

Table 1. AIMD calculation results of total energy versus time for SWSiCNT with Al-doping at Si site

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Temperature (K)
1	5.0	-3947.24	0.3980	-3946.85	134.3
2	10.0	-3947.43	0.6886	-3946.74	232.6
3	15.0	-3947.44	0.7756	-3946.66	262.1
4	20.0	-3947.41	0.7152	-3946.69	241.1
5	25.0	-3947.44	0.7111	-3946.73	239.9
6	30.0	-3947.43	0.7242	-3946.70	243.5
7	35.0	-3947.46	0.7174	-3946.75	241.1
8	40.0	-3947.53	0.7246	-3946.81	243.8
9	45.0	-3947.57	0.7273	-3946.85	244.7
10	50.0	-3947.56	0.7425	-3946.82	249.7
11	55.0	-3947.59	0.7122	-3946.88	239.2
12	60.0	-3947.62	0.6713	-3946.95	225.8
13	65.0	-3947.61	0.6329	-3946.98	212.9
14	70.0	-3947.64	0.5953	-3947.05	200.2
15	75.0	-3947.63	0.5477	-3947.09	184.2
16	80.0	-3947.60	0.4892	-3947.11	164.6
17	85.0	-3947.57	0.4370	-3947.13	146.9
18	90.0	-3947.52	0.3877	-3947.13	130.3
19	95.0	-3947.48	0.3498	-3947.13	117.5
20	100.0	-3947.45	0.3210	-3947.13	108.2
21	105.0	-3947.44	0.3058	-3947.13	103.2
22	110.0	-3947.44	0.3126	-3947.13	105.4
23	115.0	-3947.46	0.3386	-3947.12	114.1
24	120.0	-3947.50	0.3962	-3947.11	132.8
25	125.0	-3947.53	0.4907	-3947.04	164.6
26	130.0	-3947.45	0.7367	-3946.71	247.8
27	135.0	-3947.58	0.8102	-3946.77	272.5
28	140.0	-3947.54	0.7622	-3946.78	256.4
29	145.0	-3947.41	0.6150	-3946.80	206.9
30	150.0	-3947.43	0.5957	-3946.84	200.4
31	155.0	-3947.47	0.6091	-3946.86	204.9
32	160.0	-3947.33	0.4741	-3946.85	159.5
33	165.0	-3947.24	0.3808	-3946.86	128.1
34	170.0	-3947.28	0.3949	-3946.88	132.8
35	175.0	-3947.26	0.3696	-3946.89	124.3
36	180.0	-3947.26	0.3841	-3946.88	129.2
37	185.0	-3947.42	0.5232	-3946.90	176.0
38	190.0	-3947.52	0.6309	-3946.89	212.2
39	195.0	-3947.50	0.6152	-3946.89	206.9
40	200.0	-3947.55	0.6491	-3946.90	218.3

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Temperature (K)
41	205.0	-3947.63	0.7099	-3946.92	238.8
42	210.0	-3947.60	0.6712	-3946.93	225.8
43	215.0	-3947.58	0.6486	-3946.94	218.2
44	220.0	-3947.62	0.6665	-3946.96	224.2
45	225.0	-3947.55	0.5746	-3946.98	193.3
46	230.0	-3947.41	0.4431	-3946.97	149.0
47	235.0	-3947.41	0.4234	-3946.98	142.4
48	240.0	-3947.41	0.4116	-3947.00	138.4
49	245.0	-3947.35	0.3449	-3947.01	116.0
50	250.0	-3947.35	0.3590	-3947.00	120.8

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+-----+
| MD  step   time   potential   kinetic   total   instant. |
| MD                energy   energy   energy   temperature |
| MD              (fs)   (eV)   (eV)   (eV)   (K) |
+-----+
| MD    0     0.0 -3.94683e+03  8.91894e-01 -3.94593e+03    300.0 |
+-----+

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+-----+
|   step   time   potential   kinetic   total   instant. |
|           energy   energy   energy   temperature |
|          (fs)   (eV)   (eV)   (eV)   (K) |
+-----+
| MD     1     5.0 -3.94676e+03  7.32639e-01 -3.94603e+03    246.4 |
+-----+

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+-----+
|   step   time   potential   kinetic   total   instant. |
|           energy   energy   energy   temperature |
|          (fs)   (eV)   (eV)   (eV)   (K) |
+-----+
| MD     2    10.0 -3.94674e+03  5.08718e-01 -3.94623e+03    171.1 |
+-----+

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+-----+
|   step   time   potential   kinetic   total   instant. |
|           energy   energy   energy   temperature |
|          (fs)   (eV)   (eV)   (eV)   (K) |
+-----+
| MD     3    15.0 -3.94694e+03  6.23563e-01 -3.94632e+03    209.7 |
+-----+

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step	time	potential	kinetic	total	instant.
		energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)
MD 4	20.0	-3.94713e+03	7.61866e-01	-3.94636e+03	256.3

step	time	potential	kinetic	total	instant.
		energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)
MD 5	25.0	-3.94700e+03	6.43063e-01	-3.94636e+03	216.3

step	time	potential	kinetic	total	instant.
		energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)
MD 6	30.0	-3.94701e+03	6.51906e-01	-3.94635e+03	219.3

step	time	potential	kinetic	total	instant.
		energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)
MD 7	35.0	-3.94729e+03	8.65426e-01	-3.94642e+03	291.1

step	time	potential	kinetic	total	instant.
		energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)
MD 8	40.0	-3.94732e+03	8.66701e-01	-3.94645e+03	291.5

step	time	potential	kinetic	total	instant.
		energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)
MD 9	45.0	-3.94721e+03	7.92860e-01	-3.94642e+03	266.7

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 10	50.0	-3.94743e+03	9.68982e-01	-3.94646e+03		325.9

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 11	55.0	-3.94757e+03	1.08520e+00	-3.94649e+03		365.0

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 12	60.0	-3.94740e+03	9.13892e-01	-3.94649e+03		307.4

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 13	65.0	-3.94732e+03	8.23643e-01	-3.94650e+03		277.0

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 14	70.0	-3.94739e+03	8.01841e-01	-3.94659e+03		269.7

step	time	potential	kinetic	total	instant.	

			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	15	75.0	-3.94717e+03	5.97210e-01	-3.94658e+03		200.9
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	16	80.0	-3.94707e+03	5.01003e-01	-3.94657e+03		168.5
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	17	85.0	-3.94720e+03	5.99576e-01	-3.94660e+03		201.7
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	18	90.0	-3.94709e+03	5.30590e-01	-3.94656e+03		178.5
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	19	95.0	-3.94703e+03	4.20724e-01	-3.94661e+03		141.5
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	20	100.0	-3.94722e+03	5.67126e-01	-3.94666e+03		190.8
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
MD	21	105.0	-3.94731e+03	6.45506e-01	-3.94667e+03		217.1

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
MD	22	110.0	-3.94723e+03	5.74596e-01	-3.94665e+03		193.3

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
MD	23	115.0	-3.94739e+03	6.91632e-01	-3.94669e+03		232.6

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
MD	24	120.0	-3.94759e+03	8.55684e-01	-3.94673e+03		287.8

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
MD	25	125.0	-3.94750e+03	8.00504e-01	-3.94670e+03		269.3

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
MD	26	130.0	-3.94745e+03	7.36732e-01	-3.94671e+03		247.8

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	27	135.0	-3.94758e+03	8.10161e-01	-3.94677e+03	272.5

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	28	140.0	-3.94754e+03	7.62189e-01	-3.94678e+03	256.4

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	29	145.0	-3.94741e+03	6.14971e-01	-3.94680e+03	206.9

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	30	150.0	-3.94743e+03	5.95737e-01	-3.94684e+03	200.4

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	31	155.0	-3.94747e+03	6.09111e-01	-3.94686e+03	204.9

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)

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+-----+
| MD    32    160.0 -3.94733e+03  4.74069e-01 -3.94685e+03    159.5 |
+-----+

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+-----+
|  step    time    potential    kinetic    total    instant. |
|          energy    energy    energy    temperature |
|          (fs)    (eV)    (eV)    (eV)    (K) |
+-----+
| MD    33    165.0 -3.94724e+03  3.80800e-01 -3.94686e+03    128.1 |
+-----+

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+-----+
|  step    time    potential    kinetic    total    instant. |
|          energy    energy    energy    temperature |
|          (fs)    (eV)    (eV)    (eV)    (K) |
+-----+
| MD    34    170.0 -3.94728e+03  3.94929e-01 -3.94688e+03    132.8 |
+-----+

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+-----+
|  step    time    potential    kinetic    total    instant. |
|          energy    energy    energy    temperature |
|          (fs)    (eV)    (eV)    (eV)    (K) |
+-----+
| MD    35    175.0 -3.94726e+03  3.69563e-01 -3.94689e+03    124.3 |
+-----+

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+-----+
|  step    time    potential    kinetic    total    instant. |
|          energy    energy    energy    temperature |
|          (fs)    (eV)    (eV)    (eV)    (K) |
+-----+
| MD    36    180.0 -3.94726e+03  3.84140e-01 -3.94688e+03    129.2 |
+-----+

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+-----+
|  step    time    potential    kinetic    total    instant. |
|          energy    energy    energy    temperature |
|          (fs)    (eV)    (eV)    (eV)    (K) |
+-----+
| MD    37    185.0 -3.94742e+03  5.23239e-01 -3.94690e+03    176.0 |
+-----+

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+-----+

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	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	38	190.0	-3.94752e+03	6.30869e-01	-3.94689e+03		212.2
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	39	195.0	-3.94750e+03	6.15150e-01	-3.94689e+03		206.9
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	40	200.0	-3.94755e+03	6.49115e-01	-3.94690e+03		218.3
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	41	205.0	-3.94763e+03	7.09970e-01	-3.94692e+03		238.8
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	42	210.0	-3.94760e+03	6.71187e-01	-3.94693e+03		225.8
+-----+							

	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	43	215.0	-3.94758e+03	6.48556e-01	-3.94694e+03		218.2
+-----+							


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+-----+
| MD    49    245.0 -3.94735e+03  3.44924e-01 -3.94701e+03    116.0 |
+-----+

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+-----+
|  step    time    potential    kinetic    total    instant. |
|          energy    energy    energy    temperature |
|          (fs)    (eV)    (eV)    (eV)    (K) |
+-----+
| MD    50    250.0 -3.94735e+03  3.59037e-01 -3.94700e+03    120.8 |
+-----+

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+-----+
| Forces Report                                     |
+-----+

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| Index Element      Force (eV/Ang)                |
|          x        y        z  magnitude          |
+-----+
|  0   Si   0.11878   0.80333   0.69992   1.07207   |
|  1    C   0.02290  -0.38356  -0.81429   0.90040   |
|  2    C   0.10428  -0.74017  -0.59076   0.95274   |
|  3   Si   0.29198   0.04443   0.53298   0.60933   |
|  4    C  -0.34472   0.12173  -0.40678   0.54692   |
|  5   Si  -0.02574   0.69803   0.72933   1.00987   |
|  6    C   0.30229  -0.39703  -0.59112   0.77358   |
|  7   Si  -0.17079   0.68742  -0.23446   0.74612   |
|  8    C  -0.10737  -0.40793   0.58564   0.72174   |
|  9   Si   0.31486   0.38835   0.36647   0.61988   |
| 10    C  -0.27348  -0.65177  -0.31033   0.77195   |
| 11   Al   0.05967  -0.11970  -0.30218   0.33045   |
| 12    C  -0.00747  -0.29201   0.09904   0.30844   |
| 13   Si  -0.34034   0.63914   0.04894   0.72576   |
| 14    C  -0.41427   0.46457   0.15413   0.64125   |
| 15   Si  -0.69092  -0.28612  -0.28743   0.80115   |
| 16    C   0.07616  -0.81773   1.04614   1.32999   |
| 17   Si  -0.43063   0.38941  -0.88285   1.05664   |
| 18    C  -0.52933   0.03492   0.98483   1.11861   |
| 19   Si   0.93551   0.17854  -0.75637   1.21621   |
| 20    C  -0.09890  -0.37151  -0.19285   0.43010   |
| 21   Si   0.27299  -0.59571  -0.37912   0.75706   |
| 22    C   0.33092   0.22925   0.47241   0.62067   |
| 23   Si   0.60597   0.38211   0.04202   0.71761   |
+-----+

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| Net force      0.00236  -0.00202   0.01332          |
+-----+
+-----+

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Stress Report			
+-----+			
[[-7.10391835e-03 9.32356581e-04 -5.18593418e-05]			
[9.32356581e-04 -2.96118638e-03 1.84547570e-03]			
[-5.18593418e-05 1.84547570e-03 -4.51923152e-03]] eV/Ang**3			
+-----+			
+-----+			
Total Energy Analysis			
+-----+			
Electrostatic = -3857.25309 eV			
Entropy-Term = -0.00141 eV			
Exchange-Correlation = -1879.62127 eV			
External-Field = 0.00000 eV			
Hubbard-Term = -0.04011 eV			
Kinetic = 1789.76643 eV			
+-----+			
Total free energy = -3947.14946 eV			
Total energy (broadening->0) = -3947.14875 eV			
+-----+			

Table 2. AIMD calculation results of total energy versus time for SWSiCNT with Ga-doping at Si site

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Temperature (K)
0	0.0	-4045.31	0.891894	-4044.42	300.0
1	5.0	-4045.15	0.746371	-4044.41	251.1
2	10.0	-4045.04	0.622016	-4044.42	209.2
3	15.0	-4045.20	0.761397	-4044.44	256.1
4	20.0	-4045.37	0.891578	-4044.47	299.9
5	25.0	-4045.34	0.859964	-4044.48	289.3
6	30.0	-4045.35	0.895718	-4044.46	301.3
7	35.0	-4045.53	1.01353	-4044.52	340.9
8	40.0	-4045.39	0.875470	-4044.52	294.5
9	45.0	-4045.26	0.736475	-4044.52	247.7
10	50.0	-4045.47	0.891815	-4044.58	300.0
11	55.0	-4045.50	0.905289	-4044.60	304.5
12	60.0	-4045.22	0.653848	-4044.57	219.9
13	65.0	-4045.19	0.613739	-4044.58	206.4
14	70.0	-4045.40	0.770687	-4044.63	259.2
15	75.0	-4045.32	0.688420	-4044.64	231.6
16	80.0	-4045.15	0.537848	-4044.61	180.9
17	85.0	-4045.23	0.636995	-4044.59	214.3

Step Time (fs)		Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Temperature (K)
18	90.0	-4045.23	0.717311	-4044.51	241.3
19	95.0	-4045.07	0.594271	-4044.47	199.9
20	100.0	-4045.24	0.593545	-4044.64	199.6
21	105.0	-4045.40	0.703891	-4044.69	236.8
22	110.0	-4045.39	0.682764	-4044.71	229.7
23	115.0	-4045.41	0.652682	-4044.75	219.5
24	120.0	-4045.42	0.637984	-4044.78	214.6
25	125.0	-4045.44	0.638311	-4044.80	214.7
26	130.0	-4045.53	0.701893	-4044.83	236.1
27	135.0	-4045.64	0.793001	-4044.85	266.7
28	140.0	-4045.61	0.759251	-4044.85	255.4
29	145.0	-4045.52	0.662992	-4044.86	223.0
30	150.0	-4045.57	0.695707	-4044.88	234.0
31	155.0	-4045.63	0.710028	-4044.92	238.8
32	160.0	-4045.50	0.570238	-4044.93	191.8
33	165.0	-4045.47	0.520435	-4044.95	175.1
34	170.0	-4045.57	0.601049	-4044.97	202.2
35	175.0	-4045.59	0.594285	-4044.99	199.9
36	180.0	-4045.45	0.466738	-4044.98	157.0
37	185.0	-4045.39	0.408569	-4044.99	137.4
38	190.0	-4045.46	0.457079	-4045.00	153.7
39	195.0	-4045.50	0.500231	-4045.00	168.3
40	200.0	-4045.55	0.545650	-4045.00	183.5
41	205.0	-4045.62	0.640647	-4044.98	215.5
42	210.0	-4045.65	0.685311	-4044.96	230.5
43	215.0	-4045.61	0.633452	-4044.98	213.1
44	220.0	-4045.55	0.613702	-4044.93	206.4
45	225.0	-4045.55	0.577407	-4044.98	194.2
46	230.0	-4045.44	0.503735	-4044.93	169.4
47	235.0	-4045.40	0.578970	-4044.82	194.7
48	240.0	-4045.49	0.604564	-4044.89	203.4
49	245.0	-4045.32	0.445369	-4044.88	149.8
50	250.0	-4045.24	0.360813	-4044.88	121.4

+-----+						
MD	step	time	potential	kinetic	total	instant.
MD			energy	energy	energy	temperature
MD		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	0	0.0	-4.04531e+03	8.91894e-01	-4.04442e+03	300.0

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 1	5.0	-4.04515e+03	7.46371e-01	-4.04441e+03	251.1	
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 2	10.0	-4.04504e+03	6.22016e-01	-4.04442e+03	209.2	
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 3	15.0	-4.04520e+03	7.61397e-01	-4.04444e+03	256.1	
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 4	20.0	-4.04537e+03	8.91578e-01	-4.04447e+03	299.9	

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	5	25.0	-4.04534e+03	8.59964e-01	-4.04448e+03	289.3
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	6	30.0	-4.04535e+03	8.95718e-01	-4.04446e+03	301.3
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	7	35.0	-4.04553e+03	1.01353e+00	-4.04452e+03	340.9
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	8	40.0	-4.04539e+03	8.75470e-01	-4.04452e+03	294.5

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 9	45.0	-4.04526e+03	7.36475e-01	-4.04452e+03	247.7	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 10	50.0	-4.04547e+03	8.91815e-01	-4.04458e+03	300.0	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 11	55.0	-4.04550e+03	9.05289e-01	-4.04460e+03	304.5	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 12	60.0	-4.04522e+03	6.53848e-01	-4.04457e+03	219.9	

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	13	65.0	-4.04519e+03	6.13739e-01	-4.04458e+03	206.4
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	14	70.0	-4.04540e+03	7.70687e-01	-4.04463e+03	259.2
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	15	75.0	-4.04532e+03	6.88420e-01	-4.04464e+03	231.6
+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	16	80.0	-4.04515e+03	5.37848e-01	-4.04461e+03	180.9

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	17	85.0	-4.04523e+03	6.36995e-01	-4.04459e+03 214.3

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	18	90.0	-4.04523e+03	7.17311e-01	-4.04451e+03 241.3

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	19	95.0	-4.04507e+03	5.94271e-01	-4.04447e+03 199.9

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	20	100.0	-4.04524e+03	5.93545e-01	-4.04464e+03 199.6

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	21	105.0	-4.04540e+03	7.03891e-01	-4.04469e+03 236.8

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	22	110.0	-4.04539e+03	6.82764e-01	-4.04471e+03 229.7

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	23	115.0	-4.04541e+03	6.52682e-01	-4.04475e+03 219.5

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	24	120.0	-4.04542e+03	6.37984e-01	-4.04478e+03 214.6

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 25	125.0	-4.04544e+03	6.38311e-01	-4.04480e+03	214.7	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 26	130.0	-4.04553e+03	7.01893e-01	-4.04483e+03	236.1	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 27	135.0	-4.04564e+03	7.93001e-01	-4.04485e+03	266.7	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 28	140.0	-4.04561e+03	7.59251e-01	-4.04485e+03	255.4	

+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
	MD	29	145.0	-4.04552e+03	6.62992e-01	-4.04486e+03	223.0

+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
	MD	30	150.0	-4.04557e+03	6.95707e-01	-4.04488e+03	234.0
+-----+							

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	31	155.0	-4.04563e+03	7.10028e-01	-4.04492e+03 238.8
+-----+						
+-----+						

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	32	160.0	-4.04550e+03	5.70238e-01	-4.04493e+03	191.8

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 33	165.0	-4.04547e+03	5.20435e-01	-4.04495e+03	175.1	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 34	170.0	-4.04557e+03	6.01049e-01	-4.04497e+03	202.2	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 35	175.0	-4.04559e+03	5.94285e-01	-4.04499e+03	199.9	
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
MD 36	180.0	-4.04545e+03	4.66738e-01	-4.04498e+03	157.0	

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 37	185.0	-4.04539e+03	4.08569e-01	-4.04499e+03		137.4

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 38	190.0	-4.04546e+03	4.57079e-01	-4.04500e+03		153.7

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 39	195.0	-4.04550e+03	5.00231e-01	-4.04500e+03		168.3

+-----+						
+-----+						
step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD 40	200.0	-4.04555e+03	5.45650e-01	-4.04500e+03		183.5

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	41	205.0	-4.04562e+03	6.40647e-01	-4.04498e+03	215.5

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	42	210.0	-4.04565e+03	6.85311e-01	-4.04496e+03	230.5

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	43	215.0	-4.04561e+03	6.33452e-01	-4.04498e+03	213.1

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	44	220.0	-4.04555e+03	6.13702e-01	-4.04493e+03	206.4

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	45	225.0	-4.04555e+03	5.77407e-01	-4.04498e+03 194.2

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	46	230.0	-4.04544e+03	5.03735e-01	-4.04493e+03 169.4

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	47	235.0	-4.04540e+03	5.78970e-01	-4.04482e+03 194.7

+-----+						
+-----+						
	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	48	240.0	-4.04549e+03	6.04564e-01	-4.04489e+03 203.4

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
	MD	49	245.0	-4.04532e+03	4.45369e-01	-4.04488e+03 149.8

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
	MD	50	250.0	-4.04524e+03	3.60813e-01	-4.04488e+03 121.4

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	Index	Element	Force (eV/Ang)				
			x	y	z	magnitude	
	0	Si	0.10887	-0.41080	-1.05163	1.13426	
	1	C	-0.50613	1.34200	0.82062	1.65244	
	2	C	-0.03632	0.44969	-0.77201	0.89418	
	3	Si	0.56696	0.33158	-0.01193	0.65691	
	4	C	0.02703	-0.48418	-1.14340	1.24199	
	5	Si	-0.02885	-0.72526	0.10431	0.73329	
	6	C	0.24873	0.02906	-0.34427	0.42571	

Total Energy Analysis		
+-----+		
Electrostatic	= -3847.54609 eV	
Entropy-Term	= -0.00233 eV	
Exchange-Correlation	= -1975.11684 eV	
External-Field	= 0.00000 eV	
Hubbard-Term	= 6.43579 eV	
Kinetic	= 1771.13798 eV	
+-----+		
Total free energy	= -4045.09149 eV	
Total energy (broadening->0)	= -4045.09033 eV	
+-----+		

Table 3. AIMD calculation results of total energy versus time for SWSiCNT with Al-doping at C site

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Instant. Temperature (K)
0	0.0	-3962.37	0.89189	-3961.48	300.0
1	5.0	-3963.91	2.12496	-3961.79	714.8
2	10.0	-3966.61	4.75837	-3961.85	1600.5
3	15.0	-3967.95	6.11065	-3961.84	2055.4
4	20.0	-3967.78	5.91322	-3961.87	1989.0
5	25.0	-3967.23	5.32212	-3961.91	1790.2

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Instant. Temperature (K)
6	30.0	-3966.86	4.89949	-3961.96	1648.0
7	35.0	-3966.61	4.71963	-3961.89	1587.5
8	40.0	-3966.22	4.50245	-3961.71	1514.5
9	45.0	-3965.88	4.16759	-3961.71	1401.8
10	50.0	-3965.56	3.90775	-3961.65	1314.4
11	55.0	-3965.49	3.66070	-3961.83	1231.3
12	60.0	-3965.01	3.13084	-3961.88	1053.1
13	65.0	-3964.11	2.42644	-3961.69	816.2
14	70.0	-3963.58	1.99767	-3961.58	671.9
15	75.0	-3963.79	2.05895	-3961.73	692.6
16	80.0	-3964.50	2.66121	-3961.84	895.1
17	85.0	-3965.26	3.70242	-3961.55	1245.4
18	90.0	-3966.18	4.38525	-3961.80	1475.0
19	95.0	-3966.11	4.27761	-3961.83	1438.8
20	100.0	-3965.56	3.82491	-3961.73	1286.6
21	105.0	-3965.38	3.46519	-3961.92	1165.6
22	110.0	-3964.98	3.15213	-3961.83	1060.3
23	115.0	-3964.40	2.80062	-3961.59	942.0
24	120.0	-3964.19	2.47644	-3961.71	833.0
25	125.0	-3964.11	2.30922	-3961.80	776.7
26	130.0	-3964.16	2.35522	-3961.81	792.2
27	135.0	-3964.42	2.57263	-3961.84	865.3
28	140.0	-3964.48	3.09272	-3961.39	1040.3
29	145.0	-3965.56	3.88096	-3961.68	1305.4
30	150.0	-3966.08	4.30478	-3961.77	1448.0
31	155.0	-3966.36	4.72623	-3961.63	1589.7
32	160.0	-3965.86	5.09227	-3960.77	1712.9
33	165.0	-3966.56	4.84666	-3961.71	1630.2
34	170.0	-3966.12	4.28448	-3961.83	1441.1
35	175.0	-3965.36	3.58772	-3961.78	1206.8
36	180.0	-3964.90	3.09526	-3961.80	1041.1
37	185.0	-3965.00	3.26964	-3961.73	1099.8
38	190.0	-3965.32	3.69399	-3961.62	1242.5
39	195.0	-3965.45	3.82866	-3961.62	1287.8
40	200.0	-3965.39	3.84550	-3961.55	1293.5
41	205.0	-3965.27	4.09668	-3961.17	1378.0
42	210.0	-3965.54	4.22260	-3961.31	1420.3
43	215.0	-3965.44	4.18508	-3961.26	1407.7
44	220.0	-3965.71	4.55160	-3961.16	1531.0
45	225.0	-3966.27	5.03524	-3961.24	1693.7
46	230.0	-3966.81	5.48075	-3961.33	1843.5
47	235.0	-3966.92	5.57878	-3961.34	1876.5
48	240.0	-3966.07	4.97926	-3961.09	1674.8
49	245.0	-3965.47	4.44788	-3961.02	1496.1
50	250.0	-3965.38	4.41965	-3960.96	1486.6

MD	step	time	potential	kinetic	total	instant.
MD			energy	energy	energy	temperature
MD		(fs)	(eV)	(eV)	(eV)	(K)
MD	0	0.0	-3.96237e+03	8.91894e-01	-3.96148e+03	300.0

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	1	5.0	-3.96391e+03	2.12496e+00	-3.96179e+03	714.8

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
MD	2	10.0	-3.96661e+03	4.75837e+00	-3.96185e+03	1600.5

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature

		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	3	15.0	-3.96795e+03	6.11065e+00	-3.96184e+03	2055.4	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	4	20.0	-3.96778e+03	5.91322e+00	-3.96187e+03	1989.0	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	5	25.0	-3.96723e+03	5.32212e+00	-3.96191e+03	1790.2	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	6	30.0	-3.96686e+03	4.89949e+00	-3.96196e+03	1648.0	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	

		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	7	35.0	-3.96661e+03	4.71963e+00	-3.96189e+03	1587.5	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	8	40.0	-3.96622e+03	4.50245e+00	-3.96171e+03	1514.5	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	9	45.0	-3.96588e+03	4.16759e+00	-3.96171e+03	1401.8	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	10	50.0	-3.96556e+03	3.90775e+00	-3.96165e+03	1314.4	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	

		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	11	55.0	-3.96549e+03	3.66070e+00	-3.96183e+03	1231.3	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	12	60.0	-3.96501e+03	3.13084e+00	-3.96188e+03	1053.1	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	13	65.0	-3.96411e+03	2.42644e+00	-3.96169e+03	816.2	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	14	70.0	-3.96358e+03	1.99767e+00	-3.96158e+03	671.9	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	

		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	15	75.0	-3.96379e+03	2.05895e+00	-3.96173e+03	692.6	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	16	80.0	-3.96450e+03	2.66121e+00	-3.96184e+03	895.1	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	17	85.0	-3.96526e+03	3.70242e+00	-3.96155e+03	1245.4	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	18	90.0	-3.96618e+03	4.38525e+00	-3.96180e+03	1475.0	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	

			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	19	95.0	-3.96611e+03	4.27761e+00	-3.96183e+03		1438.8
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	20	100.0	-3.96556e+03	3.82491e+00	-3.96173e+03		1286.6
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	21	105.0	-3.96538e+03	3.46519e+00	-3.96192e+03		1165.6
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	22	110.0	-3.96498e+03	3.15213e+00	-3.96183e+03		1060.3
+-----+							
+-----+							

Forces Report							
+-----+							
	Index	Element	Force (eV/Ang)				
			x	y	z	magnitude	
+-----+							
	0	Si	-0.71879	-0.17943	-0.59889	0.95264	
	1	C	-0.28937	0.73280	-0.12728	0.79808	
	2	C	-0.81996	-0.71864	-0.57712	1.23363	
	3	Si	1.99034	-1.00794	1.53579	2.70852	
	4	C	-0.93253	-1.43587	-0.56057	1.80155	
	5	Si	0.09704	-1.86558	0.29869	1.89183	
	6	C	-1.52043	0.11036	-0.37196	1.56916	
	7	Si	0.67333	1.76912	-1.97540	2.73594	
	8	C	1.23494	1.63113	0.37466	2.07991	
	9	Si	-1.15443	1.47760	1.29814	2.28061	
	10	C	0.01409	-2.26273	-1.47871	2.70310	
	11	Si	0.62895	-0.54792	0.58600	1.01940	
	12	C	-0.31543	-1.94555	-0.94022	2.18374	
	13	Si	0.17243	-0.58801	2.57155	2.64355	
	14	Al	0.37583	0.58732	-0.83420	1.08724	
	15	Si	0.50891	0.70450	2.71955	2.85504	
	16	C	-0.17041	-1.46167	-0.86760	1.70829	
	17	Si	-0.94519	1.63912	-0.78732	2.04939	
	18	C	-1.21606	-0.65278	0.02144	1.38036	
	19	Si	1.21328	1.62798	-0.19233	2.03945	
	20	C	-0.69967	-0.00832	-0.73342	1.01366	
	21	Si	2.42973	1.41075	-1.30180	3.09652	
	22	C	-0.25290	-0.41639	0.72043	0.86969	

	23	Si	-0.32809	1.37078	1.24546	1.88092	
+-----+							
	Net force		-0.02441	-0.02938	0.02489		
+-----+							
+-----+							
	Total Energy Analysis						
+-----+							
	Electrostatic		= -3716.83748 eV				
	Entropy-Term		= -0.01006 eV				
	Exchange-Correlation		= -1916.27345 eV				
	External-Field		= 0.00000 eV				
	Hubbard-Term		= 2.01793 eV				
	Kinetic		= 1665.72618 eV				
+-----+							
	Total free energy		= -3965.37688 eV				
	Total energy (broadening->0)		= -3965.37185 eV				
+-----+							

Table 4. AIMD calculation results of total energy versus time for SWSiCNT with Ga-doping at C site

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Instant. Temperature (K)
0	0.0	-4063.33	0.89189	-4062.44	300.0
1	5.0	-4064.66	1.98269	-4062.68	666.9
2	10.0	-4066.35	3.66300	-4062.69	1232.1
3	15.0	-4067.74	4.80058	-4062.94	1614.7
4	20.0	-4067.70	4.80684	-4062.89	1616.8
5	25.0	-4066.56	4.10224	-4062.46	1379.8
6	30.0	-4066.49	3.78840	-4062.70	1274.3
7	35.0	-4066.60	3.80809	-4062.79	1280.9
8	40.0	-4066.12	3.39592	-4062.72	1142.3

Step	Time (fs)	Potential Energy (eV)	Kinetic Energy (eV)	Total Energy (eV)	Instant. Temperature (K)
9	45.0	-4065.67	2.96639	-4062.70	997.8
10	50.0	-4065.71	2.89914	-4062.82	975.2
11	55.0	-4065.39	2.82537	-4062.57	950.4
12	60.0	-4065.39	2.59545	-4062.79	873.0
13	65.0	-4064.86	2.17214	-4062.69	730.6
14	70.0	-4064.49	1.78163	-4062.71	599.3
15	75.0	-4063.94	1.64990	-4062.29	555.0
16	80.0	-4064.82	1.90671	-4062.91	641.3
17	85.0	-4065.38	2.33960	-4063.04	787.0
18	90.0	-4065.98	2.89360	-4063.09	973.3
19	95.0	-4066.56	3.37148	-4063.19	1134.0
20	100.0	-4066.69	3.44798	-4063.24	1159.8
21	105.0	-4066.54	3.23601	-4063.31	1088.5
22	110.0	-4066.42	3.04684	-4063.37	1024.8
23	115.0	-4066.11	2.89843	-4063.21	974.9
24	120.0	-4066.22	2.70025	-4063.52	908.3
25	125.0	-4065.50	2.45982	-4063.04	827.4
26	130.0	-4065.34	2.45697	-4062.88	826.4
27	135.0	-4065.23	2.80407	-4062.42	943.2
28	140.0	-4065.09	3.12364	-4061.96	1050.7
29	145.0	-4065.40	3.14209	-4062.25	1056.9
30	150.0	-4066.56	3.52219	-4063.03	1184.7
31	155.0	-4066.14	3.99507	-4062.14	1343.8
32	160.0	-4067.11	4.15149	-4062.95	1396.4
33	165.0	-4067.19	4.34738	-4062.84	1462.3
34	170.0	-4067.52	4.62324	-4062.89	1555.1
35	175.0	-4067.45	4.57172	-4062.88	1537.8
36	180.0	-4067.04	4.15065	-4062.89	1396.1
37	185.0	-4066.60	3.79043	-4062.81	1275.0
38	190.0	-4066.23	3.45061	-4062.77	1160.7
39	195.0	-4065.95	2.99697	-4062.96	1008.1
40	200.0	-4065.45	2.65791	-4062.79	894.0
41	205.0	-4065.73	2.68551	-4063.05	903.3
42	210.0	-4065.74	2.72605	-4063.01	916.9
43	215.0	-4065.70	2.75671	-4062.94	927.3
44	220.0	-4066.15	3.10760	-4063.04	1045.3
45	225.0	-4066.26	3.19911	-4063.06	1076.1
46	230.0	-4065.91	2.84111	-4063.07	955.6
47	235.0	-4066.00	2.80205	-4063.20	942.5
48	240.0	-4065.97	2.78554	-4063.19	937.0
49	245.0	-4065.90	2.70516	-4063.19	909.9
50	250.0	-4065.89	2.66615	-4063.23	896.8

+-----+

MD	step	time	potential	kinetic	total	instant.	
MD			energy	energy	energy	temperature	
MD		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	0	0.0	-4.06333e+03	8.91894e-01	-4.06244e+03	300.0	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	1	5.0	-4.06466e+03	1.98269e+00	-4.06268e+03	666.9	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	2	10.0	-4.06635e+03	3.66300e+00	-4.06269e+03	1232.1	
+-----+							
+-----+							
	step	time	potential	kinetic	total	instant.	
			energy	energy	energy	temperature	
		(fs)	(eV)	(eV)	(eV)	(K)	
+-----+							
MD	3	15.0	-4.06774e+03	4.80058e+00	-4.06294e+03	1614.7	
+-----+							
+-----+							

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	8	40.0	-4.06612e+03	3.39592e+00	-4.06272e+03	1142.3

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	9	45.0	-4.06567e+03	2.96639e+00	-4.06270e+03	997.8

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	10	50.0	-4.06571e+03	2.89914e+00	-4.06282e+03
						975.2

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
		(fs)	(eV)	(eV)	(eV)	(K)
+-----+						
	MD	11	55.0	-4.06539e+03	2.82537e+00	-4.06257e+03
						950.4

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	16	80.0	-4.06482e+03	1.90671e+00	-4.06291e+03	641.3

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	17	85.0	-4.06538e+03	2.33960e+00	-4.06304e+03	787.0

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	18	90.0	-4.06598e+03	2.89360e+00	-4.06309e+03	973.3

	step	time	potential	kinetic	total	instant.
			energy	energy	energy	temperature
	(fs)	(eV)	(eV)	(eV)	(eV)	(K)
+-----+						
MD	19	95.0	-4.06656e+03	3.37148e+00	-4.06319e+03	1134.0

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	48	240.0	-4.06597e+03	2.78554e+00	-4.06319e+03	937.0
+-----+						
+-----+						

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	49	245.0	-4.06590e+03	2.70516e+00	-4.06319e+03	909.9
+-----+						
+-----+						

step	time	potential	kinetic	total	instant.	
		energy	energy	energy	temperature	
	(fs)	(eV)	(eV)	(eV)	(K)	
+-----+						
MD	50	250.0	-4.06589e+03	2.66615e+00	-4.06323e+03	896.8
+-----+						
+-----+						

+-----+						
Forces Report						
+-----+						

Index	Element	Force (eV/Ang)				
		x	y	z	magnitude	
+-----+						
0	Si	-1.40047	0.41450	0.70543	1.62196	

	1	C	1.17061	-0.71716	-0.24532	1.39457	
	2	C	0.53877	0.17875	-1.06800	1.20948	
	3	Si	0.62526	-0.51512	0.42630	0.91544	
	4	C	0.29359	-0.59187	0.64128	0.92073	
	5	Si	-0.88036	-1.02909	0.68680	1.51847	
	6	C	-0.27079	-0.41282	-0.39395	0.63163	
	7	Si	-0.83648	1.67837	0.67729	1.99383	
	8	C	-0.72665	-1.43518	-1.32286	2.08272	
	9	Si	-0.54575	-0.58770	-0.81576	1.14398	
	10	C	1.53337	1.17557	0.82101	2.09934	
	11	Si	-1.01075	1.21999	-0.67679	1.72280	
	12	C	1.64836	-1.13989	-0.35377	2.03509	
	13	Si	-0.25424	-0.13636	-0.11894	0.31206	
	14	Ga	1.14138	0.01314	-0.12887	1.14871	
	15	Si	-2.39131	-0.65082	0.39674	2.50985	
	16	C	0.75612	0.07370	1.04697	1.29356	
	17	Si	-1.07873	1.29821	0.20481	1.70028	
	18	C	1.21174	-0.75218	-0.83572	1.65303	
	19	Si	0.91617	0.23907	0.99772	1.37548	
	20	C	0.90753	0.54617	0.84352	1.35405	
	21	Si	0.20701	-0.11388	-0.85161	0.88378	
	22	C	-0.95913	0.04890	-0.45917	1.06450	
	23	Si	-0.59172	1.20681	-0.17271	1.35512	

+-----+

Net force	0.00354	0.01111	0.00440	
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+-----+

+-----+

Stress Report	
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+-----+		
	[[0.00169825 0.00073565 -0.00569654]	
	[0.00073565 0.00382095 0.00076682]	
	[-0.00569654 0.00076682 -0.00155283]] eV/Ang**3	
+-----+		
+-----+		
	Total Energy Analysis	
+-----+		
	Electrostatic = -3738.67741 eV	
	Entropy-Term = -0.00740 eV	
	Exchange-Correlation = -2025.10146 eV	
	External-Field = 0.00000 eV	
	Hubbard-Term = -0.82116 eV	
	Kinetic = 1698.78927 eV	
+-----+		
	Total free energy = -4065.81815 eV	
	Total energy (broadening->0) = -4065.81445 eV	
+-----+		