

Structural, electronic and optical properties of hybrid graphitic carbon nitride and graphene nanocomposite

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1. Geometry coordinates for hybrid g-CN/G nanocomposite.

g-CN/G

4.2241786204226495	-2.4388306636060801	0.0000000000000000
0.0000000000000000	4.8776613272121603	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

C	0.3333281975965672	0.1666640987982765	0.0004871460275538
C	0.1667062236171521	0.3334124472343113	0.0004940451756642
C	0.8333359012017235	0.1666640987982765	0.0004871460275538
C	0.66666666666666715	0.3333333333333358	0.0005252400311381
C	0.3333333333333357	0.6666666666666643	0.0005470492404151
C	0.1667062236171521	0.8332937763828407	0.0004940451756642
C	0.8333359012017235	0.6666718024034327	0.0004871460275538
C	0.6665875527656887	0.8332937763828407	0.0004940451756642
C	0.8222301924887909	0.1777698075112090	0.1696880298293037
C	0.8222301924887910	0.6444603849775749	0.1696880298293037
C	0.3555396150224252	0.1777698075112090	0.1696880298293037
N	0.0000000000000000	0.0000000000000000	0.1696661458869145
N	0.9884359435831745	0.4942179717915802	0.1697068821401921
N	0.5057820282084198	0.4942179717915802	0.1697068821401921
N	0.5057820282084198	0.0115640564168254	0.1697068821401921

2. The electronic structure of the g-CN/G nanocomposite

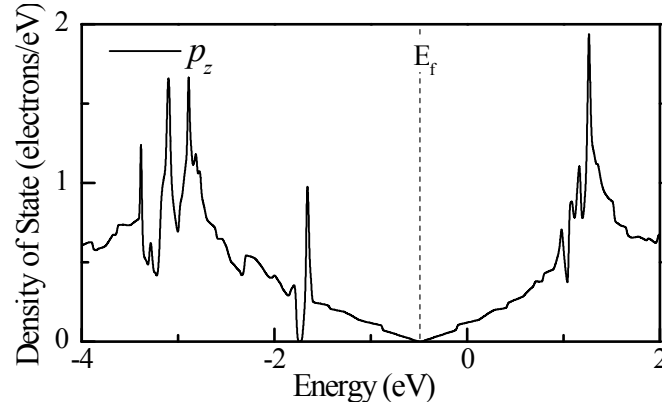


FIG. S1. The calculated partial density of state for C atoms belonged to graphene. The Fermi level is indicated by the dashed line.

3. The effect of E-field on the band gap of the g-CN/G nanocomposite

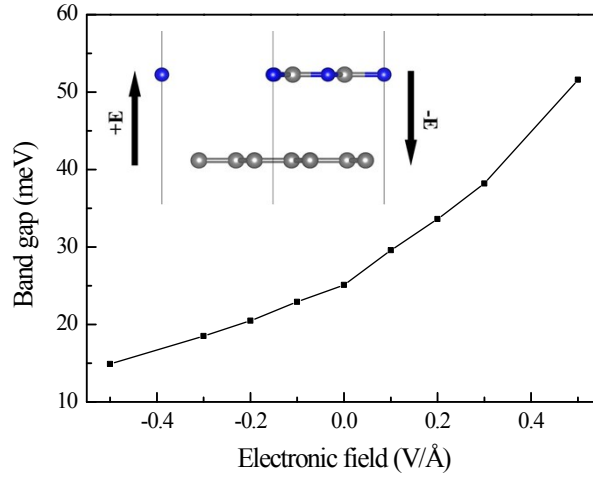


FIG. S2. Band gaps of the g-CN/G nanocomposite as a function of the external electric field (E-field). The results are calculated at the PBE level and the directions of the E-field is shown in the inset.

4. The changes in charge transfer with increasing interfacial distance

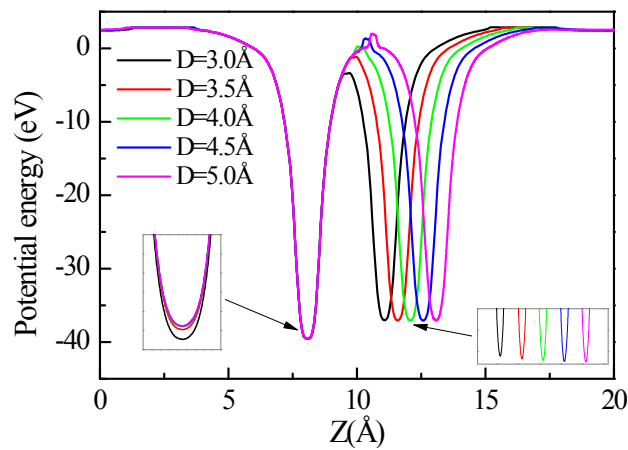


FIG. S3. XY-averaged electrostatic potentials of hybrid g-CN/G nanocomposite at different interfacial distances D

(Å) along the Z direction. Depths of potential wells of g-C₃N₄ and graphene are shown in the inset.

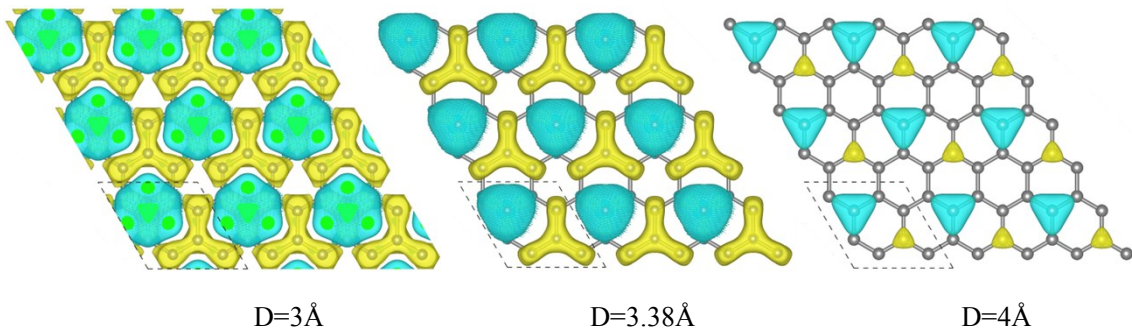


FIG. S4. The electron-hole puddle within graphene layer at different interfacial distances D (Å) along the Z direction. The yellow isosurface represents positive charge density and the cyan isosurface negative charge density. Isosurface is taken at a value of 0.0001 e/Bohr^3 .