

Supporting Information

Adsorption of Metallic, Metalloidal and Nonmetallic Adatoms on Two-Dimensional C₃N

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C₃N Structural Details

Table S1: Lattice vectors of the C₃N unitcell.

Vector	x [Å]	y [Å]	z [Å]
1	4.861	0.000	0.000
2	-2.430	4.210	0.000
3	0.000	0.000	20.000

Table S2: Atomic positions of the C₃N unitcell .

Atom	x [Å]	y [Å]	z [Å]
C	1.215	0.701	10.000
C	0.000	1.403	10.000
C	3.645	0.701	10.000
C	-1.215	3.508	10.000
C	2.430	2.806	10.000
C	1.215	3.508	10.000
C	1.215	0.701	10.000
C	0.000	1.403	10.000

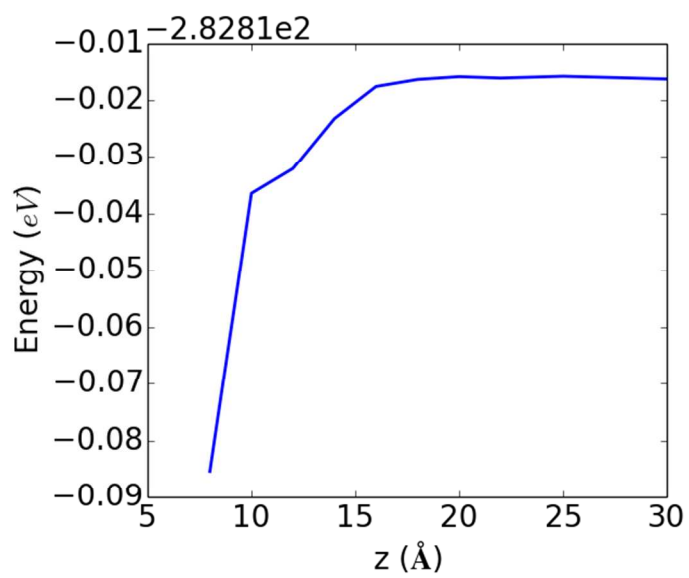


Figure S1. Total energy of the C₃N monolayer with respect to the vacuum space.