Electronic Supplementary Information (ESI) for

p-Block Element-doped Silicon Nanowires for Nitrogen Reduction Reaction: A DFT Study

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1. Si nanowire (SiNW) models

1.1 Pristine SiNW

The fully optimized pritine SiNW model with the <110> growth direction is shown in Fig. S1, which is constructed according to the report by Tachibana *et al*.[1] The pristine SiNW, which is in a supercell with the length of 12.896 (a) ×15.410 (b) ×20.779 (c) (Å) and angles of α = β = γ = 90°, consists of eight layers of silicon atoms, and each layer has three or four silicon atoms. As a result, two types of silicon atoms are exposed, i.e. Si_{3C} & Si_{2C}. Then all dangling bonds on the surface of SiNW are terminated with H adatoms.

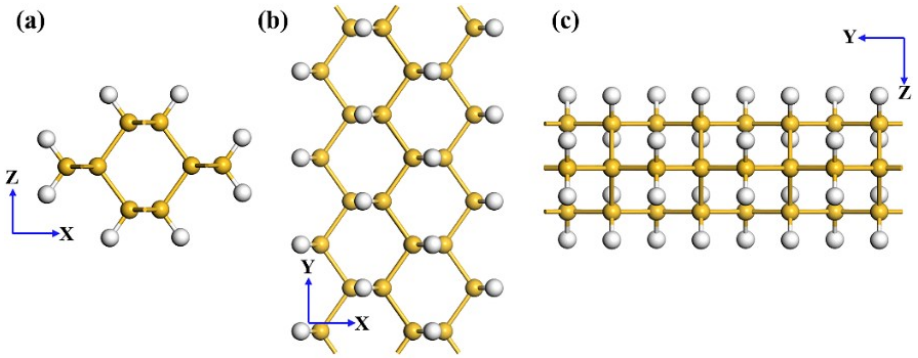

Fig. S1 Diagram of H-terminated pristine SiNW. Si (yellow), H (white).

1.2 B, C, P-doped SiNW

For checking the ability of nitrogen fixation on SiNW, one or two terminating H adatom(s) must be removed. After the remove of H adatom(s), two types of the Si atom on the surface of SiNW are exposed, i.e. three-coordinated (3C) and two-coordinated (2C). In addition, the corresponding exposed Si atom was substituted by a B (boron), C (carbon) or P (phosphorus) atom to modify the local properties of SiNW for nitrogen reduction reaction. Their models were fully relaxed during geometry optimizations (the computational setting is shown in the section of Calculation Details in the manuscript) and displayed in Fig. S2. Besides, according to SiNWs models with different active sites, shown in Fig S2, these catalysts models were also named as Si_{3C}, Si_{2C}, B_{3C}, B_{2C}, C_{3C}, C_{2C}, P_{3C}, and P_{2C}, respectively.

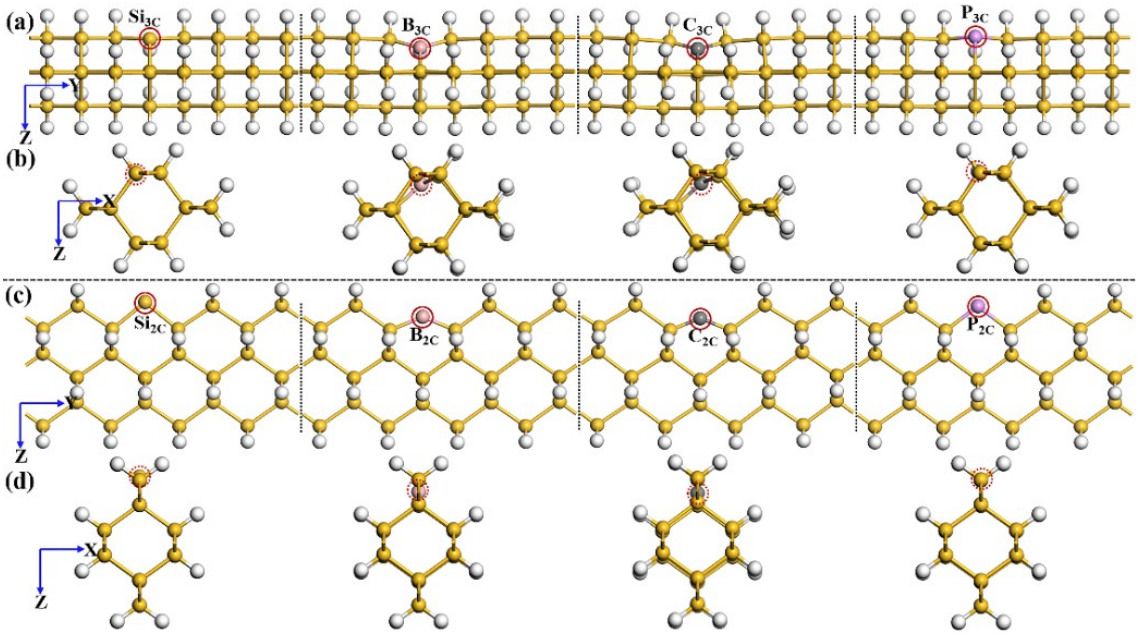

Fig. S2 Pristine and B, C and P-doped SiNWs with three-coordinated (a, b) and two-coordinated active sites (c, d). Note that, compared with the models in the upper panel (above the dash black line), the models in the lower panel were rotated by 90° along the Y axis in the supercell with the length of 12.896 (a) ×15.410 (b) ×25.779 (c) (Å) and angles of $\alpha = \beta = \gamma = 90°$. The long c lengthes (>20 Å) of two supercells can avoid the fallacious interactions from the imaginary models. Color scheme: Si (yellow), H (White), B (pink), C (grey), P (purple).

2. NRR pathways

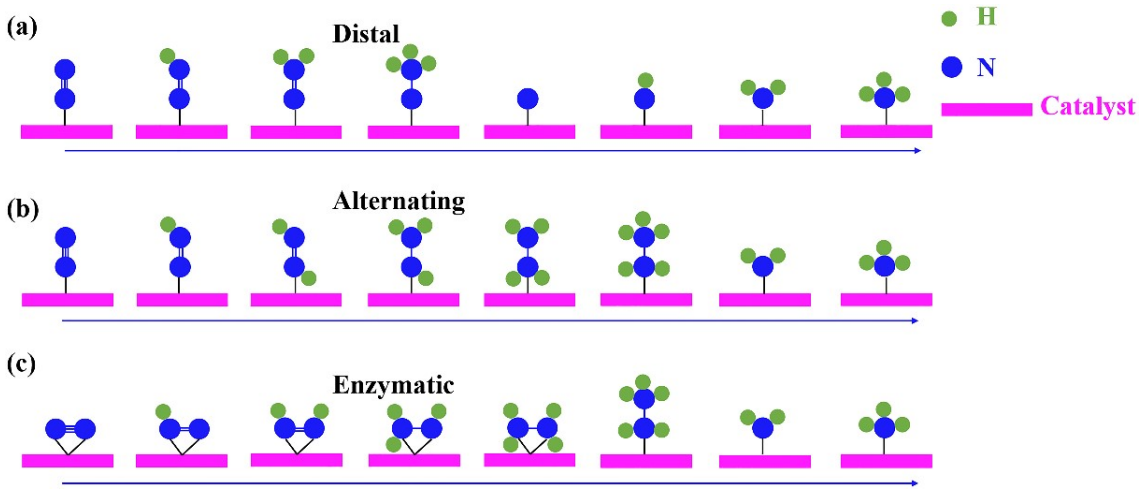

Fig. S3 Schematic diagram of NRR pathways, including (a) distal, (b) alternating and (c) enzymatic ones.

3. NRR on Si nanowires (SiNWs)

3.1 NRR pathways on Si_{3C}

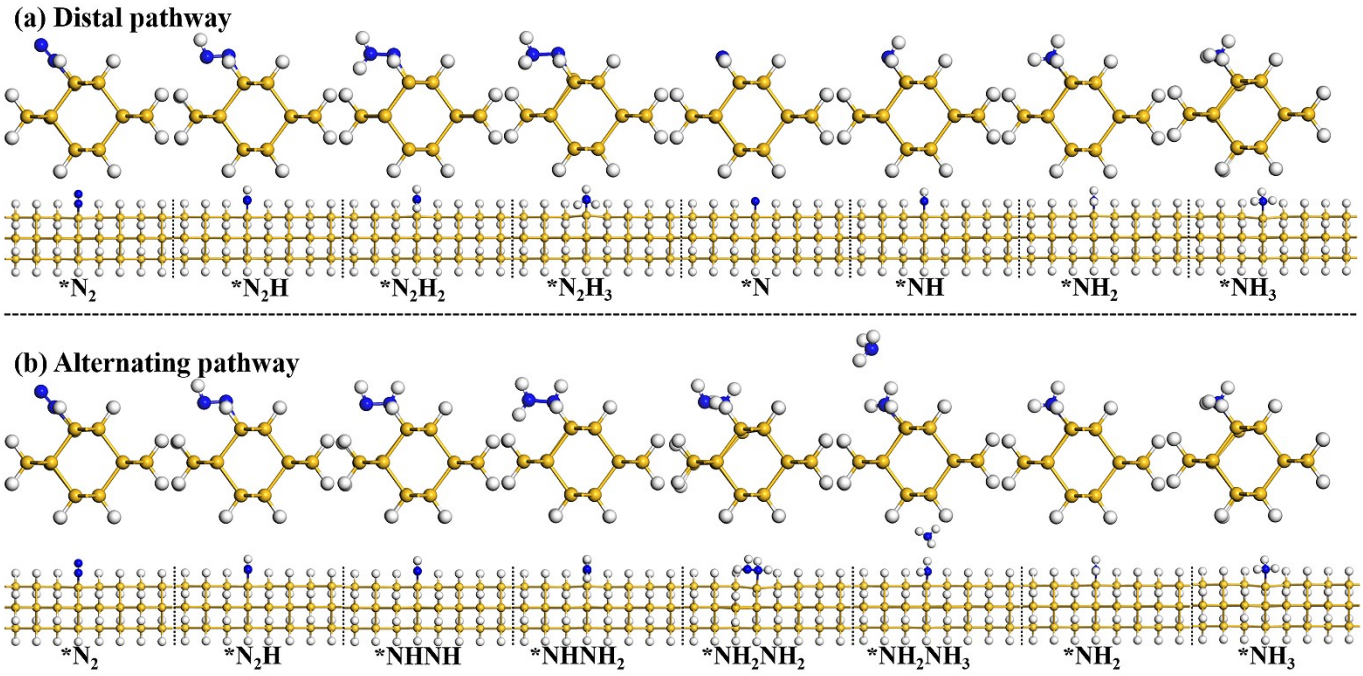

Fig. S4 NRR pathways on Si_{3C}, including (a) distal and (b) alternating reaction pathways. Color scheme: Si (yellow), H (White), N (blue).

3.2 NRR pathways on Si_{2C}

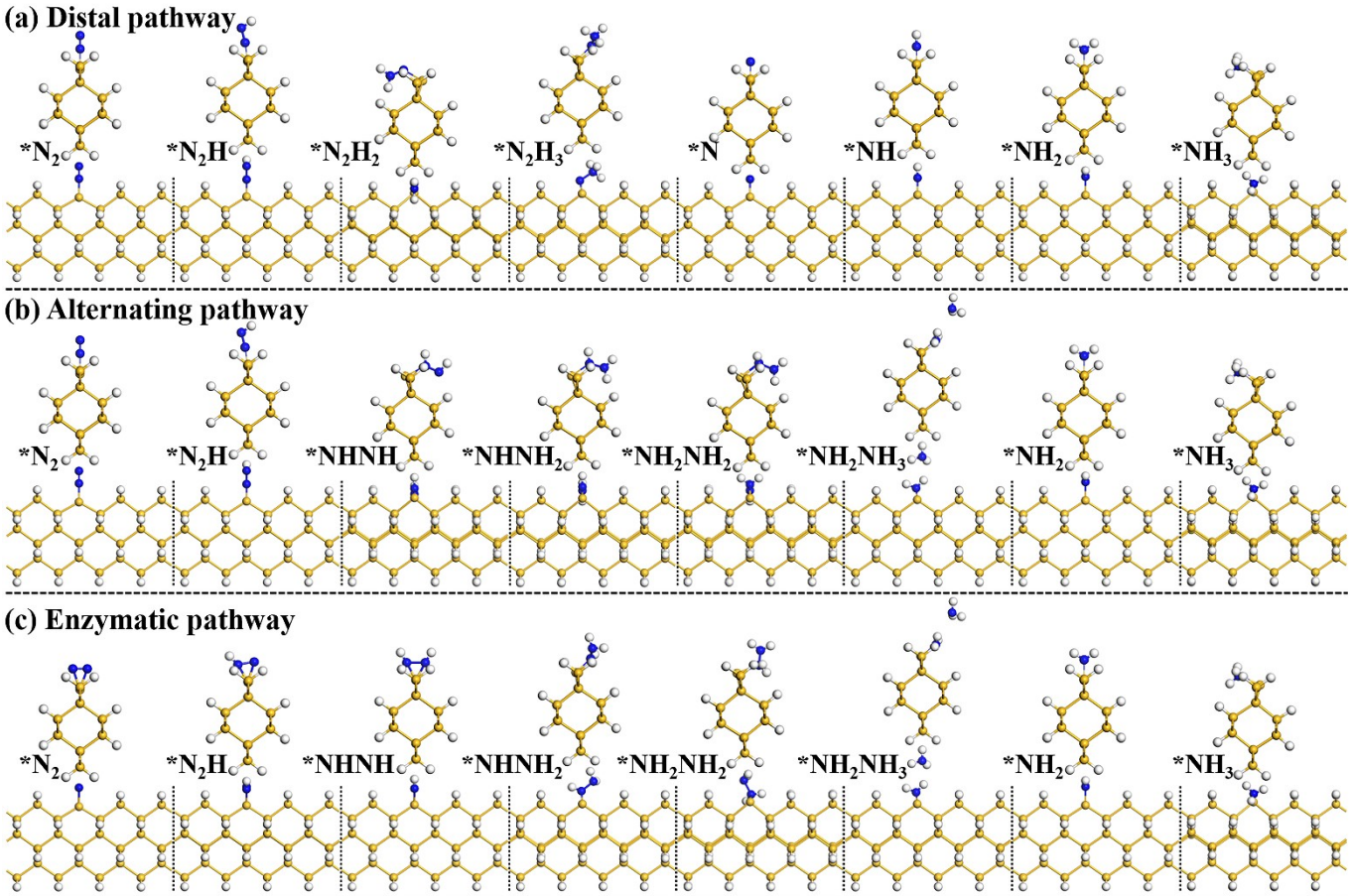

Fig. S5 NRR pathways, including the distal (a), alternating (b), and enzymatic (c) pathways, on Si_{2C} site. Color scheme: Si (yellow), H (White), N (blue).

3.3 Energy profiles of NRR on Si_{2C}

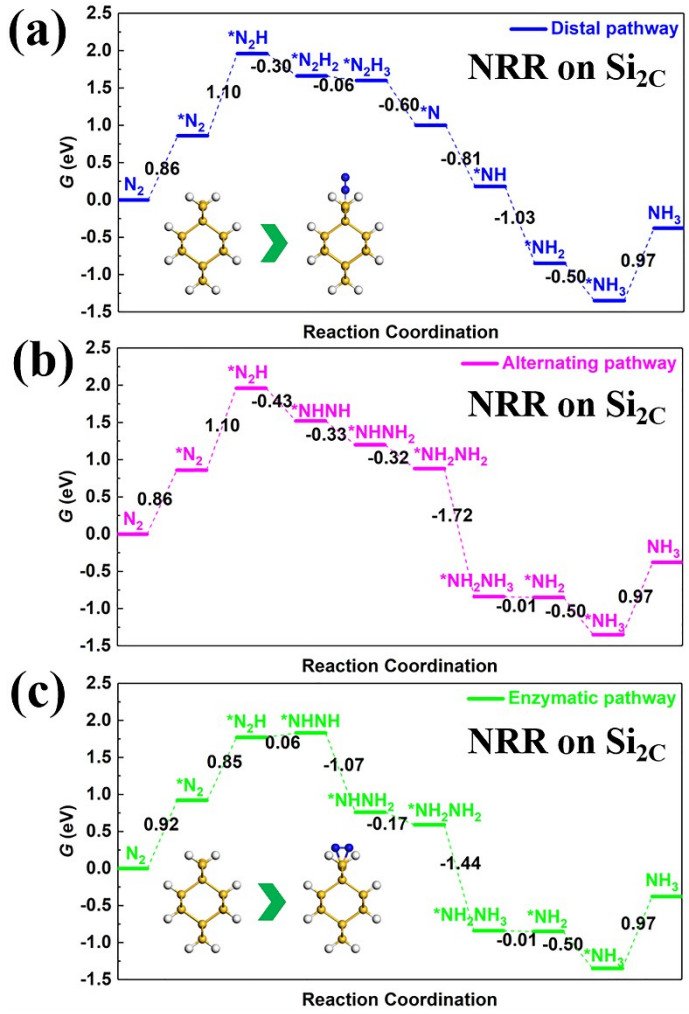

Fig. S6 Diagram of the free energy evolution along the reaction coordination, including the distal (a), alternating (b), and enzymatic (c) pathways. Insets in the images display the N_2 capture step. Color scheme: Si (yellow), H (White), N (blue).

4. Density functional theory (DFT) data

4.1 Thermochemistry of $^{1/2}N_2 + {}^{3/2}H_2 \rightarrow NH_3$

The Gibbs free energy calculation was performed as follows:

$$\Delta\mu = \Delta E_{\mathrm{DFT}} + \Delta\mathrm{ZPE} + \Delta\int C_p dT - T{\cdot}S \quad (1)$$

where μ, E, ZPE, and C_p represent the chemical potential (Gibbs freeenergy per molecular), electronic energy, zero-point energy and heat capacity, respectively. The entropy (S) consists of the translational (S_t), rational (S_r), vibrational (S_v) and electronic contributions (S_e) and thus can be expressed as:

$$S = S_t + S_r + S_v + S_e \quad (2)$$

where S_e is around zero at the foundamental electronic level.

Gases	E_{DFT}**/eV** [a]	**ZPE/eV** [b]	$\int C_p dT$ [c]	$-T{\cdot}S$ [d]	μ
H_2 (g)	-32.07	0.27	0.09	-0.40	-32.11
N_2 (g)	-2981.80	0.15	0.09	-0.59	-2982.15
NH_3 (g)	-1539.82	0.89	0.10	-0.60	-1539.43

[a] Calculated from DFT.

[b, c, d] Obtained from the NIST database (https://cccbdb.nist.gov).

4.2 Adsorption energies of N_2

Table S1 N_2 adsorption energies and binding energies of single heteroatom on SiNWs

Catalysts	**Adsorption energy/eV**		**Binding energy** (E_b)**/eV**	**Formation energy** (μ_f)**/eV**	**Active site charges/|e|**	
	End-on	Side-on			Mulliken	Hirshfeld
Si_{3C}	0.92	—	—	—	—	—
Si_{2C}	0.30	0.37	—	—	—	—
B_{3C}	-0.62	—	-8.27	-0.55	-0.252	-0.074
B_{2C}	-1.48	-0.13	-5.13	0.28	-0.059	-0.066
C_{3C}	-0.08	—	-9.02	0.19	-0.851	-0.241
C_{2C}	-1.87	-0.63	-5.30	1.65	-0.565	-0.263

P_{3C}	-0.06	—	-6.86	-1.59	-0.330	-0.120
P_{2C}	-0.05	—	-4.25	-1.36	-0.137	-0.084

5. N_2 adsorption configurations

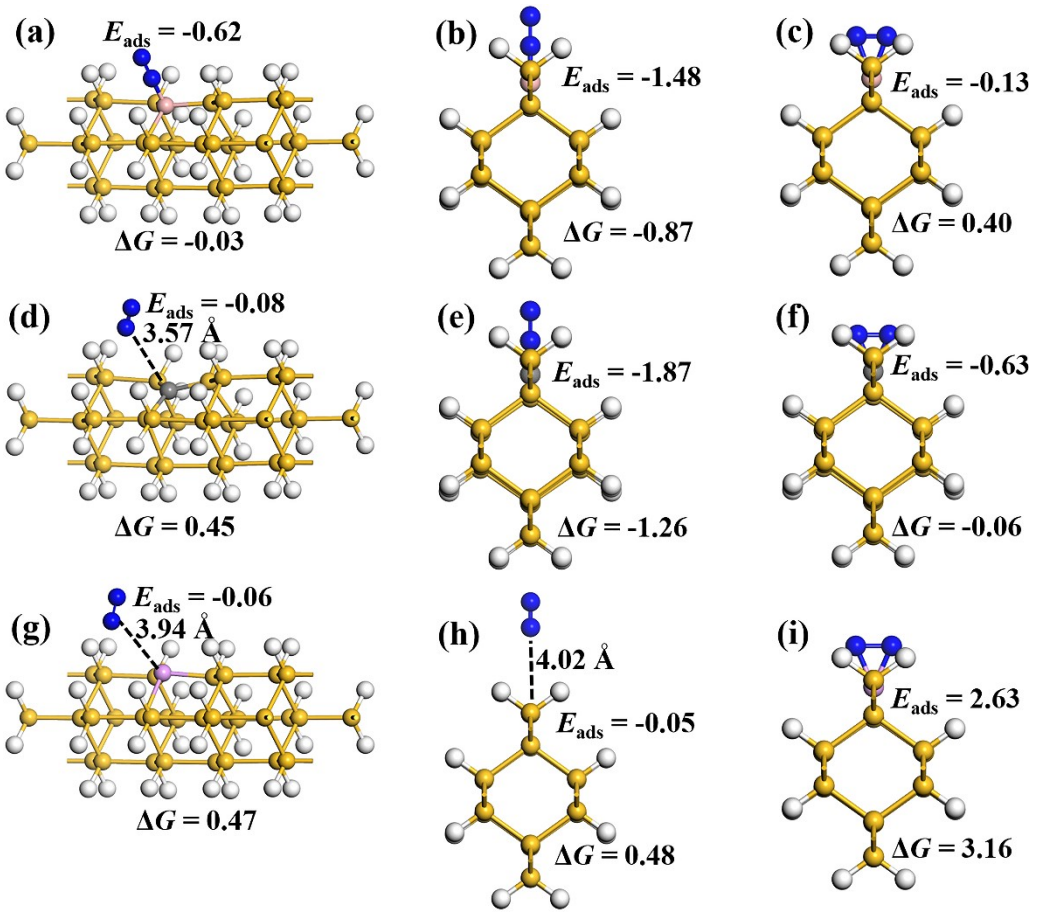

Fig. S7 N_2 adsorption configurations on B_{3C}, B_{2C}, C_{3C}, C_{2C}, P_{3C}, and P_{2C} catalysts. Black values near the dash line indicate the distance between N_2 and active sites. Color scheme: Si (yellow), H (White), N (blue).

6. NRR pathways on C_{2C}

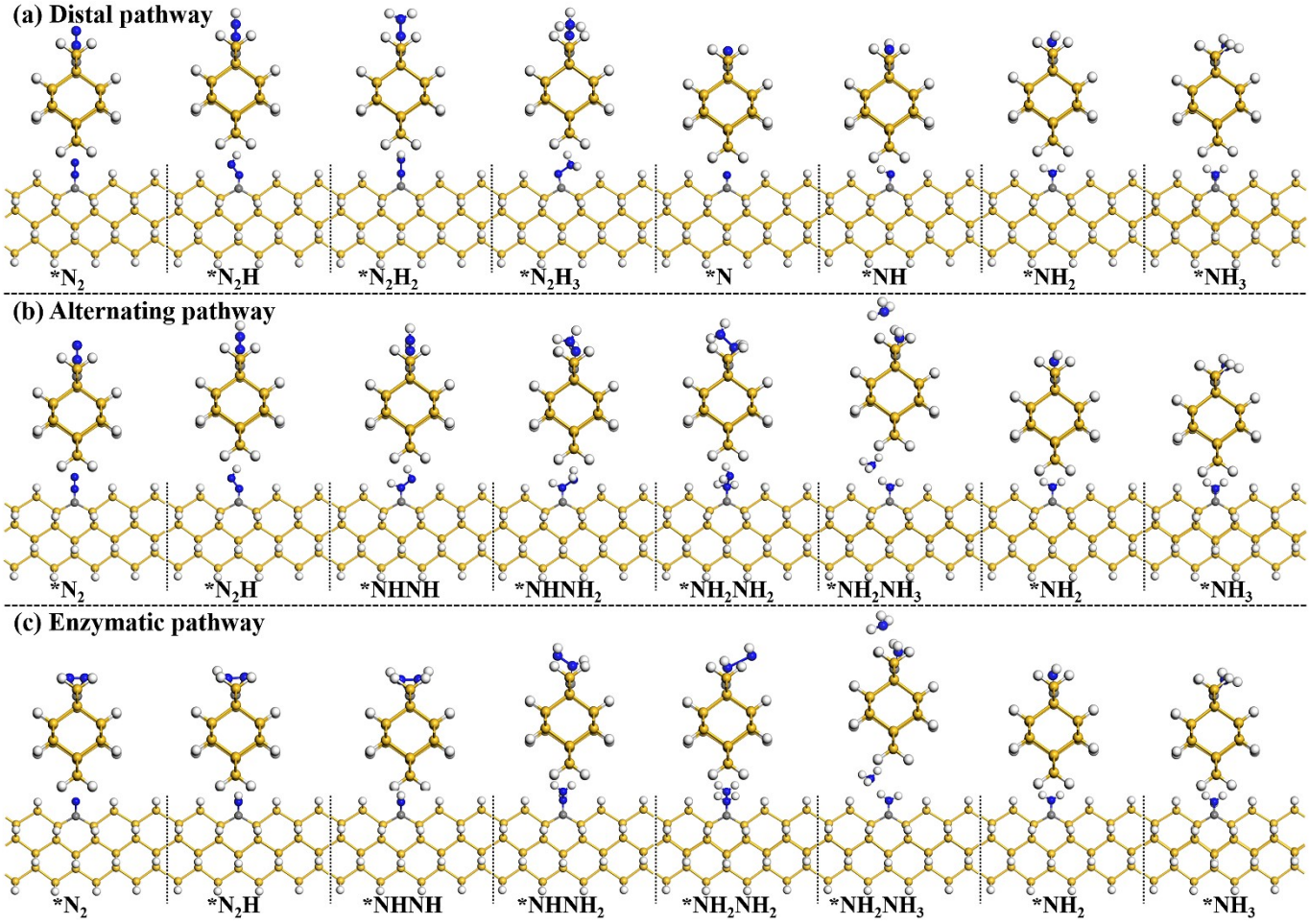

Fig. S8 NRR on C_{2C}, including the distal, alternating and enzymatic pathways. Color scheme: Si (yellow), H (White), N (blue), C (grey).

7. NRR pathways on B_{3C}

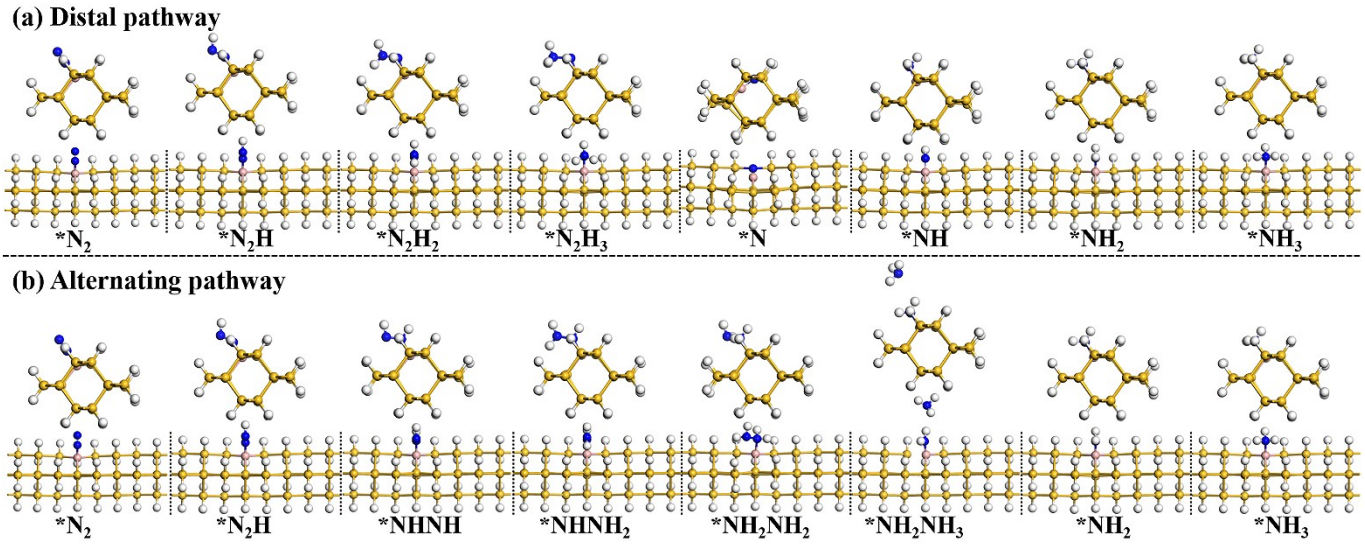

Fig. S9 NRR on B_{3C}, including the distal and alternating pathways. Color scheme: Si (yellow), H (White), N (blue), B (pink).

8. Alternating pathway on B_{2C}

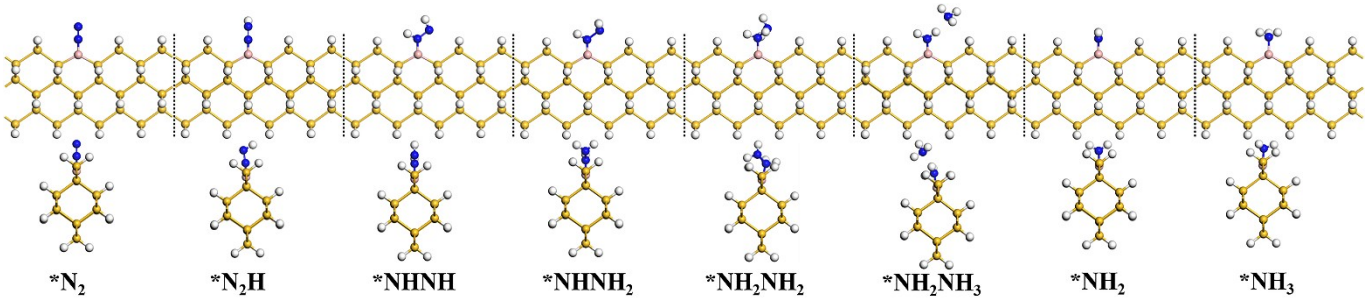

Fig. S10 The alternating pathway on B_{2C}. Color scheme: Si (yellow), H (White), N (blue), B (pink).

9. Hirshfeld analysis

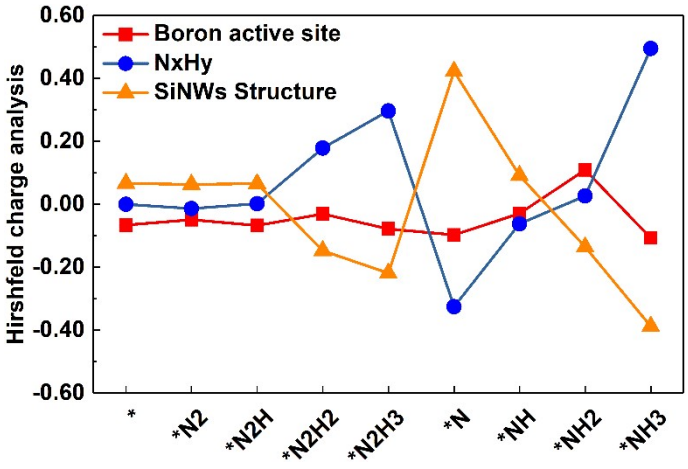

Fig. S11 Hirshfeld analysis for the optimal distal reaction pathway on B_{2C}.

10. Comparison between our work with other reports

Table S2 Comparing B_{2C} of SiNWs with other reported catalysts.

Catalysts	Limiting-potential (U_L)	Overpotential (η)	References
Diamond C(111)	-0.73 V	0.57 V	2
C-terminated (Silicon Carbide)	-0.55 V	0.39 V	3
CoNi@GDY& Mo2@GDY (Double metal dimer catalysts)	-0.52 V & -0.61 V	0.36 V & 0.45 V	4
$Ti@N_4$ & $V@N_4$ (defective graphene)	-0.69 V & -0.87 V	0.53 V & 0.71 V	5
$FeB_6(\beta)$	-0.68 V	0.52 V	6
Mo-BC_2 (Black Phosphorus)	-0.60 V	0.44 V	7
Mo_2B & Fe_2B & Co_2B	-0.82 V & -0.75 V & -0.84 V	0.66 V & 0.59 V & 0.68 V	8
Ni-WS_2 (2D substrate)	-0.86 V	0.70 V	9
1T-Mo_2C, 2H-Mo_2C, (100) edge of MoC_2	-0.52 V & -0.86 V & -0.63 V	0.36 V & 0.70 V & 0.47 V	10
Densely monodispersed Mo-N-C sites(MoN_3)	-0.63 V	0.47 V	11
MoS_2	-0.68 V	0.52 V	12
Fe-B_2N_2 site (SAC)	-0.65 V	0.49 V	13
$Ti@VB_2$	-0.61 V	0.45 V	14
Ru-PtS_2 (SAC)	-1.09 V	0.93 V	15
N_{2C} vacancy on corrugation g-C_3N_4	-1.32 V	1.16 V	16
CrB, MoB, WB, Mo_2B, & V_3B_4 (2D Metal Borides, MBenes)	-0.62 V, -0.73 V, -0.82 V, -0.78 V & -0.81 V	0.46 V, 0.57 V, 0.66 V, 0.62 V & 0.65 V	17

B_{2C} (SiNWs)	**-0.50 V**	**0.34 V**	**This work**

Therefore, it can be concluded from the above comparison (Table S2) that B-doped SiNWs (B_{2C}) would be highly promising towards NRR with a low overpotential of only 0.34 V.

11. Band structures of Si_{2C} *VS.* B_{2C}

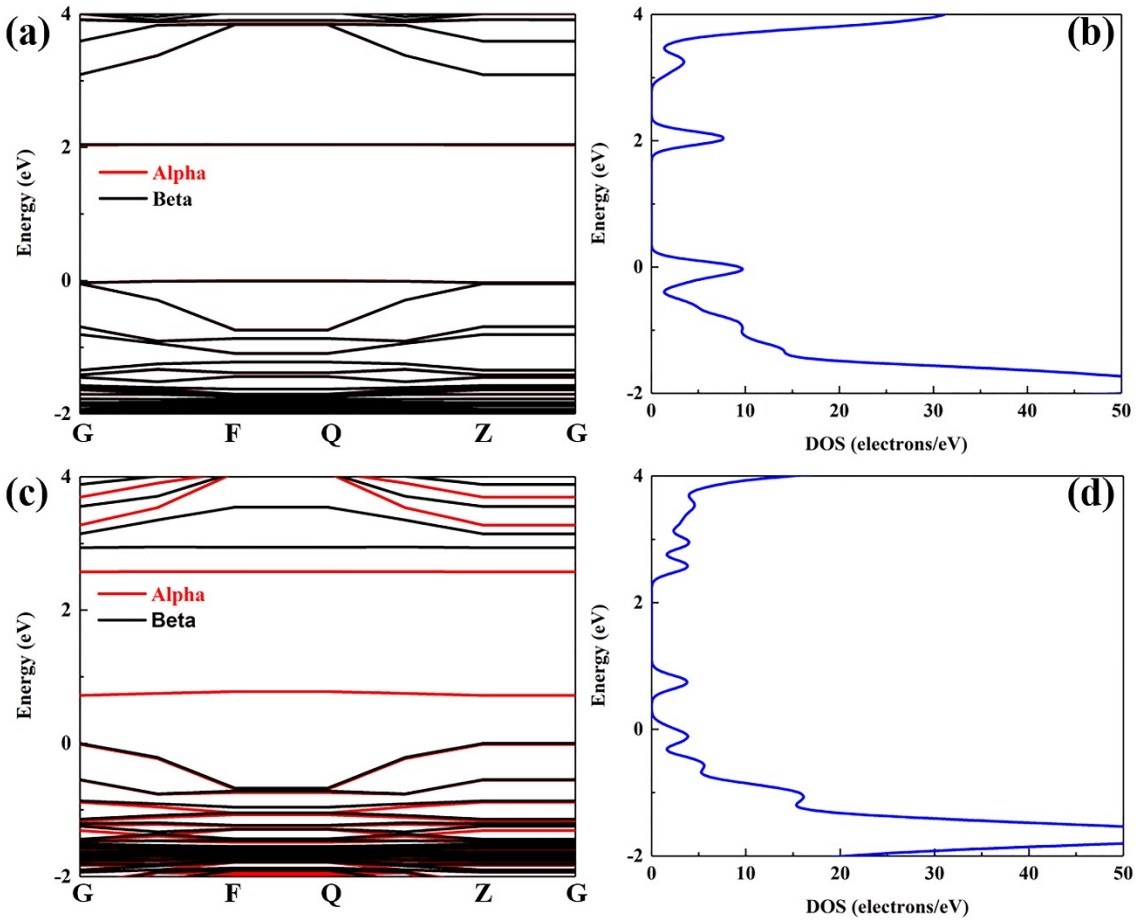

Fig. S12 Band structure and density of states (DOS) for Si_{2C} (a, b) and B_{2C} (c, d).

12. Gibbs free energy of intermediates

Table S3 NRR free energy of intermediates on Si_{3C} (Distal).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-252595.04	0.07	-252594.97	
*NN	-255575.92	0.26	-255575.66	1.46
*NNH	-255592.42	0.84	-255591.58	0.13
*NNH_2	-255608.80	0.86	-255607.94	-0.30
*NNH_3	-255625.05	1.29	-255623.76	0.24
*N	-254083.63	0.12	-254083.51	0.82
*NH	-254101.87	0.69	-254101.18	-1.61
*NH_2	-254120.09	0.74	-254119.35	-2.12
*NH_3	-254135.05	1.14	-254133.91	1.50
NH_3			-1539.43	-0.49

Table S4 NRR free energy of intermediates on Si_{3C} (Alternating).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-252595.04	0.07	-252594.97	
*NN	-255575.92	0.26	-255575.66	1.46
*NNH	-255592.42	0.84	-255591.58	0.13
*NHNH	-255608.74	0.86	-255607.88	-0.24
*$NHNH_2$	-255625.14	1.43	-255623.71	0.22
*NH_2NH_2	-255640.86	1.62	-255639.24	0.53
*NH_2NH_3	-255660.23	1.74	-255658.49	-3.20
*NH_2	-254120.09	0.74	-254119.35	-0.29
*NH_3	-254135.05	1.14	-254133.91	1.50
NH_3			-1539.43	-0.49

Table S5 NRR free energy of intermediates on Si_{2C} (Distal).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-252578.01	0.05	-252577.96	
*NN	-255559.51	0.26	-255559.25	0.86
*NNH	-255575.02	0.81	-255574.21	1.10
*NNH_2	-255591.44	0.88	-255590.56	-0.30
*NNH_3	-255607.94	1.26	-255606.68	-0.06
*N	-254067.98	0.13	-254067.85	-0.60
*NH	-254085.84	1.12	-254084.72	-0.81
*NH_2	-254102.51	0.70	-254101.81	-1.03
*NH_3	-254119.48	1.12	-254118.36	-0.50
NH_3			-1539.43	0.97

Table S6 NRR free energy of intermediates on Si_{2C} (Alternating).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-252578.01	0.05	-252577.96	
*NN	-255559.51	0.26	-255559.25	0.86
*NNH	-255575.02	0.81	-255574.21	1.10
*NHNH	-255591.59	0.89	-255590.70	-0.43
*$NHNH_2$	-255608.25	1.17	-255607.08	-0.33
*NH_2NH_2	-255624.98	1.53	-255623.45	-0.32
*NH_2NH_3	-255642.94	1.71	-255641.23	-1.72
*NH_2	-254102.51	0.70	-254101.81	-0.01
*NH_3	-254119.48	1.12	-254118.36	-0.50
NH_3			-1539.43	0.97

Table S7 NRR free energy of intermediates on Si_{2C} (Enzymatic).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-252578.01	0.05	-252577.96	
*NN	-255559.44	0.25	-255559.19	0.92
*NNH	-255575.21	0.81	-255574.40	0.85
*NHNH	-255591.19	0.80	-255590.39	0.06
*$NHNH_2$	-255608.72	1.20	-255607.52	-1.07
*NH_2NH_2	-255625.34	1.60	-255623.74	-0.17
*NH_2NH_3	-255642.94	1.71	-255641.23	-1.44
*NH_2	-254102.51	0.70	-254101.81	-0.01
*NH_3	-254119.48	1.12	-254118.36	-0.50
NH_3			-1539.43	0.97

Table S8 NRR free energy of intermediates on B_{3C} (Distal).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245394.01	0.12	-245393.89	
*NN	-248376.43	0.36	-248376.07	-0.03
*NNH	-248391.14	0.89	-248390.25	1.88
*NNH_2	-248408.18	0.99	-248407.19	-0.89
*NNH_3	-248423.62	1.32	-248422.30	0.95
*N	-246884.45	0.22	-246884.23	-1.36
*NH	-246900.34	0.75	-246899.59	0.70
*NH_2	-246918.16	0.82	-246917.34	-1.70
*NH_3	-246935.58	1.22	-246934.36	-0.96
NH_3			-1539.43	1.04

Table S9 NRR free energy of intermediates on B_{3C} (Alternating).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245394.01	0.12	-245393.89	
*NN	-248376.43	0.36	-248376.07	-0.03
*NNH	-248391.14	0.89	-248390.25	1.88
*NHNH	-248408.16	1.00	-248407.16	-0.86
*$NHNH_2$	-248424.51	1.50	-248423.01	0.20
*NH_2NH_2	-248441.46	1.68	-248439.78	-0.71
*NH_2NH_3	-248458.26	1.79	-248456.47	-0.64
*NH_2	-246918.16	0.82	-246917.34	-0.30
*NH_3	-246935.58	1.22	-246934.36	-0.96
NH_3			-1539.43	1.04

Table S10 NRR free energy of intermediates on B_{2C} (Distal).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245376.15	0.083	-245376.07	
*NN	-248359.43	0.34	-248359.09	-0.87
*NNH	-248375.71	0.76	-248374.95	0.20
*NNH_2	-248391.43	0.92	-248390.51	0.50
*NNH_3	-248408.33	1.34	-248406.99	-0.43
*N	-246867.67	0.19	-246867.48	0.08
*NH	-246885.02	0.73	-246884.29	-0.75
*NH_2	-246901.70	0.77	-246900.93	-0.59
*NH_3	-246917.96	1.19	-246916.77	0.22
NH_3			-1539.43	1.27

Table S11 NRR free energy of intermediates on B_{2C} (Alternating).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245376.15	0.083	-245376.07	
*NN	-248359.43	0.34	-248359.09	-0.87
*NNH	-248375.71	0.76	-248374.95	0.20
*NHNH	-248391.62	0.98	-248390.64	0.36
*$NHNH_2$	-248409.08	1.32	-248407.76	-1.06
*NH_2NH_2	-248423.91	1.66	-248422.25	1.56
*NH_2NH_3	-248443.24	1.92	-248441.32	-3.01
*NH_2	-246901.70	0.77	-246900.93	0.96
*NH_3	-246917.96	1.19	-246916.77	0.22
NH_3			-1539.43	1.27

Table S12 NRR free energy of intermediates on C_{2C} (Distal).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245735.55	0.096	-245735.45	
*NN	-248719.22	0.36	-248718.86	-1.26
*NNH	-248734.42	0.89	-248733.53	1.39
*NNH_2	-248749.56	0.91	-248748.65	0.94
*NNH_3	-248766.86	1.32	-248765.54	-0.83
*N	-247228.36	0.20	-247228.16	-2.05
*NH	-247245.46	0.77	-247244.69	-0.48
*NH_2	-247261.43	0.84	-247260.59	0.16
*NH_3	-247277.34	1.22	-247276.12	0.53
NH_3			-1539.43	1.24

Table S13 NRR free energy of intermediates on C_{2C} (Alternating).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245735.55	0.096	-245735.45	
*NN	-248719.22	0.36	-248718.86	-1.26
*NNH	-248734.42	0.89	-248733.53	1.39
*NHNH	-248751.51	0.99	-248750.52	-0.94
*$NHNH_2$	-248767.54	1.30	-248766.24	0.33
*NH_2NH_2	-248783.46	1.66	-248781.80	0.50
*NH_2NH_3	-248801.60	1.88	-248799.72	-1.87
*NH_2	-247261.43	0.84	-247260.59	-0.30
*NH_3	-247277.34	1.22	-247276.12	0.53
NH_3			-1539.43	1.24

Table S14 NRR free energy of intermediates on C_{2C} (Enzymatic).

Reaction intermediates	E_{DFT}/eV	ZPE/eV	G/eV	ΔG/eV
*	-245735.55	0.096	-245735.45	
*NN	-248717.98	0.32	-248717.66	-0.06
*NNH	-248733.26	0.89	-248732.37	1.35
*NHNH	-248748.44	0.87	-248747.57	0.85
*$NHNH_2$	-248766.74	1.25	-248765.49	-1.86
*NH_2NH_2	-248783.46	1.53	-248781.93	-0.39
*NH_2NH_3	-248801.60	1.88	-248799.72	-1.74
*NH_2	-247261.43	0.84	-247260.59	-0.30
*NH_3	-247277.34	1.22	-247276.12	0.53
NH_3			-1539.43	1.24

13. Optimized catalysts models

B_{3C}:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	Si	3.091235	3.896985	-0.001555
2	Si	5.759226	5.778600	1.979074
3	B	6.016213	5.778600	-1.384076
4	Si	3.091235	7.660215	-0.001555
5	Si	6.963977	7.511418	-1.839786
6	Si	4.510521	5.778600	-0.043057
7	Si	7.095850	7.713028	1.971058
8	Si	4.368289	9.625080	0.019939
9	H	2.205072	3.906168	-1.211485
10	H	2.212455	3.977154	1.210460
11	H	2.205072	7.651032	-1.211485
12	H	2.212455	7.580046	1.210460
13	H	7.843251	7.425778	-3.055228
14	H	7.975840	7.740937	3.187242
15	H	4.824409	5.778600	3.154483
16	Si	3.015387	11.550105	-0.005860
17	Si	5.747739	13.483400	1.878722
18	Si	5.715678	13.483400	-1.953995
19	Si	4.357848	13.483400	-0.025346
20	H	2.138834	11.532112	-1.221701
21	H	2.135340	11.561228	1.207645
22	H	4.824427	13.483400	-3.163178

23	H	4.882925	13.483400	3.106888
24	Si	8.431358	3.876577	0.033159
25	Si	8.431358	7.680623	0.033159
26	Si	9.807184	5.778600	0.060003
27	Si	9.771683	9.615300	-0.071606
28	H	10.701525	5.778600	-1.142780
29	H	10.666233	5.778600	1.287958
30	H	10.612510	9.574759	-1.311616
31	H	10.687256	9.619241	1.115433
32	Si	8.443313	11.553163	-0.063820
33	Si	9.790879	13.483400	-0.090584
34	H	10.651641	13.483400	-1.317761
35	H	10.686586	13.483400	1.111390
36	Si	5.724968	2.010975	-1.902029
37	Si	6.963977	4.045782	-1.839786
38	H	4.828132	2.017974	-3.107765
39	H	7.843251	4.131422	-3.055228
40	Si	5.724968	9.546225	-1.902029
41	Si	7.045728	11.516583	-1.960968
42	H	4.828132	9.539226	-3.107765
43	H	7.913591	11.516662	-3.187157
44	Si	5.749621	1.914915	1.928162
45	Si	7.095850	3.844172	1.971058
46	H	4.883099	1.880392	3.154549
47	H	7.975840	3.816263	3.187242
48	Si	5.749621	9.642285	1.928162
49	Si	7.104226	11.563291	1.875843
50	H	7.999569	11.583436	3.081591
51	H	4.883099	9.676808	3.154549
52	Si	3.015387	0.007095	-0.005860
53	Si	7.045728	0.040617	-1.960968
54	Si	7.104226	-0.006091	1.875843
55	Si	4.368289	1.932120	0.019939

56	H	2.138834	0.025088	-1.221701
57	H	2.135340	-0.004028	1.207645
58	H	7.913591	0.040538	-3.187157
59	H	7.999569	-0.026236	3.081591
60	Si	8.443313	0.004037	-0.063820
61	Si	9.771683	1.941900	-0.071606
62	H	10.612510	1.982441	-1.311616
63	H	10.687256	1.937959	1.115433

B_{2C}:

Final Coordinates (Angstroms)

ATOM		X	Y	Z
1	Si	6.467565	3.830536	3.430736
2	Si	8.380513	5.777891	0.741345
3	Si	4.554617	5.777891	0.741345
4	Si	6.467565	7.725245	3.430736
5	Si	4.551967	7.687397	-0.623335
6	Si	6.467565	5.777891	2.112473
7	Si	8.383163	7.687397	-0.623335
8	Si	6.467565	9.637003	2.056880
9	H	5.252152	3.812847	4.307614
10	H	7.682977	3.812847	4.307614
11	H	5.252152	7.742934	4.307614
12	H	7.682977	7.742934	4.307614
13	H	3.333373	7.673492	-1.501143
14	H	9.601756	7.673492	-1.501143
15	H	9.604064	5.777891	1.612427
16	H	3.331065	5.777891	1.612427

17	Si	6.467565	11.573661	3.384700
18	Si	8.373069	13.482691	0.627559
19	Si	4.562061	13.482691	0.627559
20	Si	6.467565	13.482691	2.013607
21	H	5.252364	11.587386	4.262108
22	H	7.682765	11.587386	4.262108
23	H	3.333391	13.482691	1.491749
24	H	9.601738	13.482691	1.491749
25	Si	6.467565	3.942261	-2.020232
26	Si	6.467565	7.613520	-2.020232
27	B	6.467565	5.777891	-2.764807
28	Si	6.467565	9.539935	-3.408381
29	H	5.252264	9.534907	-4.285793
30	H	7.682866	9.534907	-4.285793
31	Si	6.467565	11.520765	-2.100333
32	Si	6.467565	13.482691	-3.428381
33	H	5.253396	13.482691	-4.307428
34	H	7.681734	13.482691	-4.307428
35	Si	4.557959	1.910143	0.677321
36	Si	4.551967	3.868384	-0.623335
37	H	3.331620	1.892457	1.545160
38	H	3.333373	3.882289	-1.501143
39	Si	4.557959	9.645638	0.677321
40	Si	4.564772	11.545790	-0.708632
41	H	3.331620	9.663324	1.545160
42	H	3.332569	11.532313	-1.567512
43	Si	8.377171	1.910143	0.677321
44	Si	8.383163	3.868384	-0.623335
45	H	9.603509	1.892457	1.545160
46	H	9.601756	3.882289	-1.501143
47	Si	8.377171	9.645638	0.677321
48	Si	8.370358	11.545790	-0.708632
49	H	9.602560	11.532313	-1.567512

50	H	9.603509	9.663324	1.545160
51	Si	6.467565	-0.017880	3.384700
52	Si	4.564772	0.009991	-0.708632
53	Si	8.370358	0.009991	-0.708632
54	Si	6.467565	1.918778	2.056880
55	H	5.252364	-0.031605	4.262108
56	H	7.682765	-0.031605	4.262108
57	H	3.332569	0.023468	-1.567512
58	H	9.602560	0.023468	-1.567512
59	Si	6.467565	0.035016	-2.100333
60	Si	6.467565	2.015846	-3.408381
61	H	5.252264	2.020874	-4.285793
62	H	7.682866	2.020874	-4.285793

C_{3C}:

Final Coordinates (Angstroms)

ATOM		X	Y	Z
1	Si	3.141446	3.929712	-0.058518
2	Si	5.784342	5.778600	2.003070
3	C	5.995111	5.778600	-1.343339
4	Si	3.141446	7.627488	-0.058518
5	Si	6.917477	7.388710	-1.754228
6	Si	4.612510	5.778600	-0.063030
7	Si	7.111829	7.720153	1.992508
8	Si	4.365646	9.619601	0.016757
9	H	2.286498	3.949878	-1.290120
10	H	2.246822	4.094921	1.132168
11	H	2.286498	7.607322	-1.290120

12	H	2.246822	7.462279	1.132168
13	H	7.719367	7.201962	-3.007161
14	H	7.983671	7.773301	3.214096
15	H	4.832169	5.778600	3.164248
16	Si	3.014535	11.546986	-0.033454
17	Si	5.740838	13.483400	1.848657
18	Si	5.716852	13.483400	-1.987778
19	Si	4.356238	13.483400	-0.059323
20	H	2.145146	11.516847	-1.253969
21	H	2.128855	11.568220	1.175659
22	H	4.822535	13.483400	-3.194583
23	H	4.871660	13.483400	3.073648
24	Si	8.444864	3.884505	0.051815
25	Si	8.444864	7.672695	0.051815
26	Si	9.830359	5.778600	0.107366
27	Si	9.769121	9.615705	-0.092108
28	H	10.739287	5.778600	-1.084541
29	H	10.676959	5.778600	1.344396
30	H	10.603265	9.572154	-1.336564
31	H	10.693491	9.636995	1.087930
32	Si	8.429574	11.544759	-0.093818
33	Si	9.766265	13.483400	-0.139045
34	H	10.617550	13.483400	-1.372724
35	H	10.671981	13.483400	1.055369
36	Si	5.717434	2.077467	-1.904117
37	Si	6.917477	4.168490	-1.754228
38	H	4.815824	2.106646	-3.105820
39	H	7.719367	4.355238	-3.007161
40	Si	5.717434	9.479733	-1.904117
41	Si	7.030826	11.480048	-1.989090
42	H	4.815824	9.450554	-3.105820
43	H	7.900002	11.475823	-3.214122
44	Si	5.749563	1.917579	1.924909

45	Si	7.111829	3.837047	1.992508
46	H	4.880686	1.871277	3.149232
47	H	7.983671	3.783899	3.214096
48	Si	5.749563	9.639621	1.924909
49	Si	7.098164	11.564413	1.851390
50	H	8.000667	11.594437	3.051563
51	H	4.880686	9.685923	3.149232
52	Si	3.014535	0.010214	-0.033454
53	Si	7.030826	0.077152	-1.989090
54	Si	7.098164	-0.007213	1.851390
55	Si	4.365646	1.937599	0.016757
56	H	2.145146	0.040353	-1.253969
57	H	2.128855	-0.011020	1.175659
58	H	7.900002	0.081377	-3.214122
59	H	8.000667	-0.037237	3.051563
60	Si	8.429574	0.012441	-0.093818
61	Si	9.769121	1.941495	-0.092108
62	H	10.603265	1.985046	-1.336564
63	H	10.693491	1.920205	1.087930

C_{2C}:

Final Coordinates (Angstroms)

ATOM		X	Y	Z
1	Si	6.467565	3.804847	3.465356
2	Si	8.385025	5.777891	0.822509
3	Si	4.550104	5.777891	0.822509
4	Si	6.467565	7.750934	3.465356
5	Si	4.545552	7.654377	-0.575834

6	Si	6.467565	5.777891	2.184618
7	Si	8.389578	7.654377	-0.575834
8	Si	6.467565	9.639927	2.054510
9	H	5.251424	3.765472	4.339847
10	H	7.683706	3.765472	4.339847
11	H	5.251424	7.790309	4.339847
12	H	7.683706	7.790309	4.339847
13	H	3.341428	7.619950	-1.471330
14	H	9.593701	7.619950	-1.471330
15	H	9.610757	5.777891	1.689802
16	H	3.324372	5.777891	1.689802
17	Si	6.467565	11.588564	3.361531
18	Si	8.368071	13.482691	0.578949
19	Si	4.567059	13.482691	0.578949
20	Si	6.467565	13.482691	1.971442
21	H	5.252367	11.611378	4.238482
22	H	7.682762	11.611378	4.238482
23	H	3.335036	13.482691	1.438074
24	H	9.600094	13.482691	1.438074
25	Si	6.467565	4.081911	-1.982720
26	Si	6.467565	7.473870	-1.982720
27	C	6.467565	5.777891	-2.652663
28	Si	6.467565	9.430148	-3.394305
29	H	5.254357	9.421917	-4.276545
30	H	7.680773	9.421917	-4.276545
31	Si	6.467565	11.483144	-2.151371
32	Si	6.467565	13.482691	-3.459953
33	H	5.253832	13.482691	-4.339400
34	H	7.681297	13.482691	-4.339400
35	Si	4.567314	1.901287	0.663101
36	Si	4.545552	3.901404	-0.575834
37	H	3.333314	1.888554	1.520169
38	H	3.341428	3.935831	-1.471330

39	Si	4.567314	9.654494	0.663101
40	Si	4.574147	11.536563	-0.747920
41	H	3.333314	9.667227	1.520169
42	H	3.333288	11.508238	-1.593279
43	Si	8.367815	1.901287	0.663101
44	Si	8.389578	3.901404	-0.575834
45	H	9.601816	1.888554	1.520169
46	H	9.593701	3.935831	-1.471330
47	Si	8.367815	9.654494	0.663101
48	Si	8.360982	11.536563	-0.747920
49	H	9.601841	11.508238	-1.593279
50	H	9.601816	9.667227	1.520169
51	Si	6.467565	-0.032783	3.361531
52	Si	4.574147	0.019218	-0.747920
53	Si	8.360982	0.019218	-0.747920
54	Si	6.467565	1.915854	2.054510
55	H	5.252367	-0.055597	4.238482
56	H	7.682762	-0.055597	4.238482
57	H	3.333288	0.047543	-1.593279
58	H	9.601841	0.047543	-1.593279
59	Si	6.467565	0.072637	-2.151371
60	Si	6.467565	2.125633	-3.394305
61	H	5.254357	2.133864	-4.276545
62	H	7.680773	2.133864	-4.276545

P_{3C}:

Final Coordinates (Angstroms)

ATOM	X	Y	Z

1	Si	3.057683	3.887079	-0.002667
2	Si	5.780565	5.778600	1.940733
3	P	5.617105	5.778600	-1.996911
4	Si	3.057683	7.670121	-0.002667
5	Si	7.021472	7.594957	-1.845058
6	Si	4.462980	5.778600	-0.015029
7	Si	7.111707	7.715684	1.950604
8	Si	4.358558	9.626354	0.013291
9	H	2.171605	3.905165	-1.211540
10	H	2.197329	3.952147	1.223284
11	H	2.171605	7.652035	-1.211540
12	H	2.197329	7.605053	1.223284
13	H	7.853948	7.522253	-3.092029
14	H	7.983765	7.741594	3.173650
15	H	4.858898	5.778600	3.127646
16	Si	3.007235	11.553666	0.002796
17	Si	5.746194	13.483400	1.890058
18	Si	5.720628	13.483400	-1.939752
19	Si	4.356372	13.483400	-0.014747
20	H	2.125418	11.542269	-1.209755
21	H	2.134092	11.562154	1.221796
22	H	4.838259	13.483400	-3.155677
23	H	4.881742	13.483400	3.118996
24	Si	8.461704	3.872759	0.021056
25	Si	8.461704	7.684441	0.021056
26	Si	9.835376	5.778600	0.036524
27	Si	9.798717	9.622145	-0.055362
28	H	10.712595	5.778600	-1.179279
29	H	10.710837	5.778600	1.253653
30	H	10.651271	9.605333	-1.288586
31	H	10.703250	9.626346	1.140930
32	Si	8.456046	11.552977	-0.043399
33	Si	9.803687	13.483400	-0.064389

34	H	10.668259	13.483400	-1.289339
35	H	10.694557	13.483400	1.141715
36	Si	5.723355	1.978356	-1.906264
37	Si	7.021472	3.962243	-1.845058
38	H	4.844234	2.002861	-3.124135
39	H	7.853948	4.034947	-3.092029
40	Si	5.723355	9.578844	-1.906264
41	Si	7.062515	11.531392	-1.944369
42	H	4.844234	9.554339	-3.124135
43	H	7.925778	11.526173	-3.173845
44	Si	5.748725	1.922497	1.918682
45	Si	7.111707	3.841516	1.950604
46	H	4.883645	1.903640	3.146952
47	H	7.983765	3.815606	3.173650
48	Si	5.748725	9.634703	1.918682
49	Si	7.100190	11.560024	1.885588
50	H	7.985835	11.569754	3.099319
51	H	4.883645	9.653560	3.146952
52	Si	3.007235	0.003534	0.002796
53	Si	7.062515	0.025808	-1.944369
54	Si	7.100190	-0.002824	1.885588
55	Si	4.358558	1.930846	0.013291
56	H	2.125418	0.014931	-1.209755
57	H	2.134092	-0.004954	1.221796
58	H	7.925778	0.031027	-3.173845
59	H	7.985835	-0.012554	3.099319
60	Si	8.456046	0.004223	-0.043399
61	Si	9.798717	1.935055	-0.055362
62	H	10.651271	1.951867	-1.288586
63	H	10.703250	1.930854	1.140930

P_{2C}:

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	Si	6.467565	3.833015	3.424520
2	Si	8.388148	5.777891	0.740597
3	Si	4.546981	5.777891	0.740597
4	Si	6.467565	7.722766	3.424520
5	Si	4.548899	7.674607	-0.640748
6	Si	6.467565	5.777891	2.103859
7	Si	8.386231	7.674607	-0.640748
8	Si	6.467565	9.631378	2.047811
9	H	5.251972	3.815794	4.300718
10	H	7.683157	3.815794	4.300718
11	H	5.251972	7.739987	4.300718
12	H	7.683157	7.739987	4.300718
13	H	3.334013	7.660674	-1.522387
14	H	9.601117	7.660674	-1.522387
15	H	9.608848	5.777891	1.615017
16	H	3.326281	5.777891	1.615017
17	Si	6.467565	11.567017	3.379600
18	Si	8.377583	13.482691	0.639080
19	Si	4.557546	13.482691	0.639080
20	Si	6.467565	13.482691	2.018259
21	H	5.252595	11.574289	4.257042
22	H	7.682534	11.574289	4.257042
23	H	3.332576	13.482691	1.507985
24	H	9.602554	13.482691	1.507985
25	Si	6.467565	3.956236	-2.019008
26	Si	6.467565	7.599545	-2.019008
27	P	6.467565	5.777891	-3.400446

28	Si	6.467565	9.542942	-3.381816
29	H	5.252918	9.532682	-4.259719
30	H	7.682211	9.532682	-4.259719
31	Si	6.467565	11.528082	-2.085172
32	Si	6.467565	13.482691	-3.423236
33	H	5.252570	13.482691	-4.300364
34	H	7.682559	13.482691	-4.300364
35	Si	4.560819	1.922358	0.664823
36	Si	4.548899	3.881174	-0.640748
37	H	3.333449	1.921481	1.530863
38	H	3.334013	3.895107	-1.522387
39	Si	4.560819	9.633423	0.664823
40	Si	4.560294	11.548135	-0.701210
41	H	3.333449	9.634300	1.530863
42	H	3.332233	11.537420	-1.565429
43	Si	8.374310	1.922358	0.664823
44	Si	8.386231	3.881174	-0.640748
45	H	9.601681	1.921481	1.530863
46	H	9.601117	3.895107	-1.522387
47	Si	8.374310	9.633423	0.664823
48	Si	8.374835	11.548135	-0.701210
49	H	9.602896	11.537420	-1.565429
50	H	9.601681	9.634300	1.530863
51	Si	6.467565	-0.011236	3.379600
52	Si	4.560294	0.007646	-0.701210
53	Si	8.374835	0.007646	-0.701210
54	Si	6.467565	1.924403	2.047811
55	H	5.252595	-0.018508	4.257042
56	H	7.682534	-0.018508	4.257042
57	H	3.332233	0.018361	-1.565429
58	H	9.602896	0.018361	-1.565429
59	Si	6.467565	0.027699	-2.085172
60	Si	6.467565	2.012839	-3.381816

61	H	5.252918	2.023099	-4.259719
62	H	7.682211	2.023099	-4.259719

14. References

1. Y. Ikeda, M. Senami and A. Tachibana, *AIP Adv.*, 2012, **2**, 042168.
2. Z. Guo, S. Qiu, H. Li, Y. Xu, S. J. Langford and C. Sun, *Diamond Relat. Mater.*, 2021, **111**, 108210.
3. Z. Guo, S. Qiu, H. Li, Y. Xu, S. J. Langford and C. Sun, *Phys. Chem. Chem. Phys.*, 2020, **22**, 21761-21767.
4. L. J. Arachchige, Y. Xu, Z. Dai, X. L. Zhang, F. Wang and C. Sun, *J. Mater. Sci. Technol.*, 2021, **77**, 244-251.
5. C. Choi, S. Back, N.-Y. Kim, J. Lim, Y.-H. Kim and Y. Jung, *ACS Catal.*, 2018, **8**, 7517-7525.
6. Q. Li, C. Liu, S. Qiu, F. Zhou, L. He, X. Zhang and C. Sun, *J. Mater. Chem. A*, 2019, **7**, 21507-21513.
7. Q. Li, S. Qiu, C. Liu, M. Liu, L. He, X. Zhang and C. Sun, *J. Phys. Chem. C*, 2019, **123**, 2347-2352.
8. X. Liu, Y. Jiao, Y. Zheng and S.-Z. Qiao, *ACS Catal.*, 2020, **10**, 1847-1854.
9. X. Ma, J. Hu, M. Zheng, D. Li, H. Lv, H. He and C. Huang, *Appl. Surf. Sci.*, 2019, **489**, 684-692.
10. B. Zhang, J. Zhou, S. R. Elliott and Z. Sun, *J. Mater. Chem. A*, 2020, **8**, 23947-23954.
11. K. Ye, M. Hu, Q.-K. Li, Y. Han, Y. Luo, J. Jiang and G. Zhang, *J. Phys. Chem. Lett.*, 2020, **11**, 3962-3968.
12. L. Zhang, X. Ji, X. Ren, Y. Ma, X. Shi, Z. Tian, A. M. Asiri, L. Chen, B. Tang and X. Sun, *Adv. Mater.*, 2018, **30**, 1800191.
13. D. Jiao, Y. Liu, Q. Cai and J. Zhao, *J. Mater. Chem. A*, 2021, **9**, 1240-1251.
14. L. Ge, W. Xu, C. Chen, C. Tang, L. Xu and Z. Chen, *J. Phys. Chem. Lett.*, 2020, **11**, 5241-5247.
15. L. Cai, N. Zhang, B. Qiu and Y. Chai, *ACS Appl. Mater. Interfaces*, 2020, **12**, 20448-20455.

16. C. Ren, Y. Zhang, Y. Li, Y. Zhang, S. Huang, W. Lin and K. Ding, *J. Phys. Chem. C*, 2019, **123**, 17296-17305.

17. X. Guo, S. Lin, J. Gu, S. Zhang, Z. Chen and S. Huang, *Adv. Funct. Mater.*, 2021, **31**, 2008056.