_8 cluster, carbon atoms prefer forming

kernels at the structural centre. The ground state of $Si_5C_8(a)$ has a $C_s(I)$ geometry with a ring of carbon atoms. $Si_5C_8(b)$ lies 0.363 eV above $Si_5C_8(a)$ in energy. We note that there are two rings in $Si_5C_8(b)$: One is made of a cycle of repeating Si-C-C-Si structures, the other one is a cycle made of Si-C pairings. The energy of $Si_5C_8(c)$ is 1.035 eV higher than that of $Si_5C_8(a)$. Next, for the Si_6C_7 cluster, $Si_6C_7(a)$ is the lowest-energy structure. The planar structure $Si_6C_7(b)$ with C_2 symmetry is 0.435 eV higher than $Si_6C_7(a)$ in energy. The other $C_s(II)$ structure, $Si_6C_7(c)$, lies 0.563 eV above $Si_6C_7(a)$ in energy.

There exist a number of isomers as stable structures in the case of six carbon atoms. For the Si_7C_6 cluster, $Si_7C_6(a)$ in Fig. 1 has the lowest energy. $Si_7C_6(b)$ with C_{2v} symmetry is 0.743 eV less stable than $Si_7C_6(a)$. The third stable isomer $Si_7C_6(c)$ is a C_{3v} structure with a binding energy of -57.328 eV, which is 1.274 eV higher than $Si_7C_6(a)$. Subsequently, $Si_8C_5(a)$ with $C_s(I)$ symmetry is the most stable structure with three carbon atoms bonded at the center of the structure. Another stable structure $Si_8C_5(b)$ is 0.199 eV higher than $Si_8C_5(a)$ in energy. The structure $Si_8C_5(c)$ with $C_s(II)$ symmetry is 0.407 eV less stable than $Si_8C_5(a)$.

$Si_9C_4(a)$ and $Si_9C_4(b)$ are two different structures with an energy difference of 0.422 eV. $Si_9C_4(a)$ has the lowest energy. $Si_9C_4(c)$ is 0.495 eV higher than $Si_9C_4(a)$ in energy. $Si_{10}C_3(a)$, $Si_{10}C_3(b)$ and $Si_{10}C_3(c)$ are the stable structures for the $Si_{10}C_3$ clusters. $Si_{10}C_3(a)$ is the most stable structure. $Si_{10}C_3(c)$ is slightly (about 0.019 eV) higher than $Si_{10}C_3(b)$ in energy. $Si_{10}C_3(b)$ is 0.619 eV higher than $Si_{10}C_3(a)$ in energy. For the $Si_{11}C_2$ cluster, the lowest-energy structure, $Si_{11}C_2(a)$, lies 0.093 eV below $Si_{11}C_2(b)$. $Si_{11}C_2(c)$ is 0.101 eV higher than $Si_{11}C_2(a)$ in energy. For the $Si_{12}C$ cluster, $Si_{12}C(a)$ is obtained as the ground state, which agrees with the structures proposed by Li et al. [25]. $Si_{12}C(b)$ and $Si_{12}C(c)$ are 0.163 eV, 0.834 eV less stable than $Si_{12}C(a)$, respectively. It is found that carbon atoms prefer the surface sites to the center sites in the ground states of $Si_{11}C_2$ and $Si_{12}C$.
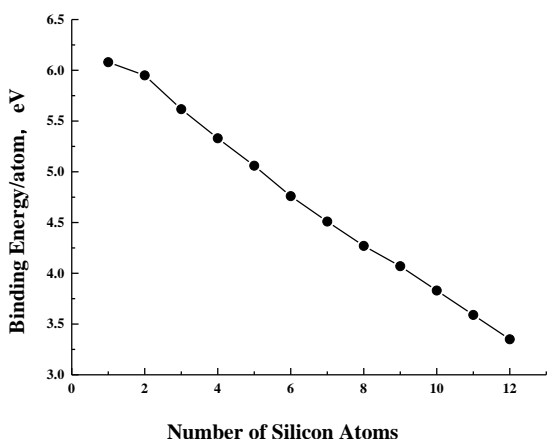
$$E_{BE} = [E_{total} - nE_{si} - (13 - n)E_c]/13, \qquad (1)$$

where E_{si}, E_c, and E_{total} are the energies of isolated Si and C atoms and of the Si_nC_{13-n} cluster, respectively. The binding energy per atom versus the number of silicon atoms in the Si_nC_{13-n} ($n = 1 - 12$) clusters is shown in Fig. 2. It is found that the stability of Si_nC_{13-n} ($n = 1 - 12$) clusters increases as the number of carbon atoms increases.

A vibrational frequency calculation is important for predicting structural stability. To determine the ground state of Si_nC_{13-n} ($n = 1 - 12$) clusters, we chose at least five configurations with low binding energies and calculated the corresponding vibrational frequencies.

Table 1. Vibration frequencies of Si_nC_{13-n} ($n = 1 - 12$) clusters

No	v, cm^{-1}	I, km/mol	No	v, cm^{-1}	I, km/mol
1	41.7	0.00	7	55.2	0.16
	2169.3	911.06		1349.7	5.70
2	33.8	1.17	8	30.0	0.05
	2144.1	0.00		1736.6	305.39
3	43.0	1.61	9	36.6	0.21
	2039.0	134.74		1066.7	27.99
4	62.9	0.29	10	40.0	0.24
	1959.1	8.23		950.0	13.32
5	48.0	1.15	11	75.9	1.35
	1824.2	90.94		1371.8	12.14
6	22.2	0.08	12	49.9	0.06
	1461.4	9.99		697.5	25.45

In Table 1, the lowest vibrational frequencies (cm^{-1}) and the highest infrared spectral (IR) intensities (km/mol) of the ground states for Si_nC_{13-n} ($n = 1 - 12$) clusters are listed, the km in the IR intensity represents kilometer. It can be clearly seen that the ground states obtained here are actually equilibrium states without imaginary frequencies.

The HOMO-LUMO gaps of the lowest-energy structures versus the number of silicon atoms in the binary clusters are plotted in Fig. 3. It is found that the HOMO-LUMO gaps of the ground states range from about 0.422 to 1.716 eV, indicating both high chemical stability and semi-conductivity, except for the cases of Si_6C_7 and $Si_{12}C$.
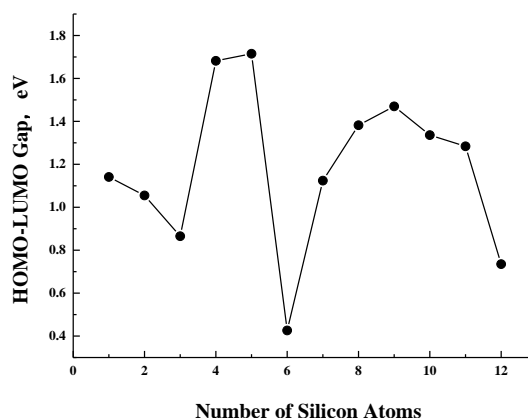

Fig. 2. Binding energy per atom (in eV) for Si_nC_{13-n} ($n = 1 - 12$) clusters versus the number of silicon atoms in (Si_nC_{13-n} ($n = 1 - 12$)) the clusters

In order to study the stability of Si_nC_{13-n} ($n = 1 - 12$) clusters, we have calculated the binding energies of all the lowest-energy structures obtained here. The binding energy is defined as

Fig. 3. HOMO-LUMO gap (in eV) versus the number of silicon atoms in Si_nC_{13-n} ($n = 1 - 12$) clusters

We plot the HOMO of the lowest-energy structures of Si_nC_{13-n} ($n = 1 - 12$) in Fig. 4. It clearly shows that the frontier molecular orbitals are mainly accumulating in silicon, which results from the fact that the majority of Si atoms exhibit small coordination number and the

unsaturated Si atoms apparently show great chemical reactivity. The geometry and stability of the clusters are closely related to the bonding features and charge distributions. Analysis of the Mülliken population shows significant charge transfer from silicon to carbon. It is found that in the ground states of Si_nC_{13-n} ($n = 8, 9, 11, 12$), most carbon atoms gain charge whereas the silicon atoms lose charge and a few silicon atoms located on the edge of the structures acquire negative charges.
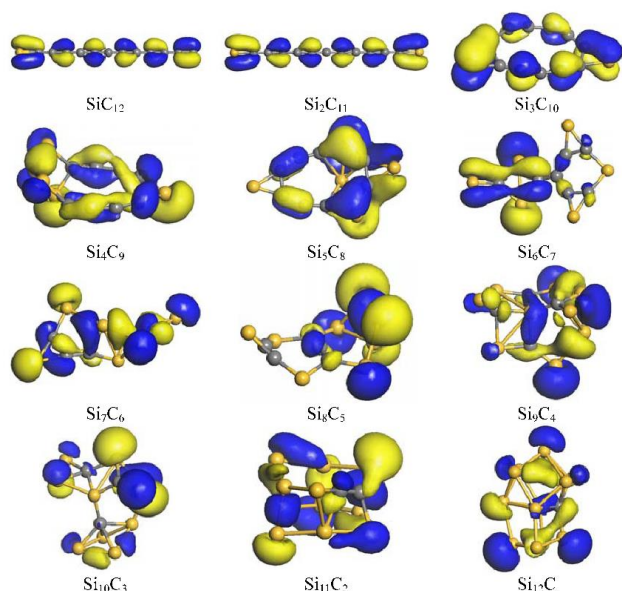

Fig. 4. The HOMO of the Si_nC_{13-n} clusters ($n = 1 - 12$). The isodensity surfaces correspond to 0.030 e/a.u.^{3}, where e represents electron

4. CONCLUSIONS

Geometries, binding energies and electronic structures of Si_nC_{13-n} ($n = 1 - 12$) clusters have been investigated using all-electron DFT. As the number of silicon atoms increases, the lowest-energy structures transform from planar structures (ring or chain) to 3D structures. We find that in the equilibrium geometries of the Si_nC_{13-n} ($n = 1 - 4$) clusters, silicon atoms prefer to bond at one or two end(s) of the C chain or ring and the lowest-energy structures are all planar structures except for the case of Si_4C_9. Moreover, the lowest-energy configurations of Si_nC_{13-n} ($n = 4 - 12$) clusters are all 3D structures. The most stable structures of the Si_nC_{13-n} ($n = 5 - 10$) clusters show that carbon atoms preferentially take up positions in the centre of the structures, whereas for the $Si_{11}C_2$ and $Si_{12}C$ clusters, carbon atoms prefer locating at the surface sites. Based on the calculation of the HOMO-LUMO gaps of the ground states, it is found that except for Si_6C_7 and $Si_{12}C$, the lowest-energy structures of Si_nC_{13-n} ($n = 1 - 12$) have high chemical stability and semi-conductivity. Analysis of the Mülliken population shows that significant charge transfer takes place from the silicon atoms to the carbon atoms.

Acknowledgments

REFERENCES

1. **Raghavachari, K., Binkley, J.S.** Structure, Stability, and Fragmentation of Small Carbon Clusters *Journal of Chemical Physics* 87 (4) 1987: pp. 2191 – 2197. https://doi.org/10.1063/1.453145

2. **Shen, L.N., Graham, W.R.M.** Observation of an Infrared Frequency of the C_4 Molecule *Journal of Chemical Physics* 91 (8) 1989: pp. 5115 – 5116. https://doi.org/10.1063/1.457603

3. **Arnold, D.W., Bradforth, S.E., Kitsopoulos, T.N., Neumark, D.M.** Vibrationally Resolved Spectra of C_2–C_{11} by Anion Photoelectron Spectroscopy *Journal of Chemical Physics* 95 (12) 1991: pp. 8753 – 8764. https://doi.org/10.1063/1.461211

4. **Froudakis, G., Zdetsis, A., Engels, B., Peyerimhoff, S.D.** A Comparative Abinitio Study of the Si_2C_4, Si_3C_3, and Si_4C_2 Clusters *Journal of Chemical Physics* 101 (8) 1994: pp. 6790 – 6799. https://doi.org/10.1063/1.468334

5. **Nakajima, A., Taguwa, T., Nakao, K., Gomei, M., Kishi, R., Iwata, S., Kaya, K.** Photoelectron Spectroscopy of Silicon – Carbon Cluster Anions *Surface Review & Letters* 3 (01) 1996: pp. 411 – 415. https://doi.org/10.1063/1.469731

6. **Zdetsis, A.D., Froudakis, G., Mühlhäuser, M., Thümnel, H.** Abinitio Study of Electronic, Structural, and Vibrational Properties of the Si_4C Cluster *Journal of Chemical Physics* 104 (7) 1996: pp. 2566 – 2573. https://doi.org/10.1063/1.471004

7. **Hunsicker, S., Jones, R.O.** Structure and Bonding in Mixed Silicon–Carbon Clusters and their Anions *Journal of Chemical Physics* 105 (12) 1996: pp. 5048 – 5060. https://doi.org/10.1063/1.472350

8. **Xia, B.Y., Cai, W.S., Shao, X.G., Guo, Q.X., Maigret, B., Pan, Z.X.** Chiral Recognition Study for the Inclusion Complexes of Amino Acids with A-Cyclodextrin Using a Fast Annealing Evolutionary Algorithm *Chemical Research in Chinese Universities* 546 (1) 2002: pp. 33 – 38. https://doi.org/10.1016/S0166-1280(01)00434-1

9. **Pradhan, P., Ray, A.K.** A Density Functional Study of the Structures and Energetics of Small Hetero-Atomic Silicon–Carbon Nanoclusters *Journal of Molecular Structure Theochem* 716 (1) 2004: pp. 109 – 130. https://doi.org/10.1016/j.theochem.2004.11.019

10. **Yadav, P.S., Yadav, R.K., Agrawal, S., Agrawal, B.K.** Theoretical Study of the Physical Properties of Binary Si_mC_n Clusters: An Ab Initio Study *Physica E: Low-Dimensional Systems and Nanostructures* 33 (1) 2006: pp. 249 – 262. https://doi.org/10.1016/j.physe.2006.03.132

11. **Jiang, Z., Xu, X., Wu, H., Zhang, F., Jin, Z.** Structure and Stability of Si_nC_{m-n} Clusters *Journal of Molecular Structure Theochem* s 589 – 590 (s 1 – 3) 2002: pp. 103 – 109. https://doi.org/ 10.1016/S0166-1280(02)00251-8

12. **Jiang, Z., Xu, X., Wu, H., Zhang, F., Jin, Z.** First Principles Studies on the Structures, Electronic States and Stability of $Si_nC_m^+$ Cationic Clusters *Journal of Molecular Structure Theochem* 624 (1 – 3) 2003: pp. 61 – 67.

https://doi.org/10.1016/S0166-1280(02)00738-8

13. **Wang, H., Lu, W.C., Sun, J., Li, Z.S., Sun, C.C.** Theoretical Investigation on the Structures of Silicon and Carbon Hetero Clusters *Chemical Physics Letters* 423 (1 – 3) 2006: pp. 87 – 93. https://doi.org/10.1016/j.cplett.2006.03.031

14. **Wang, X., Wang, B., Chen, G., Zhao, J.** Theoretical Identification of the Lowest-Energy Structure of $(SiC)_{12}$ Herocluster: Segregation of C and Si in Planar and Cage Structures *Chemical Physics* 355 (1) 2009: pp. 31 – 36. https://doi.org/10.1016/j.chemphys.2008.10.051

15. **Li, Q.X., Lu, W.C., Zang, Q.J., Zhao, L.Z., Wang, C.Z., Ho, K.M.** Carbon-Rich C_9Si_n (n = 1 – 5) Clusters from Ab Initio Calculations *Computational & Theoretical Chemistry* 963 (2 – 3) 2011: pp. 439 – 447. https://doi.org/10.1016/j.comptc.2010.11.010

16. **Azeezullanazrulla, M., Joshi, K., Israel, S., Krishnamurty, S.** Structure and Stability of a Silicon Cluster On Sequential Doping with Carbon Atoms *Physica E: Low-Dimensional Systems and Nanostructures* 76 2016: pp. 173 – 180. https://doi.org/10.1016/j.physe.2015.10.012

17. **Tang, Y., Lu, J., Yan, X., Lin, X., Zhu, H.** Growth Pattern and Electronic Property of $Si_{12}C_{12}$-assembled Structures *Superlattices & Microstructures* 100 2016: pp. 483 – 489. https://doi.org/10.1016/j.spmi.2016.10.004

18. **Byrd, J.N., Lutz, J.J., Jin, Y., Ranasinghe, D.S., Jr, J.A.M., Perera, A., Duan, X.F., Burggraf, L.W., Sanders, B.A., Bartlett, R.J.** Predictive Coupled-Cluster Isomer Orderings for some Si_nC_m (m,n ≤ 12) Clusters: A Pragmatic Comparison Between DFT and Complete Basis Limit Coupled-Cluster Benchmarks *Journal of Chemical Physics* 145 (2) 2016: pp. 961 – 1189. https://doi.org/ 10.1063/1.4955196

19. **Koohi, M., Amiri, S.S., Shariati, M.** Silicon Impacts On Structure, Stability and Aromaticity of $C_{20-n}Si_n$ Heterofullerenes (n = 1 – 10): A Density Functional Perspective *Journal of Molecular Structure* 1127 2017: pp. 522 – 531. https://doi.org/10.1016/j.molstruc.2016.08.012

20. **Delley, B.** An All-electron Numerical Method for Solving the Local Density Functional for Polyatomic Molecules *Journal of Chemical Physics* 92 (1) 1990: pp. 508 – 517. https://doi.org/10.1063/1.458452

21. **Delley, B.** Analytic Energy Derivatives in the Numerical Local-Density-Functional Approach *Journal of Chemical Physics* 94 (11) 1991: pp. 7245 – 7250. https://doi.org/10.1063/1.460208

22. **Becke, A.D.** A Multicenter Numerical Integration Scheme for Polyatomic Molecules *Journal of Chemical Physics* 88 (4) 1988: pp. 2547 – 2553. https://doi.org/ 10.1063/1.454033

23. **Lee, C., Yang, W., Parr, R.G.** Development of the Colle-Salvetti Correlation-Energy Formula Into a Functional of the Electron Density *Physical Review B Condensed Matter* 37 (2) 1988: pp. 785. https://doi.org/ 10.1103/PhysRevB.37.785

24. **Li, S.D., Zhao, Z.G., Zhao, X.F., Wu, H.S., Jin, Z.H.** Structural and Electronic Properties of Semiconductor Binary Microclusters A_mB_n (A,B = Si, Ge, C): A B3LYP-DFT Study *Physical Review B* 64 (19) 2001: pp. 195312. https://doi.org/ 10.1103/PhysRevB.64.195312

25. **Chu, Q.Y., Li, B.X., Yu, J.** Stability of Carbon-Doped Silicon Clusters: FP-LMTO Molecular Dynamics Calculations *Journal of Molecular Structure Theochem* 806 (1 – 3) 2007: pp. 67 – 76. https://doi.org/10.1016/j.theochem.2006.11.005