

Article

DFT Study on the Gas-Phase Cluster Formation Mechanism in SiC CVD

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Abstract

This study employs density functional theory and quantum chemical calculations to investigate the gas-phase nucleation and growth mechanisms during chemical vapor deposition of silicon carbide. Based on thermodynamic stability evaluations of large clusters under various configurations, the lowest-energy ground-state structure was determined. The Gibbs free energy (ΔG) calculations of pure silicon clusters (Si_n), single-carbon silicon clusters (Si_nC), and double-carbon silicon clusters (Si_nC_2) were conducted at different temperatures. The findings reveal that silicon atoms promote cluster growth. The special 2D-to-3D configurational transition attenuates the reaction's spontaneity. During the initial nucleation stage, the system tends to form Si_nC ; however, as the size increases, it evolves into the more stable Si_nC_2 . This study reveals gas-phase cluster formation at the atomic scale, providing a theoretical foundation for suppressing detrimental gas-phase nucleation.

Keywords: SiC; chemical vapor deposition; density functional theory; cluster

1. Introduction

Silicon carbide (SiC) films exhibit high density, excellent thermal stability, and corrosion resistance [1–3], rendering them desirable for applications involving high thermal loads and harsh chemical environments, including aerospace, nuclear reactors, and cutting or abrasive tools [2,4]. Currently, common methods for preparing SiC films include the pack cementation method [5], physical vapor deposition [6], and chemical vapor deposition (CVD) [7]. CVD is widely used for coating preparation because of its advantages, including high substrate bonding strength, superior deposition purity, and a high, controllable deposition rate [8,9].

In SiC-CVD processes, precursor systems are typically categorized into two types: Si-C-H systems [10,11] and Si-C-Cl-H systems [12,13]. Although the Si-C-Cl-H system can suppress gas-phase nucleation and improve precursor utilization efficiency, the Si-C-H system is more widely used in practical applications because of its advantages, including non-corrosiveness, simple exhaust gas treatment, and environmental friendliness [14]. However, the Si-C-H system is prone to side reactions and nanoparticle formation in the reactor, requiring a comprehensive understanding of its gas-phase nucleation pathways to enhance coating quality and control defects [15].

Gas-phase nucleation wastes reaction precursors and reduces the efficiency of film growth. Furthermore, the nanoparticles generated through this process can contaminate



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both the reactor walls and deposited films [16]. Previous studies have conducted extensive investigations to address this issue. Vorob et al. [17] numerically investigated the gas-phase nucleation and subsequent transport behavior of silicon clusters in a vertical rotating disk reactor. Kollmuss et al. [18] determined that the incomplete pyrolysis of propane at low temperatures is responsible for the gas-phase nucleation of silicon species. Hong et al. [19] proposed that the gas-phase polymerization reactions between C_2H_2 and SiH_2 play a significant role in particle formation. Swihar and Girschick [20] developed an extensive chemical kinetic model detailing the formation of silicon hydride clusters during silane pyrolysis. However, existing studies are limited to pure silicon systems or individual reaction pathways, and a systematic understanding of the microscopic growth mechanisms of silicon–carbon clusters and the thermodynamic evolution governing their early-stage gas-phase nucleation remains lacking.

Motivated by these considerations, this study employs quantum chemical calculations to systematically investigate the gas-phase mechanisms of nanoparticle precursor formation during the SiC-CVD process. Specifically, the formation and growth evolution pathways of pure silicon clusters (Si_n), single-carbon silicon clusters (Si_nC), and double-carbon silicon clusters (Si_nC_2) are analyzed at practical deposition temperatures. This study aims to elucidate the thermodynamic processes of gas-phase nucleation and to provide theoretical support for optimizing the SiC-CVD process and suppressing gas-phase nucleation.

2. Calculation Method and Validation

The gas-phase reaction mechanism (R1–R17) is adopted based on the 17-reaction Si–C–H kinetic model developed by Allendorf [21], large clusters (e.g., Si_6 , Si_5C , and Si_4C_2) are treated as particle embryos during gas-phase nucleation [22]. By integrating Kremer’s insights on cluster growth via Si_2H_2 and SiH_2 [23], a synergistic reaction network is proposed, as shown in Figure 1, detailing the formation and growth pathways of pure silicon clusters (Si_n , $n = 2–6$), single-carbon silicon clusters (Si_nC , $n = 2–5$), and double-carbon silicon clusters (Si_nC_2 , $n = 2–4$).

The free energy of each reaction was calculated using the Gaussian 16 program package [24] based on density functional theory (DFT), and the reaction direction was assessed based on the free energy difference (ΔG) between the reactants and the products. A $\Delta G < 0$ is a requirement for a reaction to be spontaneous. First, geometric optimization and harmonic vibrational frequency analysis were performed using the DFT B3LYP/cc-pVTZ method. High-accuracy single-point energy calculations were performed using the high-level electron correlation method CCSD(T) in conjunction with the cc-pVQZ basis set. To evaluate the temperature-dependent thermodynamic properties across the CVD thermal gradient (300 K to 1900 K) [25], these properties were calculated using the Shermo program [26] by combining high-accuracy single-point energies with thermodynamic corrections. Precursor gases are typically introduced at 300 K and transported across a steep thermal boundary layer toward the heated susceptor, which usually operates between 1700 K and 1900 K. By evaluating the thermodynamic driving forces across this specific gradient, this study captures the continuous evolution of gas-phase species from initial room-temperature mixing to severe high-temperature pyrolysis near the growth surface. During the extraction process, the contributions of electronic and spatial degeneracies of isolated atoms and open-shell radical clusters to the electronic entropy and total free energy were explicitly considered and corrected.

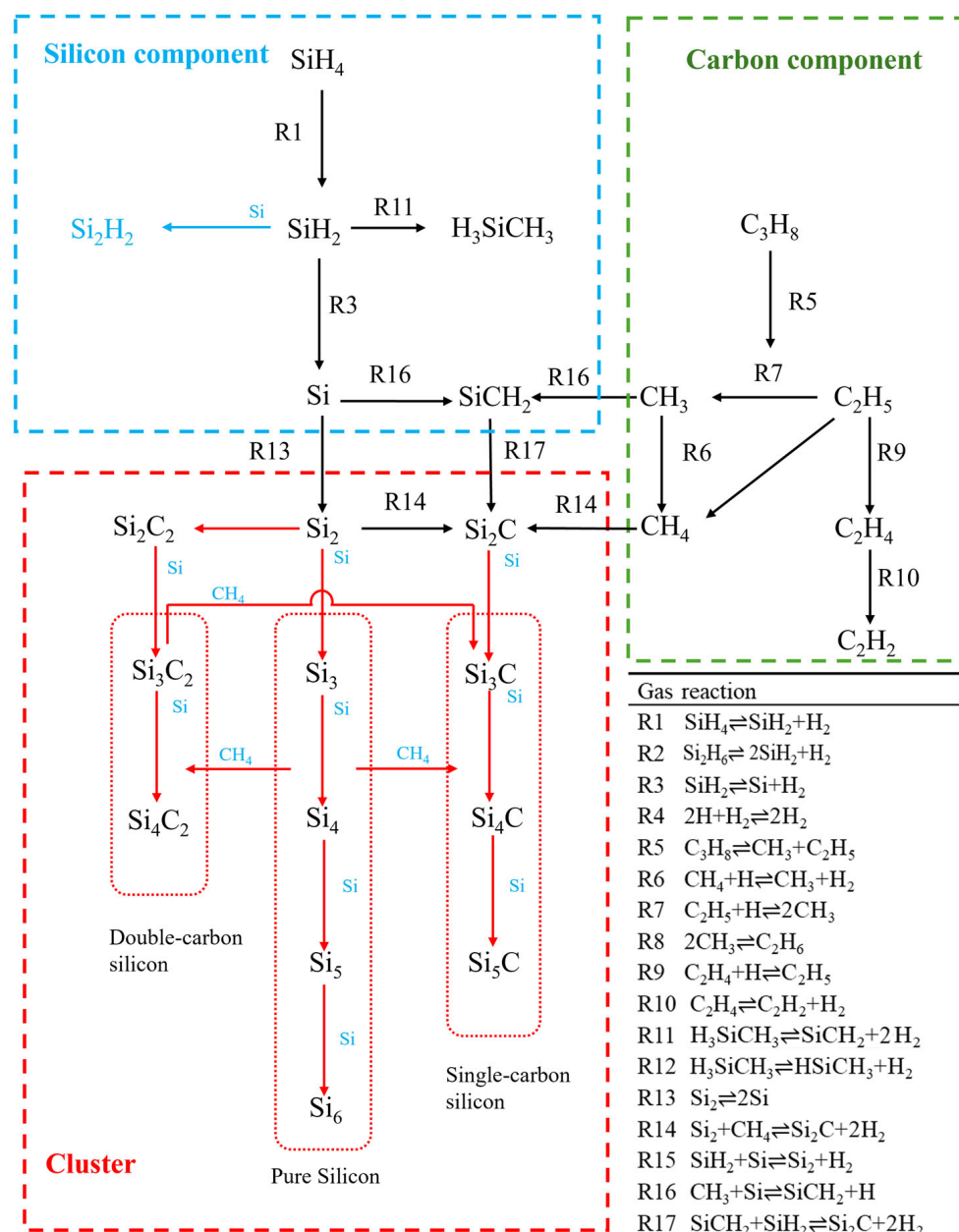


Figure 1. Schematic diagram of cluster formation and growth pathways.

To account for the systematic overestimation of harmonic vibrational frequencies and the inherent anharmonicity of molecular motions, scaling factors derived from the benchmark study by Merrick et al. [27] were utilized. Specifically, the zero-point vibrational energy, thermal enthalpy correction, and entropy were scaled by 0.9882, 0.9946, and 0.9997, respectively. This calibration effectively eliminates the bias introduced by anharmonic effects in the macroscopic thermodynamic properties.

To validate the reliability of the selected method and basis set for treating silicon–carbon systems, a test was conducted on the equilibrium geometry of the double-carbon silicon cluster Si_3C_2 . The calculated total energy and bond lengths were compared with literature values. The calculated data and literature comparisons are shown in Table 1. The optimized structure aligns with previous reports, confirming the validity of the computational model employed in this study.

Table 1. Comparison of the calculated total energy (in Eh) and bond lengths (in Å) of the lowest-energy Si₃C₂ with literature values.

Cluster (Symmetry, State)	Calculation Method	Bonds Lengths	$\Delta r = r_{\text{this study}} - r_{\text{literature}} $	Literature
Si ₃ C ₂ (C _{2v} , ¹ A ₁)	B3PW91/6-31G(d)	$r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.57$	$\Delta r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 0.04$	[28]
		$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.72$	$\Delta r(\text{Si}_{(1)}-\text{C}_{(1)}) = 0$	
		$r(\text{C}_{(1)}-\text{Si}_{(2)}) = 1.92$	$\Delta r(\text{C}_{(1)}-\text{Si}_{(2)}) = 0.01$	
		$r(\text{C}_{(1)}-\text{C}_{(2)}) = 1.36$	$\Delta r(\text{C}_{(1)}-\text{C}_{(2)}) = 0$	
	MP2/DZ2P//CCSD(T)	$r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.67$	$\Delta r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 0.06$	[29]
		$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.68$	$\Delta r(\text{Si}_{(1)}-\text{C}_{(1)}) = 0.04$	
		$r(\text{C}_{(1)}-\text{Si}_{(2)}) = 1.92$	$\Delta r(\text{C}_{(1)}-\text{Si}_{(2)}) = 0.01$	
		$r(\text{C}_{(1)}-\text{C}_{(2)}) = 1.37$	$\Delta r(\text{C}_{(1)}-\text{C}_{(2)}) = 0.01$	
	MBPT(2)/6-31G*//MBPT(4)/6-31G*	$r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.53$	$\Delta r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 0.08$	[30]
		$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.73$	$\Delta r(\text{Si}_{(1)}-\text{C}_{(1)}) = 0.01$	
		$r(\text{C}_{(1)}-\text{Si}_{(2)}) = 1.91$	$\Delta r(\text{C}_{(1)}-\text{Si}_{(2)}) = 0.02$	
		$r(\text{C}_{(1)}-\text{C}_{(2)}) = 1.37$	$\Delta r(\text{C}_{(1)}-\text{C}_{(2)}) = 0.01$	
	B3LYP/cc-pVTZ//CCSD(T)/cc-pVQZ	$r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.61$	-	This study
		$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.72$		
		$r(\text{C}_{(1)}-\text{Si}_{(2)}) = 1.93$		
		$r(\text{C}_{(1)}-\text{C}_{(2)}) = 1.36$		

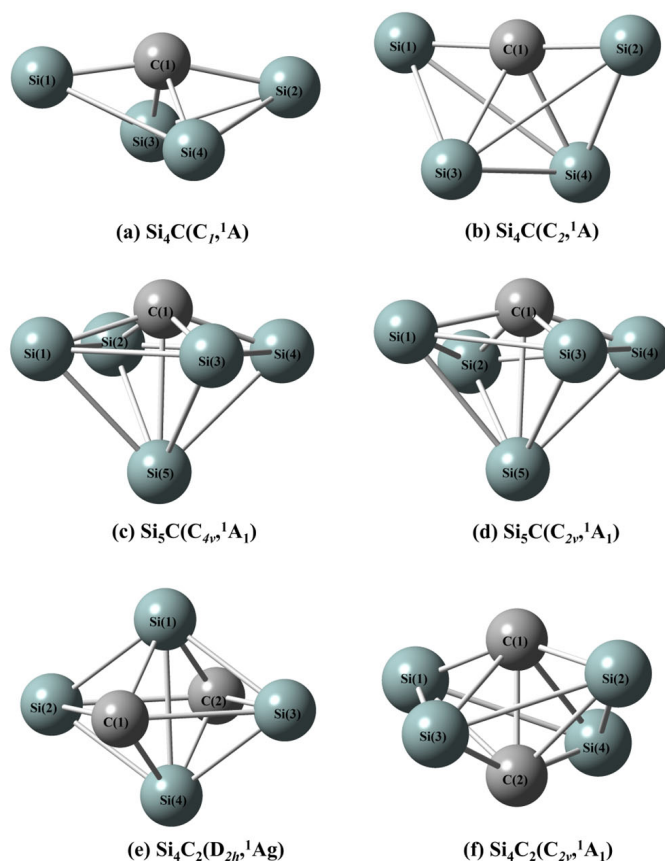
Structural isomerism becomes increasingly pronounced as cluster size increases. Therefore, identifying the global energy minimum that corresponds to the most stable ground-state structure is a fundamental prerequisite for accurate thermodynamic calculations [31]. Structural optimizations were systematically conducted, and the thermodynamic stability of multiple potential isomers for large clusters, including Si₄C, Si₅C, and Si₄C₂, was screened. The structural symmetries and electronic ground states of these clusters were obtained from the literature [28,31]. They are depicted in Figure 2, with the calculated data and literature comparisons tabulated in Table 2. Since the ground-state structures of the Si₆ and Si₃C₂ clusters have been conclusively established in prior research [32–34], their validated global minimum configurations, Si₆(C_{2v}, ¹A₁) and Si₃C₂(C_{2v}, ¹A₁), were used directly.

Table 2. Comparison of the calculated total energy (in Eh) and bond lengths (in Å) of the lowest-energy Si₄C, Si₅C, and Si₄C₂ with literature values.

Cluster (Symmetry, State)	Calculation Method	Bonds Lengths	Total Energy	Literature
Si ₄ C(C ₁ , ¹ A)	HF/6-31G*//CCSD(T)/6-31G*	$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.76$	−1193.89	[35]
		$r(\text{Si}_{(2)}-\text{C}_{(1)}) = 1.87$		
		$r(\text{Si}_{(3)}-\text{C}_{(1)}) = 1.92$		
		$r(\text{Si}_{(1)}-\text{Si}_{(3)}) = 2.61$		
		$r(\text{Si}_{(2)}-\text{Si}_{(3)}) = 2.42$		
	B3LYP/cc-pVTZ//CCSD(T)/cc-pVQZ	$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.78$	−1194.196	This study
		$r(\text{Si}_{(2)}-\text{C}_{(1)}) = 1.92$		
		$r(\text{Si}_{(3)}-\text{C}_{(1)}) = 1.91$		
		$r(\text{Si}_{(1)}-\text{Si}_{(3)}) = 2.62$		
		$r(\text{Si}_{(2)}-\text{Si}_{(3)}) = 2.41$		
Si ₄ C(C ₂ , ¹ A)	B3LYP/cc-pVTZ//CCSD(T)/cc-pVQZ	$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.77$	−1194.199	This study
		$r(\text{Si}_{(3)}-\text{C}_{(1)}) = 2.15$		
		$r(\text{Si}_{(1)}-\text{Si}_{(3)}) = 2.39$		
		$r(\text{Si}_{(1)}-\text{Si}_{(4)}) = 3.20$		

Table 2. Cont.

Cluster (Symmetry, State)	Calculation Method	Bonds Lengths	Total Energy	Literature
$\text{Si}_5\text{C}(\text{C}_{4v}, {}^1\text{A}_1)$	B3PW91/6-31G(d)	$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.89$ $r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.44$ $r(\text{C}_{(1)}-\text{Si}_{(5)}) = 1.89$	-	[28]
	B3LYP/cc-pVTZ// CCSD(T)/cc-pVQZ	$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.89$ $r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.55$ $r(\text{C}_{(1)}-\text{Si}_{(5)}) = 2.26$	has imaginary frequency	This study
$\text{Si}_5\text{C}(\text{C}_{2v}, {}^1\text{A}_1)$	B3LYP/cc-pVTZ// CCSD(T)/cc-pVQZ	$r(\text{Si}_{(1)}-\text{C}_{(1)}) = 1.77$ $r(\text{Si}_{(3)}-\text{C}_{(1)}) = 2.15$ $r(\text{Si}_{(1)}-\text{Si}_{(3)}) = 2.39$ $r(\text{Si}_{(1)}-\text{Si}_{(4)}) = 3.20$	-1483.32	This study
$\text{Si}_4\text{C}_2(\text{D}_{2h}, {}^1\text{A}_g)$	SCF/DZP//MP2/6-31G*	$r(\text{C}_{(1)}-\text{Si}_{(1)}) = 2.00$ $r(\text{C}_{(1)}-\text{Si}_{(2)}) = 2.22$ $r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.30$	-1231.96	[36]
	B3LYP/cc-pVTZ// CCSD(T)/cc-pVQZ	$r(\text{C}_{(1)}-\text{Si}_{(1)}) = 1.94$ $r(\text{C}_{(1)}-\text{Si}_{(3)}) = 2.30$ $r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.40$	-1232.09	This study
$\text{Si}_4\text{C}_2(\text{C}_{2v}, {}^1\text{A}_1)$	SCF/DZP//MP2/6-31G*	$r(\text{C}_{(1)}-\text{Si}_{(1)}) = 2.11$ $r(\text{C}_{(1)}-\text{Si}_{(2)}) = 2.37$ $r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.30$	-1231.96	[36]
	B3LYP/cc-pVTZ// CCSD(T)/cc-pVQZ	$r(\text{C}_{(1)}-\text{Si}_{(1)}) = 1.80$ $r(\text{C}_{(1)}-\text{Si}_{(3)}) = 2.18$ $r(\text{Si}_{(1)}-\text{Si}_{(2)}) = 2.59$	-1232.24	This study

Figure 2. Optimized geometric structures of Si_4C , Si_5C , and Si_4C_2 .

The calculations reveal that the $\text{Si}_4\text{C}(\text{C}_{2v}, {}^1\text{A}_1)$ and $\text{Si}_4\text{C}_2(\text{C}_{2v}, {}^1\text{A}_1)$ exhibit the lowest total system energies of -1194.199 Eh and -1232.24 Eh. Respectively, compared to other candidate geometries such as $\text{Si}_4\text{C}(\text{C}_1, {}^1\text{A})$ at -1194.196 Eh and $\text{Si}_4\text{C}_2(\text{D}_{2h}, {}^1\text{A}_g)$ at -1232.090 Eh. Vibrational frequency analysis indicates that the highly symmetric $\text{Si}_5\text{C}(\text{C}_{4v}, {}^1\text{A}_1)$ configuration possesses imaginary frequencies. Guided by the criteria of stable stationary points on the potential energy surface and the energy minimization principle, $\text{Si}_4\text{C}(\text{C}_{2v}, {}^1\text{A}_1)$, $\text{Si}_4\text{C}_2(\text{C}_{2v}, {}^1\text{A}_1)$, and $\text{Si}_5\text{C}(\text{C}_{2v}, {}^1\text{A}_1)$ were established as the standard large cluster geometries for modeling the gas-phase growth.

3. Results and Discussion

3.1. Pure Silicon Cluster Growth

In gas-phase reactions, the initial pyrolysis of precursor gases dominates the early chemical processes. Compared with C_2H_5 , which possesses a higher dissociation energy, silane undergoes homolysis or dehydrogenation at lower temperatures, generating highly reactive Si atoms and hydrogen-containing intermediates such as SiH_2 and Si_2H_2 . Consequently, the initial nucleation stage of the system is primarily characterized by the growth of pure silicon clusters (Si_n , $n = 2-6$), with the optimized configurations illustrated in Figure 3. The structural symmetries and electronic ground states of these clusters were adopted in accordance with previous studies [34].

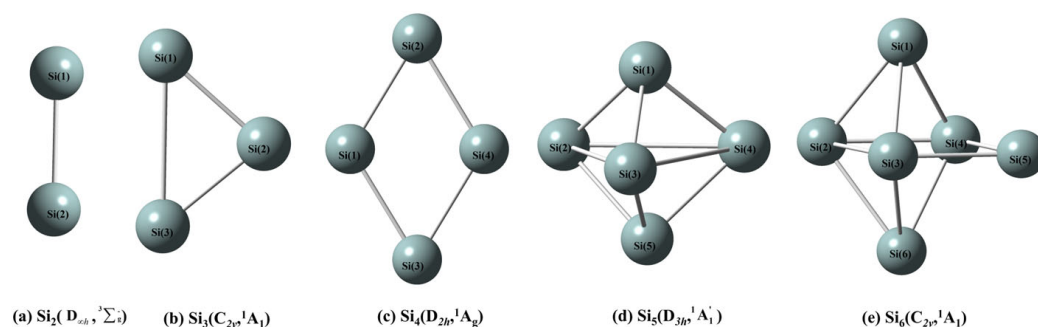


Figure 3. Optimized geometric structures of Si_n .

This study investigates four parallel reaction pathways for the gas-phase growth of pure silicon clusters. These pathways are driven by three fundamental mechanisms: the direct association of free Si atoms with silicon clusters, and the reactions of SiH_2 and Si_2H_2 with pure silicon clusters. These reaction schemes are as follows:



Figure 4 illustrates the evolution of the Gibbs free energy (ΔG) for the gas-phase growth of Si_n within the temperature range of 300 K to 1900 K. First, the ΔG values for all four reaction pathways remain negative across the entire temperature range, indicating that the gas-phase nucleation and aggregation of Si_n are spontaneous from a thermodynamic perspective. Furthermore, the free energy variation is strongly size-dependent. Notably, at the Si_4 size node (reactions G(4), G(9), G(14), and G(18)), a significant decline in the thermodynamic driving force is observed relative to adjacent sizes (ΔG becomes less negative). At the atomic level, this occurs because the Si_4 cluster exists as a highly stable 2D planar rhombus. The addition of a fifth Si atom disrupts this planar stability, forcing drastic spatial deformation of the silicon framework to form the global minimum 3D trigonal bipyramidal structure. The energy barrier accompanying this 2D-to-3D geometric

transition macroscopically translates into a diminished release of free energy, thereby lowering the relative spontaneity of this growth step.

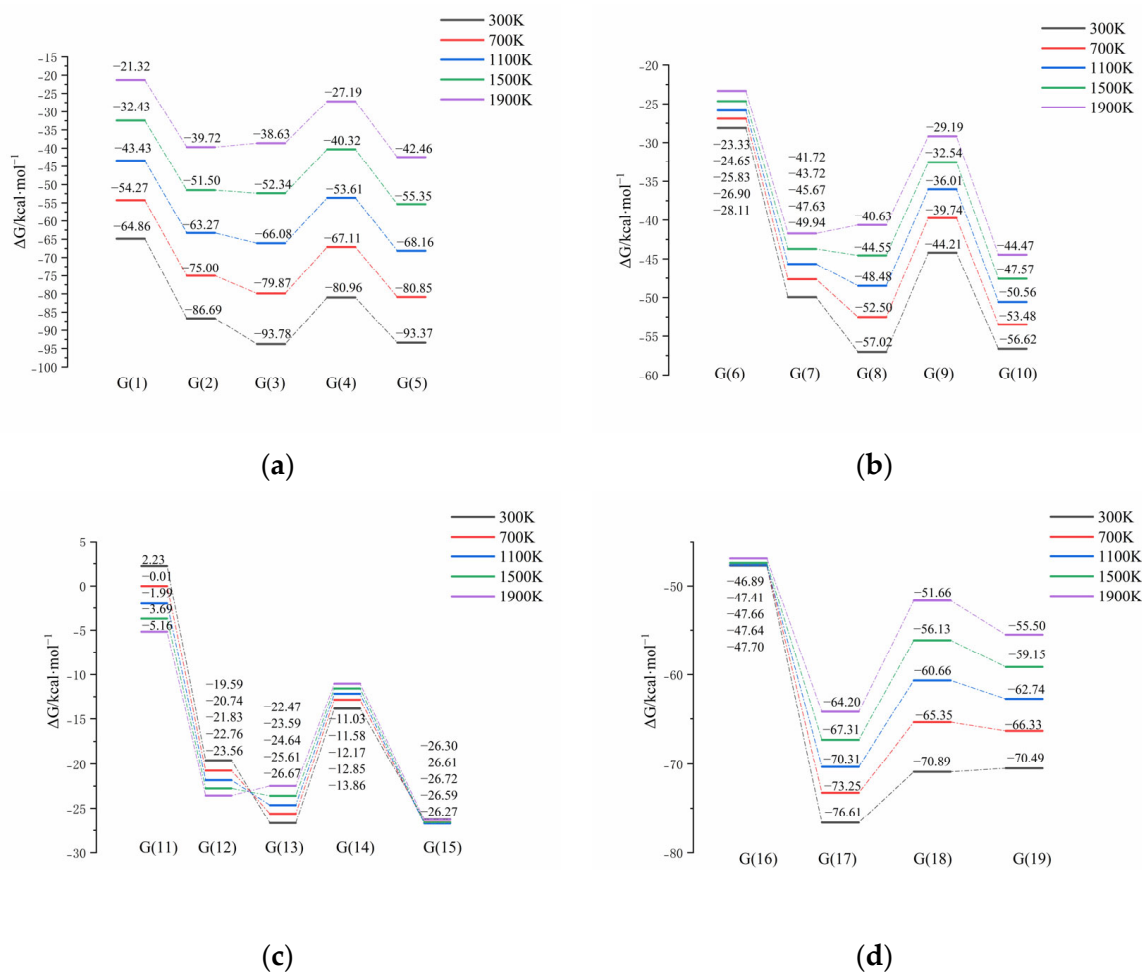


Figure 4. Evolution of ΔG for Si_n in the temperature range from 300 K to 1900 K. (a) denotes reactions (G1)–(G5); (b) denotes reactions (G6)–(G10); (c) denotes reactions (G11)–(G15); (d) denotes reactions (G16)–(G19);

The ΔG values of pathways (G1)–(G5) are highly sensitive to temperature variations. Constrained by a severe entropy penalty ($\Delta S < 0$), their thermodynamic spontaneity sharply declines at high temperatures. Conversely, pathways (G11)–(G15) maintain thermodynamic ($\Delta S \approx 0$) stability. Subsequent analysis reveals that the addition of double Si atoms via Si_2H_2 is more prone to occur than single Si atom addition, exhibiting a more negative free energy and exceptional spontaneity compared with SiH_2 -driven growth.

3.2. Single-Carbon Atom Doping and Growth

The formation of Si_n lays the foundation for subsequent nucleation; however, the gas-phase assembly of Si_n is merely the start of early-stage nanoparticle aggregation. During the actual process, carbon atoms are continuously incorporated into the silicon framework to form stable Si_nC_n nanoparticle precursors. This section broadens the research scope from pure silicon systems to the silicon–carbon system, focusing specifically on the formation and growth mechanisms of single-carbon silicon clusters (Si_nC , $n = 2–5$). The optimized configurations of the Si_nC are depicted in Figure 5. The structural symmetries and electronic ground states of these clusters were adopted in accordance with previous studies [28,31,35].

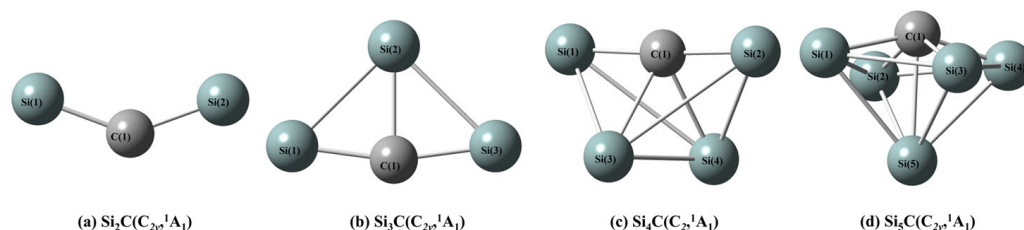


Figure 5. Optimized geometric structures of the Si_nC .

This study investigates six growth pathways for Si_nC , encompassing the initial carbonization of Si_n and the subsequent silicidation growth of Si_nC . The specific reactions are as follows:

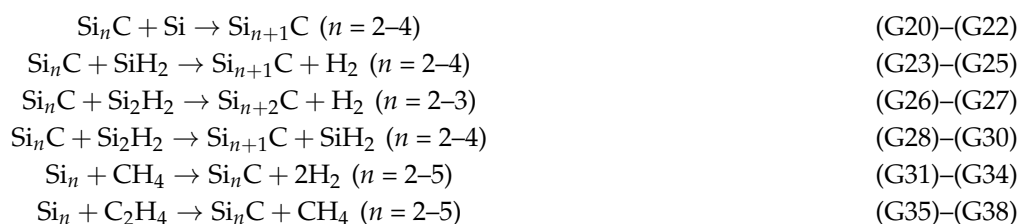


Figure 6 depicts how the change in ΔG varies with temperature and cluster size during the gas-phase formation and growth of Si_nC . The growth of Si_nC clusters shares thermodynamic features similar to those of Si_n . The pathway involving the direct addition of Si atoms demonstrates the strongest reaction spontaneity. As the degree of silicidation deepens (increasing n), the thermodynamic driving force decays, and the Gibbs values become more positive. Specifically, a drastic drop in the negative free energy occurs during the formation of Si_4C . Reaction G(29) even exhibits non-spontaneous behavior ($\Delta G > 0$). The underlying mechanism that drives this phenomenon closely aligns with the reasons for the sudden increase in free energy during pure Si cluster growth.

Driven by an increase in gas-phase molecules, the significant positive entropy change ($\Delta S > 0$) in reactions (G31)–(G34) renders them less spontaneous or even non-spontaneous at low temperatures. A comparison of carbonization agents indicates that C_2H_4 favors addition reactions more strongly at low temperatures. While CH_4 carbonization proceeds spontaneously throughout the entire temperature range, its high-temperature thermodynamic driving force remains weaker than that of C_2H_4 (reflected by a less negative ΔG value).

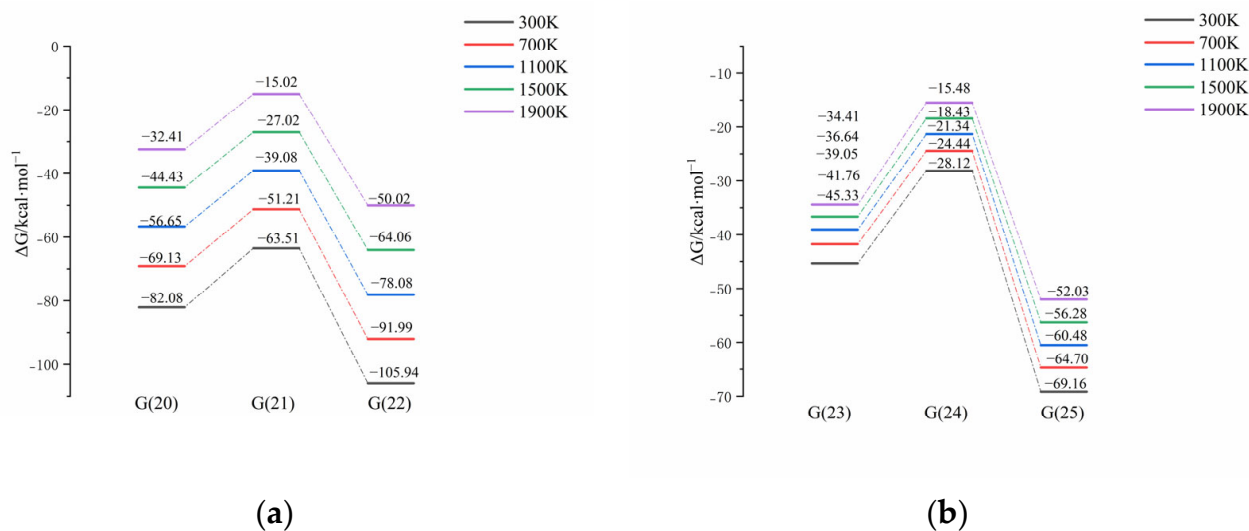


Figure 6. Cont.

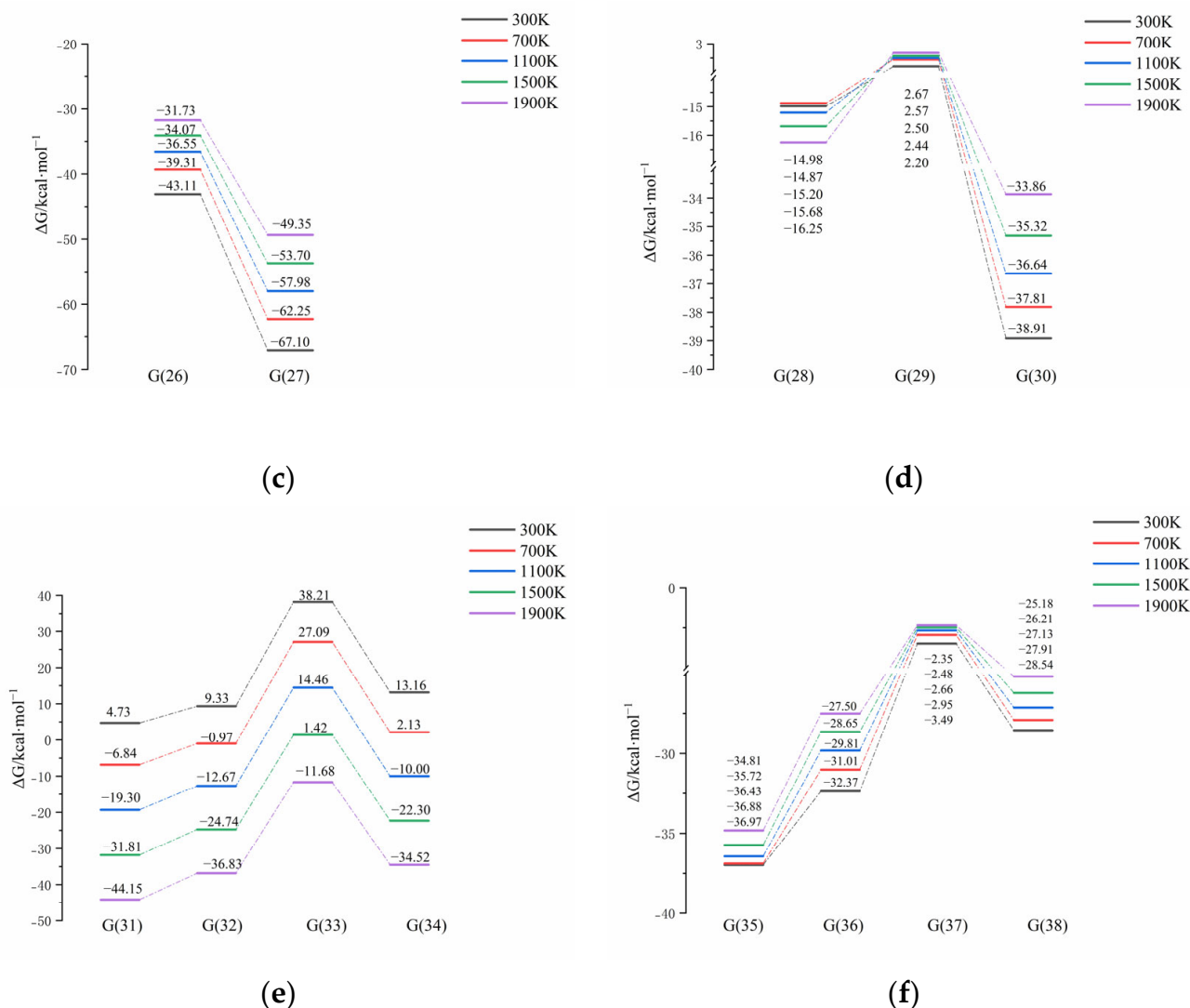


Figure 6. Evolution of ΔG for Si_nC in the temperature range from 300 K to 1900 K. (a) denotes reactions (G20)–(G22); (b) denotes reactions (G23)–(G25); (c) denotes reactions (G26)–(G27); (d) denotes reactions (G28)–(G30); (e) denotes reactions (G31)–(G34); (f) denotes reactions (G35)–(G38).

3.3. Double-Carbon Atom Addition and Growth

As the gas-phase reactions progress, this study further investigates the formation and growth pathways of double-carbon silicon clusters (Si_nC_2), a stage characterized by profound carbon enrichment within the clusters. The optimized geometries of these Si_nC_2 clusters are depicted in Figure 7. The structural symmetries and electronic ground states of these clusters were adopted in accordance with previous studies [28,36]. Thaddeus [37] identified the SiC_2 radical as a compact cyclic ring with C_{2v} symmetry.

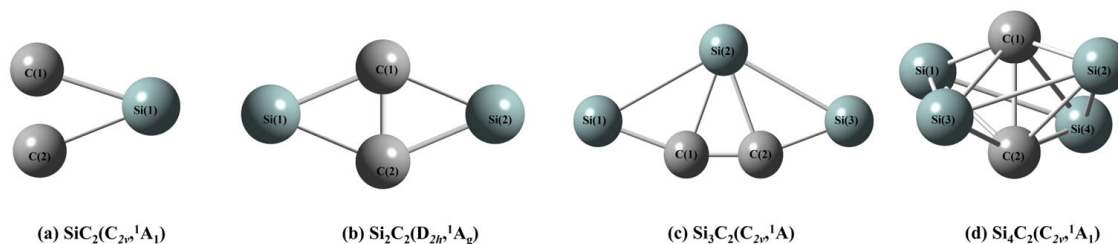


Figure 7. Optimized geometric structures of the Si_nC_2 .

This study investigates four formation pathways for Si_nC_2 , including progressive growth of Si_nC_2 , direct addition of double-carbon sources, and secondary carbonization of Si_nC . The specific reactions are as follows:

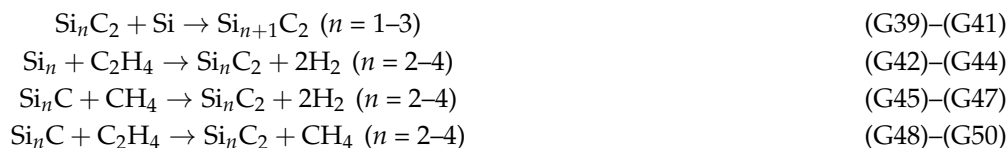


Figure 8 illustrates the ΔG variations during Si_nC_2 gas-phase formation and growth, confirming silicidation as a vital, spontaneous process ($\Delta G < 0$). The direct carbonization of pure Si clusters into double-carbon clusters features a specific equilibrium temperature. A comparison of CH_4 and C_2H_4 carbonization demonstrates that while initial small clusters thermodynamically prefer Si_nC formation, the continuously growing cluster skeletons predominantly exist as the more stable di-carbon species Si_nC_2 .

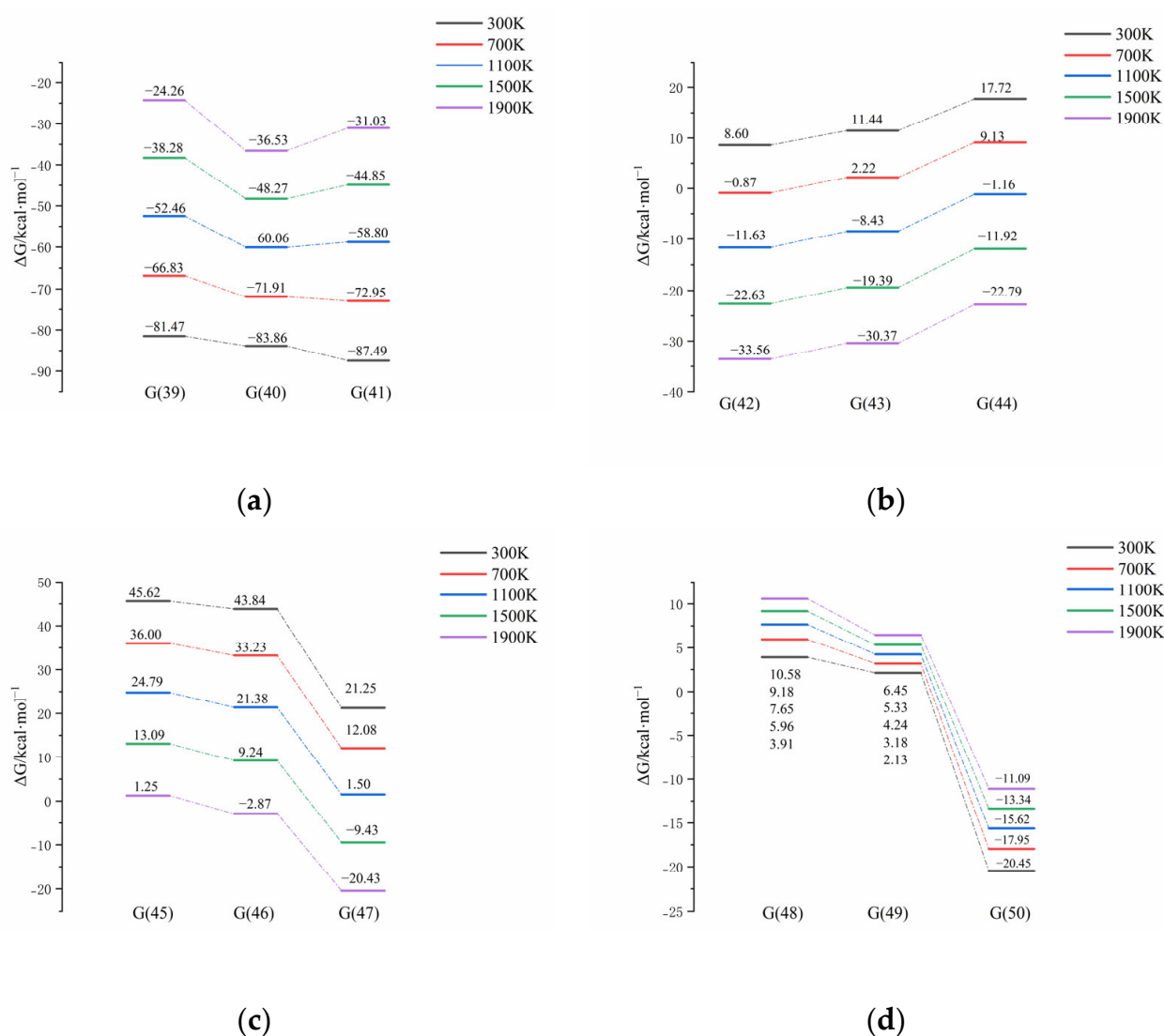


Figure 8. Evolution of ΔG for Si_nC_2 in the temperature range from 300 K to 1900 K. (a) denotes reactions (G39)–(G41); (b) denotes reactions (G42)–(G44); (c) denotes reactions (G45)–(G47); (d) denotes reactions (G48)–(G50).

4. Conclusions

In this study, DFT was systematically employed to investigate the formation and growth mechanisms of nanoparticle precursors, including Si_n , Si_nC , and Si_nC_2 , during the early-stage gas-phase nucleation in SiC-CVD. By analyzing the changes under various temperature conditions, the following key conclusions are drawn:

- (1) Continuous silicidation fundamentally drives cluster growth. Specifically, direct free Si atom addition yields the most negative, indicating the maximum thermodynamic spontaneity. Nevertheless, the inherent entropy reduction during successive silicidation leads to a decline in spontaneity as temperature increases.
- (2) The thermodynamic behavior of the clusters is highly size-dependent. Specifically, 2D-to-3D structural transitions, exemplified by the formation of Si_5 and Si_4C , disrupt the original planar stability, imposing a substantial deformation barrier during the 3D topological reconstruction.
- (3) During early gas-phase reactions, the system thermodynamically prefers Si_nC , whereas continuously growing clusters predominantly exist as the more stable Si_nC_2 . Additionally, as a reactant, ethylene is more prone to low-temperature addition reactions than methane.

Although this study establishes a thermodynamic foundation for early-stage cluster evolution, future investigations incorporating kinetic barrier evaluations and transition state theory are needed to fully capture the dynamic behavior of gas-phase nucleation under complex reactor conditions.

Author Contributions: P.S.: Writing—original draft, methodology, and investigation. S.T.: Writing—original draft and data curation. L.F.: Writing—review and editing and methodology. X.Y.: investigation. L.L.: supervision. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this study.

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