

## A multifunctional material of two-dimensional g-C<sub>4</sub>N<sub>3</sub>/graphene bilayer

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### 1. Geometry coordinates for g-C<sub>4</sub>N<sub>3</sub>/graphene bilayer.

g-C<sub>4</sub>N<sub>3</sub>/graphene

4.2401872388267243	-2.4480733664876904	0.0000000000000000	
0.0000000000000000	4.8961467329753816	0.0000000000000000	
0.0000000000000000	0.0000000000000000	20.0000000000000000	
C	0.3332752595999153	0.1666376393186937	0.0049711917219071
C	0.1666910034969860	0.3333820943013919	0.0050376857153438
C	0.8333623742542073	0.1666376312872657	0.0049711915002391
C	0.6666666959989627	0.3333332980038435	0.0050237481158959
C	0.3333333443078175	0.6666666616158849	0.0051924340427263
C	0.1666910449861092	0.8333089493091350	0.0050376859693841
C	0.8333623664040246	0.6667247463040482	0.0049711916437687
C	0.6666179000577799	0.8333089908302185	0.0050376856634173
C	0.8276646853012366	0.1723353075260974	0.1645950067259960
C	0.8276646882934173	0.6553293796726081	0.1645950082619692
C	0.3446706155049810	0.1723353057090478	0.1645950082752989
C	0.999999986028385	0.0000000023491751	0.1645319484150320
N	0.9837374038780240	0.4918686992284194	0.1644356606200859
N	0.5081313028873424	0.4918687045946228	0.1644356627102539
N	0.5081313064263568	0.0162625999495560	0.1644356606186932

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## 2. The changes in charge transfer with increasing interfacial distance

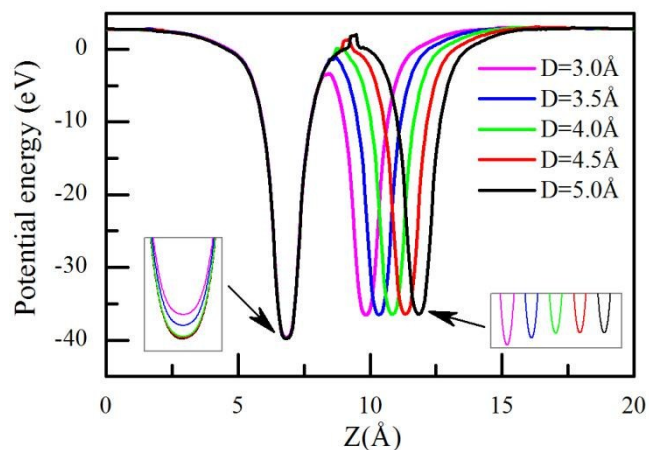


FIG. S1. XY-averaged electrostatic potentials of hybrid g-C<sub>4</sub>N<sub>3</sub>/graphene bilayer at different interfacial distances  $D$  (Å) along the Z direction. Depths of potential wells of graphene and g-C<sub>4</sub>N<sub>3</sub> are shown in the inset.

## 3. The ferromagnetic (FM), antiferromagnetic (AFM) and non-magnetic (NM) configurations

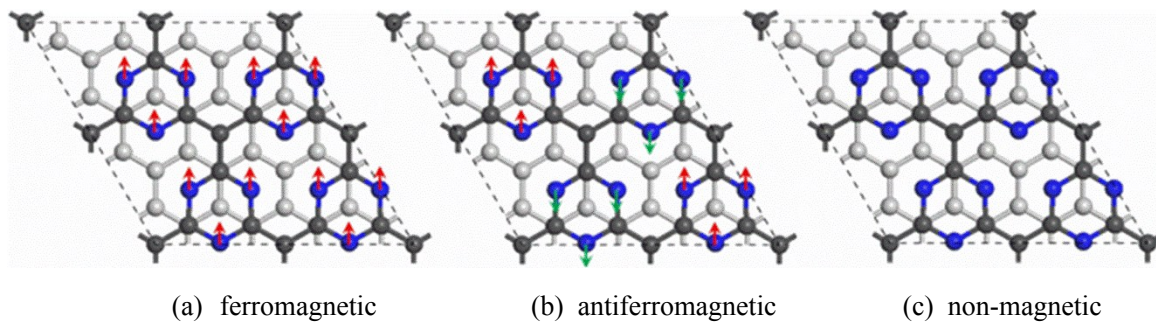


FIG. S2. The equilibrium configurations and local magnetic arrangements for (a) FM, (b) AFM, and (c) NM states.