

Supporting Information

Structural details for monolayer C₃N

Here is the POSCAR information for optimized C₃N monolayer unit cell with lattice geometry and atom positions.

-----monolayer C₃N unit cell POSCAR file begins-----

C3N UNIT CELL

1.0000000000000000

4.2088834623923717 -2.429999999999998 0.0000000000000000

0.0000000000000000 4.859999999999994 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.0000000000000000

C N

6 2

Direct

0.3333894736219791 0.1666947368109896 -0.0000000000000000

0.8333052631890104 0.1666947368109896 -0.0000000000000000

0.8333052631890104 0.6666105263780209 0.0000000000000000

0.6666105263780209 0.8333052631890104 0.0000000000000000

0.1666947368109896 0.8333052631890104 0.0000000000000000

0.1666947368109896 0.3333894736219791 -0.0000000000000000

0.6666666666666643 0.3333333333333357 -0.0000000000000000

0.3333333333333357 0.6666666666666643 -0.0000000000000000

-----monolayer C₃N supercell (3 × 3 × 1) POSCAR file begins-----

C3N SUPERCELL

1.0000000000000000

12.557812874522490 -7.250256643538519 0.0000000000000000

0.0000000000000000 14.500513287077009 0.0000000000000000

0.0000000000000000 0.0000000000000000 30.000055465349799

C N

54 18

Direct

0.1107173257825827 0.0553586628912914 0.0000000000000000

0.2779746704420422 0.0553586628912912 0.0000000000000000

0.2779746704420422 0.2226160075507505 0.0000000000000000

0.2226160075507508 0.2779746704420420 0.0000000000000000

0.0553586628912917 0.2779746704420419 0.0000000000000000

0.0553586628912917 0.1107173257825827 0.0000000000000000

0.4440506591159160 0.0553586628912913 0.0000000000000000

0.6113080037753756 0.0553586628912912 0.0000000000000000

0.6113080037753756 0.2226160075507506 0.0000000000000000

0.5559493408840842 0.2779746704420421 0.0000000000000000

0.3886919962246250 0.2779746704420419 0.0000000000000000

0.3886919962246250 0.1107173257825827 0.0000000000000000

0.7773839924492496 0.0553586628912913 0.0000000000000000

0.9446413371087091 0.0553586628912913 0.0000000000000000

0.9446413371087091 0.2226160075507506 0.0000000000000000

0.8892826742174177	0.2779746704420421	0.0000000000000000
0.7220253295579586	0.2779746704420420	0.0000000000000000
0.7220253295579586	0.1107173257825827	0.0000000000000000
0.1107173257825827	0.3886919962246246	0.0000000000000000
0.2779746704420422	0.3886919962246244	0.0000000000000000
0.2779746704420422	0.5559493408840837	0.0000000000000000
0.2226160075507508	0.6113080037753753	0.0000000000000000
0.0553586628912917	0.6113080037753753	0.0000000000000000
0.0553586628912917	0.4440506591159159	0.0000000000000000
0.4440506591159160	0.3886919962246246	0.0000000000000000
0.6113080037753756	0.3886919962246244	0.0000000000000000
0.6113080037753756	0.5559493408840838	0.0000000000000000
0.5559493408840842	0.6113080037753753	0.0000000000000000
0.3886919962246250	0.6113080037753753	0.0000000000000000
0.3886919962246250	0.4440506591159159	0.0000000000000000
0.7773839924492496	0.3886919962246247	0.0000000000000000
0.9446413371087091	0.3886919962246245	0.0000000000000000
0.9446413371087091	0.5559493408840839	0.0000000000000000
0.8892826742174177	0.6113080037753754	0.0000000000000000
0.7220253295579586	0.6113080037753753	0.0000000000000000
0.7220253295579586	0.4440506591159160	0.0000000000000000
0.1107173257825827	0.7220253295579580	0.0000000000000000
0.2779746704420422	0.7220253295579576	0.0000000000000000
0.2779746704420422	0.8892826742174170	0.0000000000000000
0.2226160075507508	0.9446413371087086	0.0000000000000000

0.0553586628912917	0.9446413371087087	0.0000000000000000
0.0553586628912917	0.7773839924492493	0.0000000000000000
0.4440506591159160	0.7220253295579580	0.0000000000000000
0.6113080037753756	0.7220253295579577	0.0000000000000000
0.6113080037753756	0.8892826742174171	0.0000000000000000
0.5559493408840842	0.9446413371087088	0.0000000000000000
0.3886919962246250	0.9446413371087086	0.0000000000000000
0.3886919962246250	0.7773839924492492	0.0000000000000000
0.7773839924492496	0.7220253295579580	0.0000000000000000
0.9446413371087091	0.7220253295579580	0.0000000000000000
0.9446413371087091	0.8892826742174174	0.0000000000000000
0.8892826742174177	0.9446413371087088	0.0000000000000000
0.7220253295579586	0.9446413371087088	0.0000000000000000
0.7220253295579586	0.7773839924492494	0.0000000000000000
0.2222222222222222	0.1111111111111110	0.0000000000000000
0.1111111111111112	0.2222222222222223	0.0000000000000000
0.5555555555555556	0.1111111111111111	0.0000000000000000
0.4444444444444444	0.2222222222222223	0.0000000000000000
0.8888888888888890	0.1111111111111110	0.0000000000000000
0.7777777777777782	0.2222222222222224	0.0000000000000000
0.2222222222222222	0.4444444444444443	0.0000000000000000
0.1111111111111112	0.5555555555555556	0.0000000000000000
0.5555555555555556	0.4444444444444443	0.0000000000000000
0.4444444444444444	0.5555555555555556	0.0000000000000000
0.8888888888888890	0.4444444444444443	0.0000000000000000

0.7777777777777782	0.555555555555556	0.000000000000000
0.222222222222222	0.777777777777777	0.000000000000000
0.111111111111112	0.888888888888890	0.000000000000000
0.555555555555556	0.777777777777777	0.000000000000000
0.444444444444444	0.888888888888890	0.000000000000000
0.888888888888890	0.777777777777777	0.000000000000000
0.777777777777782	0.888888888888891	0.000000000000000