Electronic Supplementary Materials for:

Reassessing structural models of graphitic carbon nitride for reliable photocatalytic predictions

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[*] *Corresponding authors: t.frankcombe@unsw.edu.au, yun.liu@anu.edu.au.*
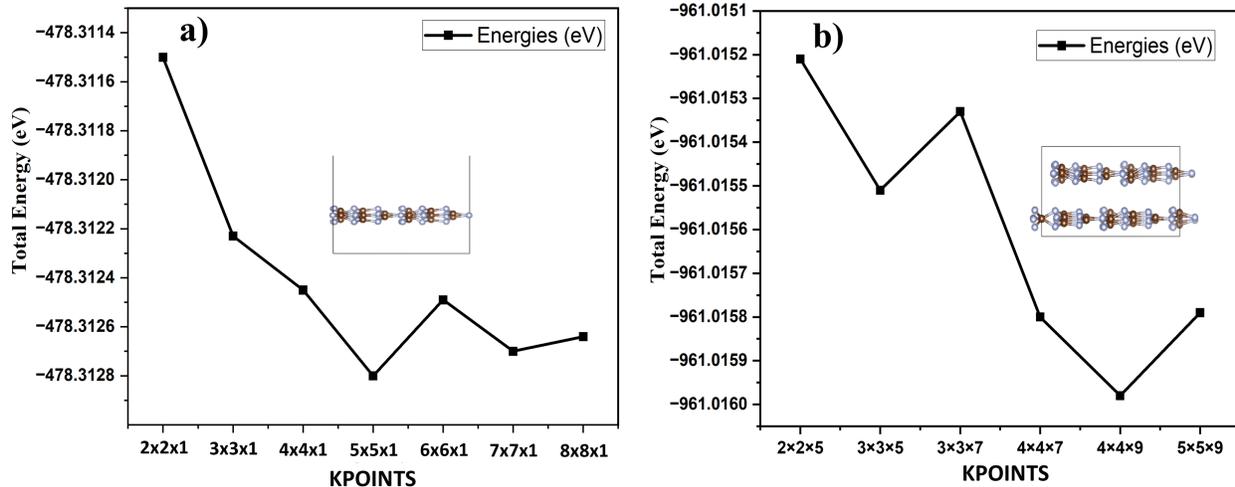[‡] *These authors contributed equally to this work.*

Figure S1 Convergence tests of the total energy with respect to the k-point sampling for the monolayer and bulk g-C_3N_4 structures considered in this work. (a) Total energy variation for the buckled g-C_3N_4 monolayer using Γ-centered grids ranging from $2 \times 2 \times 1$ to $8 \times 8 \times 1$. (b) Convergence behaviour for the corrugated bulk model using progressively denser k-point Γ-centered meshes.

As shown in Fig. S1, the energy differences between successive Γ-centered k-point meshes are on the order of $\sim 10^{-3}$ meV atom^{-1} for both the monolayer (56 atoms) and bulk (112 atoms) g-C_3N_4 models, corresponding to a range of approximately 0.001–0.006 meV atom^{-1}. These values are far below the typical convergence threshold of 1 meV atom^{-1}, confirming that the selected $3 \times 3 \times 1$ and $3 \times 3 \times 7$ k-point meshes used in this work provide well-converged Brillouin-zone sampling while maintaining computational efficiency. The reported energy differences per atom were obtained by dividing the total energy variation between successive k-point meshes by the number of atoms in the supercell.

Table S1 Relative total energies (in eV) of planar and buckled g-C_3N_4 models calculated using different exchange–correlation (XC) functionals.

XC Functional	Planar Reference Model 1	Buckled Model 2	Buckled Model 3	Buckled Model 4	Buckled Model 5
GGA-PBE	0.00	-0.96	-1.26	-2.86	-1.46
r^{2}SCAN	0.00	–	–	-2.90	–
HSE06	0.00	–	–	-2.64	–

2

Table S2 Interlayer binding energies, E_b, of different g-C_3N_4 stacking registries.

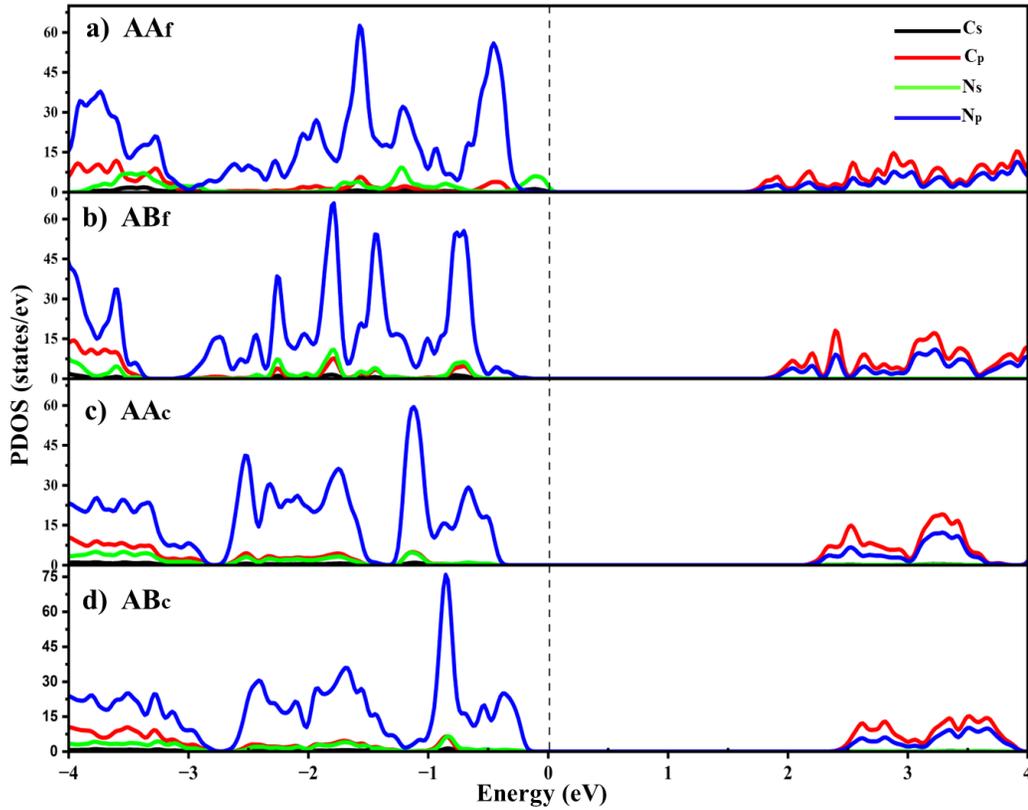| Stacking registry	E_b (eV Å^{-2})	E_b (J m^{-2})
AA_f	0.0060	0.0965
AB^*c	0.0072	0.1160
AA_c	0.0085	0.1359
AB^*c_2	0.0093	0.1484
AB^*c_1	0.0093	0.1489
ABc_1	0.0120	0.1928
ABc_2	0.0120	0.1928
ABc_3	0.0121	0.1933
AB^*f	0.0151	0.2415
AB^*c_3	0.0168	0.2699

Figure S2 PDOS of flat and buckled stacking configurations for AA and AB* registries of heptazine-based g-C_3N_4.

Table S3 Structural and electronic properties of g-C$_3$N$_4$ models from previous DFT studies and a representative corrugated bulk structure (AB$_{c3}$) from this work optimized using different exchange–correlation functionals.

Space group	Planarity/geometry	Relaxation Method	Lattice constant (Å)	Buckling height (Å)	PBE band gap (eV)	HSE06 band gap (eV)	Ref.
$P\bar{6}m2$	Planar/bulk	HSE06-D3	$a = 14.14$, $c = 6.38$	–	–	2.30	[1]
$P\bar{6}m2$	Non-planar/bulk	HSE06-D3	$a = 13.78$, $c = 6.98$	–	–	2.91	[1]
–	Non-planar/monolayer	PBE-D3	$a = 13.82$, $b = 12.24$	–	1.88	2.91	[2]
$Pca21$	Non-planar/monolayer	PBE-optB86b-vdW	$a = 11.81$, $b = 13.18$	Layer1 = 3.15	1.99	3.04	[3]
$P321$	Non-planar/monolayer	PBE-optB86b-vdW	$a = b = 11.81$,	Layer1 = 2.08	2.15	2.82	[3]
$C2221$	Non-planar/bulk	HSE06-D3	$a = 13.80$, $c = 6.68$	–	–	2.87	[4]
$Aba2$	Non-planar/monolayer	HSE06-D3	$a = 13.51$, $c = 6.95$	–	–	3.17	[4]
$Amm2$	Planar/bulk	HSE06-D3	$a = 14.12$, $c = 6.75$	–	–	2.66	[4]
$Cmcm$	Planar/bulk	PBE-D2	$a = 14.30$, $c = 7.06$	–	–	2.60	[5]
$P6_3/mmc$	Planar/bulk	PBE-D2	$a = 14.29$, $c = 6.92$	–	–	2.40	[5]
$P1$	Non-planar/bulk	PBE-D3(BJ)	$a = 13.90$, $c = 6.97$	Layer1 = 1.32, Layer 2 = 1.40	1.60	2.81	This work
$P1$	Non-planar/bulk	TPSS-D3(BJ)	$a = 13.86$, $c = 6.96$	Layer1 = 1.32, Layer2 = 1.40	1.60	2.81	This work
$P1$	Non-planar/bulk	r^{2}SCAN-D3(BJ)	$a = 13.81$, $c = 6.76$	Layer1 = 1.32, Layer2 = 1.40	1.60	2.81	This work
$P1$	Non-planar/bulk	r^{2}SCAN	$a = 13.79$, $c = 7.12$	Layer1 = 1.35, Layer2 = 1.46	1.51	2.86	This work
$P1$	Non-planar/bulk	HSE06-D3(BJ)	$a = 13.77$, $c = 6.99$	Layer1 = 1.30, Layer2 = 1.41	–	2.86	This work

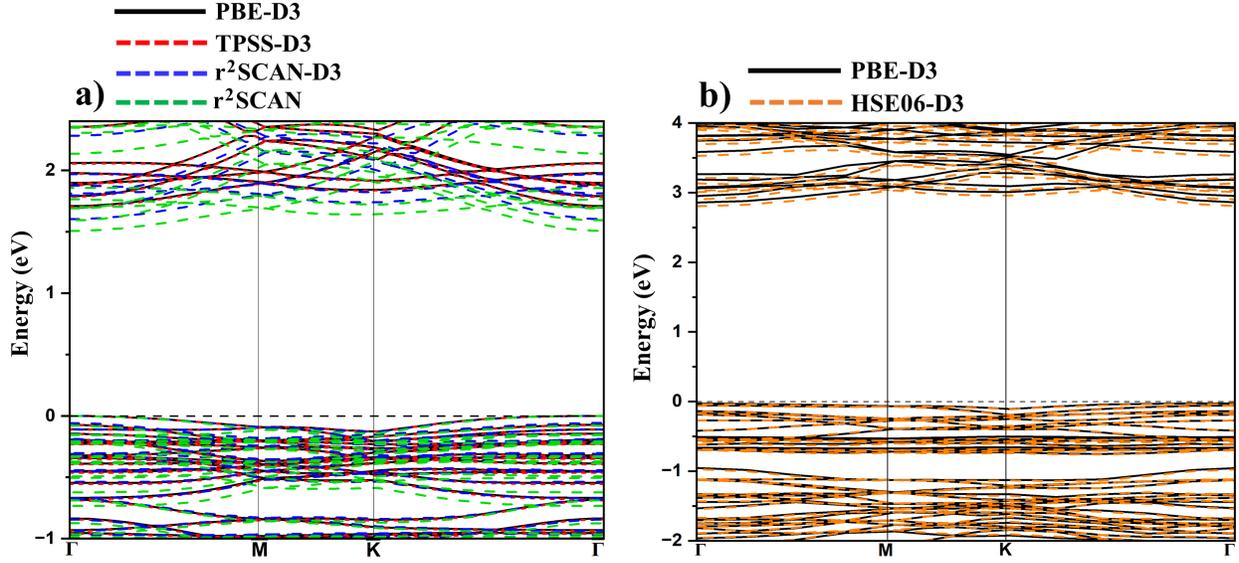**Figure S3** (a) PBE band structures of bulk g-C_3N_4 evaluated at geometries optimized using (i) PBE-D3 (ii) TPSS-D3 (iii) r^{2}SCAN and (iv) r^{2}SCAN functionals. (b) HSE06 band structures of bulk g-C_3N_4 evaluated at geometries optimized using (i) PBE-D3 and (ii) HSE06-D3 functionals.

To evaluate the sensitivity of the predicted electronic structure to the structural relaxation method, a representative bulk g-C_3N_4 stacking configuration (AB$_c$) was fully optimized using several exchange-correlation (XC) functionals (PBE-D3, TPSS-D3, r^{2}SCAN-D3, r^{2}SCAN, and HSE06-D3). The resulting structural parameters (Table S3) show only minor variations in the lattice constants ($a = 13.77$–13.90 Å, $c = 6.76$–7.12 Å) and buckling heights (Layer 1 ≈ 1.30–1.35 Å; Layer 2 ≈ 1.40–1.46 Å), indicating that the corrugated bulk framework is robust with respect to the choice of XC functional. The corresponding band structures (Fig. S3) display very similar dispersions, with PBE band gaps varying modestly between 1.51 and 1.60 eV depending on the relaxed geometry, while HSE06 calculations yield band gaps of 2.8–2.86 eV. These results indicate that the electronic structure of bulk g-C_3N_4 is only weakly affected by the relaxation functional, confirming the reliability of the PBE-D3 optimized geometry used in the main calculations.

Table S4 PBE band gaps E_g (in eV) of pristine, P-doped, and Ni-doped g-C_3N_4 for different structural motifs.

Structural motif	E_g (pure)	E_g (P-doped)	E_g (Ni-doped)
2D planar	1.25	0.24	0.00
2D buckled	1.87	1.62	0.13
3D buckled	1.71	0.99	0.00

5

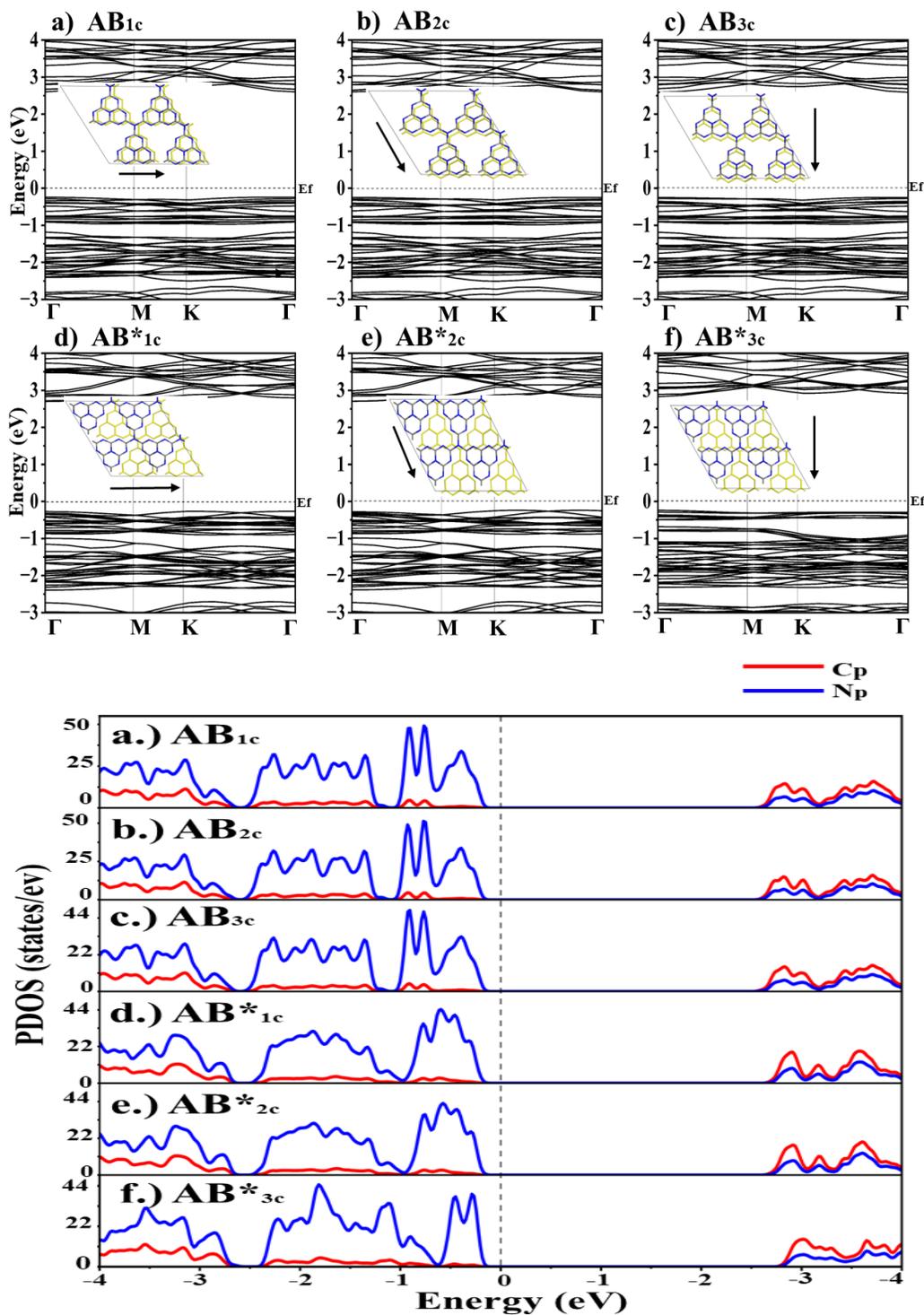**Figure S4** HSE06 band structures and PDOS of different corrugated stacking motifs for heptazine-based g-C_3N_4. The asterisk (*) and subscript "c" refer to $180°$ rotation and corrugated models, respectively.

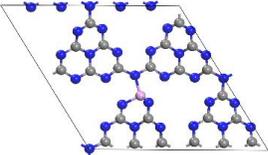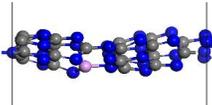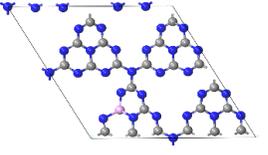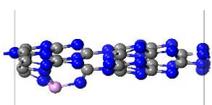| S/N	Dopant sites	E_f (eV)	Structural Model	
			Top View	Side View
1	P@C1	0.54		
2	P@C2	0.83		
3	P@C3	0.87		
4	P@C4	0.54		
5	P@C5	0.87		
6	P@Int	1.65		
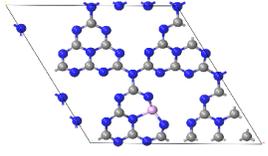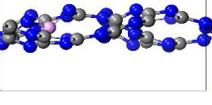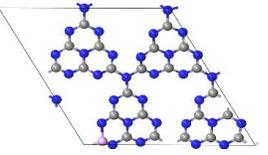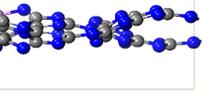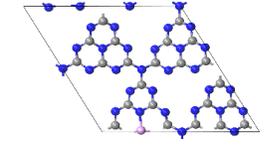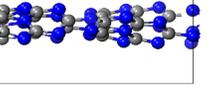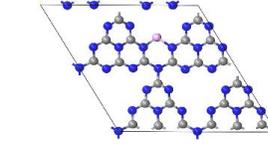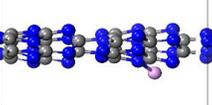
Figure S5 Possible P dopant sites in buckled g-C_3N_4 monolayer (C1–C5 and interstitial position), including their corresponding formation energies.

S/N	Dopant sites	E_f (eV)	Structural Model	
			Top View	**Side View**
1	P@N1	0.99		
2	P@N2	0.88		
3	P@N3	0.99		
4	P@N4	1.90		
5	P@N5	0.60		
6	P@N6	0.88		
7	P@N7	0.60		
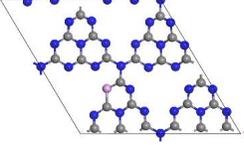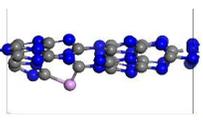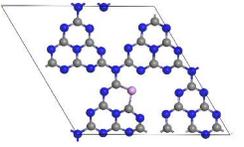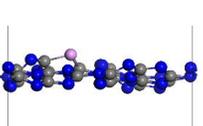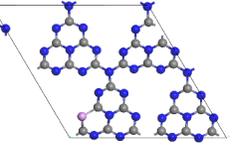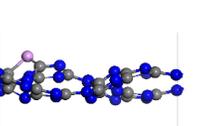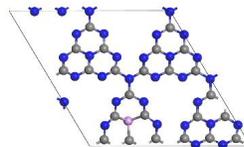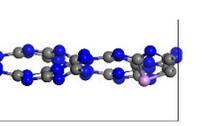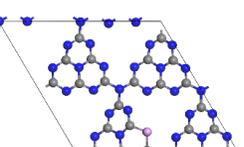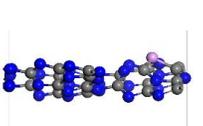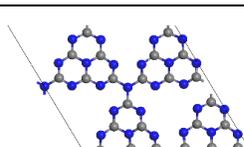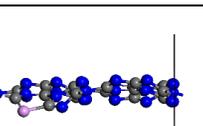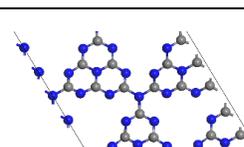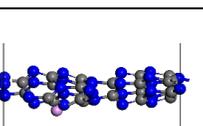
Figure S6 Possible P dopant sites in buckled g-C_3N_4 monolayer (N1–N7), including their corresponding formation energies.
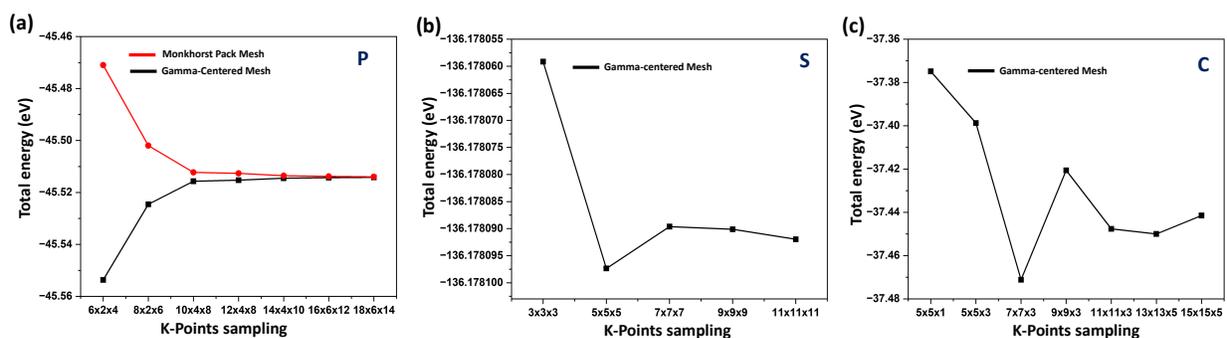
Figure S7 K-point convergence tests showing the variation of total energy with k-point sampling density for the pure elemental phases used to obtain the chemical potentials (per-atom energies): (a) black phosphorus, (b) orthorhombic sulfur (α-S), and (c) carbon (graphite).
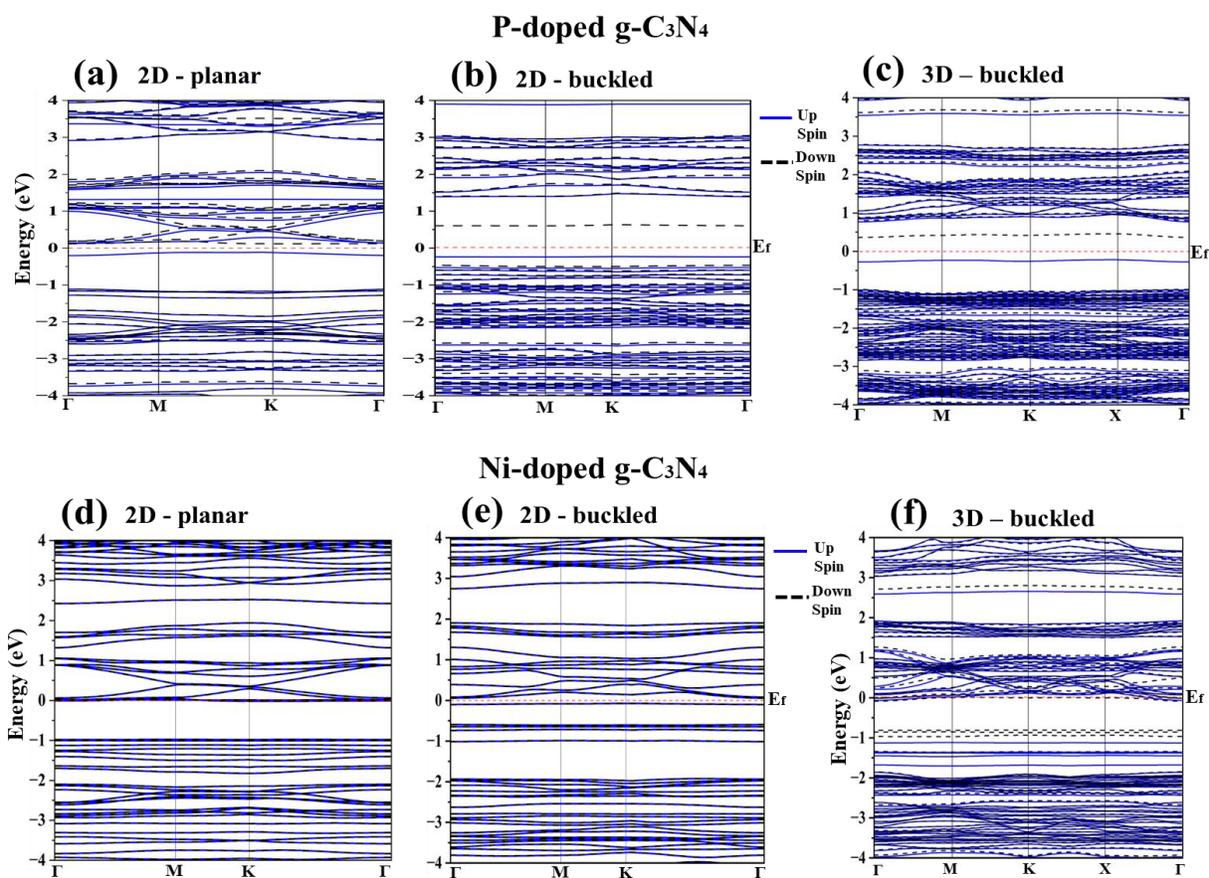
Figure S8 Electronic band structures of P- and Ni-doped g-C_3N_4 in planar 2D, buckled 2D, and buckled 3D configurations.

1. Optimized structure of the buckled monolayer g-C$_3$N$_4$ used in this work.

```
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  -6.9272965831589515   11.9984296410823301    0.0000000000000000
   0.0000000000000000    0.0000000000000000   20.0000000000000000
   C     N
  24    32
Direct
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  0.6170604947644862    0.5555376249581461    0.1822785433516864
  0.9402165084829417    0.8786957097990099    0.1998686788673643
  0.9421766680379032    0.7175721351482146    0.2140966271386824
  0.7781844683026196    0.5535822591512768    0.1680481663604342
  0.7743806261133375    0.7213761385769288    0.1910747462367568
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  0.4421672280341282    0.7175564305588795    0.1680512143458144
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0.9951243388458700    0.3281738416414290    0.1587825174762613
0.8429832935197081    0.0090657416323050    0.2251442566994835
0.6647365684866408    0.1633935770033037    0.1852014036052018
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```

2. Optimized structures of selected corrugated stacking configurations of bulk g-C$_3$N$_4$ used in this work.

    a. Corrugated AA Stacking pattern

```
Corrugated_AA_g-C3N4_bulk
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 0.0002876212973206    -0.0002223893738684      7.1819621818604338
   C      N
  48     64
Direct
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  0.6169833986862256    0.5554297360782776    0.1182618367262987
  0.9396941013906569    0.8784448159240451    0.1617194944615437
  0.9427581881800505    0.7180265336303220    0.1991230103415933
  0.7775779155134688    0.5527235599861777    0.0797574580917856
  0.7739537520538093    0.7212298177801735    0.1405500781850030
  0.4392838164861463    0.0565188366190082    0.1392856201766234
  0.1169840579517564    0.0554291768659491    0.1182582732207527
  0.4396934785881167    0.3784450626617435    0.1617245005290578
  0.4427591542369056    0.2180269404496889    0.1991111082704310
  0.2775781906139550    0.0527242664679501    0.0797442612271552
  0.2739538137558222    0.2212296879317255    0.1405510981254052
  0.4392286224874403    0.5564659869937554    0.1393125727830986
  0.1173043112524732    0.5560576132960564    0.1617314765163677
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0.2777228184111923   0.5529963531322523   0.1991492278332025
0.2745163424714418   0.7217942730532563   0.1405435134548330
0.9392301615897038   0.0564662911304535   0.1393025751936367
0.6173048032924328   0.0560572916213339   0.1617051542749771
0.9403203875293172   0.3787647080928969   0.1182630262921138
0.9430253810272634   0.2181700441692789   0.0797535395837352
0.7777229921346198   0.0529954166559103   0.1991288842570214
0.7745175894964654   0.2217940186522428   0.1405223003771964
0.9392292325133603   0.5564791057292461   0.6383791083348934
0.6172969207110005   0.5560568060337361   0.6159929293328372
0.9403060118823943   0.8787707055017192   0.6594441995788154
0.9430138987629729   0.7181784999468769   0.6979423551394018
0.7777196540205326   0.5529990065454359   0.5785586603820357
0.7745058888879346   0.7217966158271090   0.6371770511625753
0.4392306966995875   0.0564801883983664   0.6383601168429840
0.1172977862863068   0.0560559676435211   0.6159893287985229
0.4403057869185944   0.3787709776516816   0.6594504553023649
0.4430154148557043   0.2181790388322243   0.6979317315559161
0.2777203755613780   0.0529996725941557   0.5785457354903597
0.2745062182629670   0.2217961333991928   0.6371808129894400
0.4392790050255165   0.5565291213510148   0.6383972610380989
0.1169843391646939   0.5554473021407953   0.6594400907847695
0.4396967286321514   0.8784586434620967   0.6159601706327921
0.4427579086913506   0.7180354498978097   0.5785664336626677
0.2775757730613795   0.5527424173404383   0.6979509332483460
0.2739564836828726   0.7212473844920150   0.6371659910337242
0.9392808913448090   0.0565293821796058   0.6383867256067641
0.6169851117255223   0.0554468039507467   0.6594123830444063
0.9396982393150007   0.3784587052404764   0.6159641861217394
0.9427616150623259   0.2180373590018426   0.5785604200035090
0.7775761824826865   0.0527412374375236   0.6979292402942338
0.7739577766316998   0.2212465479257952   0.6371401794551449
0.9993582011654439   0.9959525432157116   0.1395174400878962
0.9879195096450032   0.6539065752952461   0.2285713768336367
0.6674123214029636   0.5004056939756547   0.0543020677930737
0.8317928799236229   0.8305792012624161   0.1228519421410299
0.9950200305840602   0.8281284602060829   0.2247554557044807
0.8418483125865692   0.5077107692318654   0.0499536046531935
0.6646463205570680   0.6630925696310247   0.1589979195264517
0.8318269006909603   0.6635983255045358   0.1396187459150019
0.4993576031092652   0.4959530293519275   0.1395248104996393
0.4879214043072678   0.1539067523326344   0.2285516311374214
0.1674126125497066   0.0004060538226380   0.0542926569810123
0.3317916713644705   0.3305793389520730   0.1228616634791471
0.4950200719377436   0.3281276047237948   0.2247529414525489
0.3418482233597542   0.0077108868149168   0.0499367277049361
0.1646465243427834   0.1630906987206432   0.1590033934291984
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0.3318278433210358	0.1635987977259224	0.1396062061763981
0.4997956912423064	0.9963894994483655	0.1395055871121206
0.4880339193678477	0.6538968845989840	0.0499528547274176
0.1676238467470627	0.5007408808454458	0.2247962983510152
0.3326560454155572	0.8311030793555030	0.1589899700300449
0.4953407822658305	0.8283333026875432	0.0543010153830608
0.3418454674694958	0.5078354487014339	0.2285951736218120
0.1651689992857930	0.6639548908577709	0.1228353890847523
0.3321502761014850	0.6639230233639927	0.1396204399803234
0.9997953535508922	0.4963891547646729	0.1395278334140708
0.9880385384672484	0.1538992813523342	0.0499500457385550
0.6676232735650161	0.0007404085600843	0.2247737453257219
0.8326546679324419	0.3311005373245187	0.1589803475055325
0.9953457127609080	0.3283360155609911	0.0543117798515531
0.8418446531068984	0.0078343707484163	0.2285788068710943
0.6651691381800635	0.1639534004475168	0.1228052872920457
0.8321506837045619	0.1639220626658877	0.1396018729529829
0.9997869618937770	0.9963938450452094	0.6381807727269040
0.9880287439031200	0.6539118300306942	0.7277446256171438
0.6676190248742498	0.5007380136451255	0.5529278054269220
0.8326412786987183	0.8311044553061120	0.6187296546684568
0.9953307777060354	0.8283451623892099	0.7233905409926333
0.8418482258933471	0.5078444805773622	0.5490942594739944
0.6651580337034968	0.6639547495783701	0.6548915485240788
0.8321420843284678	0.6639277153478844	0.6380895407920508
0.4997862964315824	0.4963944588917893	0.6381888939063473
0.4880313655465135	0.1539122027054025	0.7277262285899547
0.1676197490050380	0.0007385197478648	0.5529170629621439
0.3326402090889784	0.3311042771701920	0.6187426816155651
0.4953316230563574	0.3283444580394431	0.7233882286711918
0.3418488810433830	0.0078449154500127	0.5490777611382240
0.1651584602072025	0.1639523703047549	0.6548995101269320
0.3321433199793438	0.1639278669718512	0.6380793061678713
0.4993614204313926	0.9959691525086113	0.6381439135855407
0.4879154115055856	0.6539094390766119	0.5491139715073202
0.1674096077390741	0.5004234308430650	0.7233971123440558
0.3317986178015792	0.8305987552850004	0.6548538414486355
0.4950178034504686	0.8281346829571523	0.5529123807758075
0.3418443712749171	0.5077290562585987	0.7277528393079694
0.1646504044427786	0.6631107641732216	0.6187160501208453
0.3318295964358388	0.6636155399830670	0.6380994032179056
0.9993608202887627	0.4959685989190566	0.6381648321092774
0.9879202792439696	0.1539114605218271	0.5491097640165492
0.6674093871167165	0.0004229581961091	0.7233735311995780
0.8317970162455278	0.3305955875409998	0.6548390518806438
0.9950229997028115	0.3281371665078162	0.5529214080703720
0.8418441161931490	0.0077281628829915	0.7277369811475387
0.6646506255507940	0.1631086357906577	0.6186816187918038

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     0.8318300174571031    0.1636139191809479    0.6380775216745863
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b. Corrugated AB Stacking pattern

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13.9939381243969141    -0.0075249775942331     0.2521386052797668
-7.0033613276809650    12.1163532868388213    -0.2421420337994773
 0.1393529857019180    -0.0739627512486262     7.6028347690852796
   C      N
  48     64
Direct
   0.9390893942837213    0.5556768725874806    0.1393221764048734
   0.6169006702007991    0.5539561980354428    0.1269530439080104
   0.9388531292484431    0.8774452046706258    0.1553551729971590
   0.9430768701371720    0.7188001027817948    0.1829054573310976
   0.7767257248813448    0.5499437271339531    0.0964484803432547
   0.7742736161850758    0.7190457689188169    0.1429603804188146
   0.4390892586011657    0.0556770531619604    0.1392943788419486
   0.1169007534181577    0.0539561428619163    0.1269387228086764
   0.4388510567143525    0.3774449539117473    0.1553696393593573
   0.4430750460402080    0.2187983268580154    0.1828963177387068
   0.2767258568721649    0.0499459939292148    0.0964233789263496
   0.2742725961755059    0.2190463922109296    0.1429643543978343
   0.4391030297387755    0.5557069100238227    0.1396835536930918
   0.1173242575528457    0.5559928370015126    0.1545680718172930
   0.4408944614356331    0.8778996980009590    0.1261672129654083
   0.4449867771820589    0.7181183079475499    0.0962357380608489
   0.2759134153970851    0.5517203553414906    0.1827095935999029
   0.2757428370502817    0.7204921140654059    0.1418270784364171
   0.9391023085918909    0.0557056278386365    0.1396652859376523
   0.6173235773781692    0.0559330860221752    0.1545453515420079
   0.9408950255903813    0.3778988628444062    0.1261954222891377
   0.9449885743491580    0.2181196713744552    0.0962405842086217
   0.7759121393497365    0.0517181598674597    0.1826814046759183
   0.7757423354581809    0.2204914646252271    0.1418355012634243
   0.0605129503093612    0.4387500530149915    0.6380464782656892
   0.3822980123592664    0.4385157559043376    0.6231243811202638
   0.0587159645238998    0.1165580505566826    0.6514997741462822
   0.0546161109664598    0.2763348703287475    0.6815003232517738
   0.2237049569663371    0.4427255614356626    0.5950221771110427
   0.2238707738558119    0.2739611028919768    0.6358439967638325
   0.5605138335272419    0.9387515148082398    0.6380171846790187
   0.8822968419884714    0.9385160657803777    0.6231046636692548
   0.5587161373085747    0.6165597807577544    0.6515122148836735
   0.5546172735330583    0.7763384283419795    0.6814864502932201
   0.7237053853875772    0.9427251971195504    0.5949923444215282
   0.7238700402601325    0.7739623251766922    0.6358411706310664
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 0.5605350103050623    0.4387821631934432    0.6384242080206319
 0.8827278134762443    0.4405228558245470    0.6507576351543408
 0.5607794169471410    0.1170251720411006    0.6223010320833537
 0.5565541518747329    0.2756657848838841    0.5948025483040212
 0.7228947078941043    0.4445187508437539    0.6813182534653601
 0.7253611220849107    0.2754267532238248    0.6347023705077329
 0.0605331143931943    0.9387801174223649    0.6384074034592491
 0.3827280162865482    0.9405232880900002    0.6507227526748803
 0.0607785494252512    0.6170239081503813    0.6223179883332424
 0.0565497841281239    0.7756615675257054    0.5948056107494815
 0.2228945195578520    0.9445178274030893    0.6812893034023235
 0.2253620045841993    0.7754277579108666    0.6346841393720686
-0.0014333071302605    0.9951988639950304    0.1402196006609722
 0.9916897455269136    0.6590902113653698    0.2027305134407915
 0.6674003499191271    0.4973433493887847    0.0755854618627890
 0.8310240859962208    0.8276622842794129    0.1250085699771772
 0.9951175166895444    0.8286430688788982    0.2030088581415991
 0.8373731801470383    0.5011300875374674    0.0753070532030224
 0.6652494463644217    0.6617716209686719    0.1633559786581764
 0.8315715780038604    0.6622928552374985    0.1406021982090228
 0.4985665670509394    0.4951995119356712    0.1402381555627806
 0.4916873848373523    0.1590877333975725    0.2027123017690916
 0.1674010964724202   -0.0026531716017342    0.0755586747265946
 0.3310219059139098    0.3276642820847625    0.1250282585355712
 0.4951150859980201    0.3286404718137354    0.2030123984196002
 0.3373735439255602    0.0011326340564712    0.0752745637433408
 0.1652486558083110    0.1617707158104018    0.1633589817909606
 0.3315705958581913    0.1622933418229537    0.1405893213163466
 0.4995802615098074    0.9961884773230599    0.1394834258086511
 0.4938178913687518    0.6574500564467463    0.0755181111359682
 0.1660147584359621    0.4996905966357326    0.2028106021318668
 0.3329520995797820    0.8294734895438541    0.1619926851689044
 0.4976631813211453    0.8274528004425818    0.0753142043091187
 0.3355248525428063    0.5030672408999924    0.2029450703053764
 0.1671566632729753    0.6637285127618057    0.1235484887360594
 0.3325047734584530    0.6632178977324035    0.1400566236709544
-0.0004191537502717    0.4961890239167485    0.1395166678450792
 0.9938212014076283    0.1574526752952963    0.0755177377152952
 0.6660119771058710   -0.0003135736887135    0.2027748791503877
 0.8329530973401345    0.3294722899373577    0.1620237830692231
 0.9976659386134097    0.3274569518975648    0.0753351265241277
 0.8355214609745515    0.0030617052175726    0.2029097839428232
 0.6671577501452296    0.1637314536581937    0.1235498797033178
 0.8325048390333958    0.1632173558713953    0.1400486668336159
 0.0000363115532789    0.9982651499698356    0.6381991894072589
 0.0057907912333421    0.3370103297333269    0.7022165679675321
 0.3336021341511720    0.4947588050653303    0.5748869910483515
 0.1666521405673726    0.1649813482939073    0.6156275495484562
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0.0019441605392302    0.1669952628552499    0.7023920482645187
0.1640913077710118    0.4913747173079063    0.5747767890681974
0.3324582095830691    0.3307115787524936    0.6540822044531627
0.1671066230450187    0.3312337299698345    0.6376960311803831
0.5000363421970526    0.4982659281948519    0.6382206382457187
0.5057926126527320    0.8370147382391618    0.7021946925268510
0.8336026159318274    0.9947567519780303    0.5748546117508951
0.6666527901199478    0.6649819858253175    0.6156410902067403
0.5019457599342809    0.6669996846231955    0.7023935430373747
0.6640913921240681    0.9913751277641345    0.5747425066176598
0.8324575664841242    0.8307139945003080    0.6540799485395671
0.6671067249657506    0.8312347933680496    0.6376758947579974
0.5010615313478447    0.9992756505187615    0.6374487297875089
0.5079386858079850    0.3353744855076701    0.5749911154753814
0.8322252212612987    0.4971218264829136    0.7021925849900463
0.6686107817032950    0.1668094042267902    0.6526262273185233
0.5045090753252451    0.1658267341901875    0.5746602050427210
0.6622422667807425    0.4933272549453202    0.7024582476884017
0.8343825012774052    0.3327127329320618    0.6142859886894317
0.6680563322515065    0.3321741290053896    0.6371199954260603
0.0010614541529623    0.4992745887716319    0.6374811980050581
0.0079324648085650    0.8353683105638335    0.5749922178561504
0.3322263908374351    0.9971232472785476    0.7021540999412826
0.1686124386251311    0.6668099375943228    0.6526231530759818
0.0045036837096046    0.6658209490900353    0.5746820139230018
0.1622428395864243    0.9933277731805517    0.7024296785517885
0.3343830332968799    0.8327132082708605    0.6142551466909468
0.1680554335669110    0.8321725737497324    0.6371038134526310
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    c. Corrugated AB$_{3c}$ Stacking pattern

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Corrugated_AB_3c_g-C3N4_bulk
1.00000000000000
13.8778216988194742     0.0056398121145604     0.0159572731997013
-6.9326068395638059    12.0662382462042572    -0.0010496279981677
 0.0065209808430480     0.0017203145418332     6.9739682597215005
  C        N
 48       64
Direct
  0.9981486443691665   0.5001049924091276   0.1957675706404842
  0.6752925017955675   0.4989644303617879   0.1616796970325396
  0.9986026604073359   0.8228350523394425   0.2113836640264708
  0.0008482950301740   0.6620908713190019   0.2462917565049736
  0.8365858186503061   0.4963428032528867   0.1300755422400997
  0.8333113165769959   0.6651846896652742   0.1797010836971893
  0.4981493068726977   0.0001083522498533   0.1957581299648510
  0.1752919779517512   0.9989618715576825   0.1616604939641419
  0.4986039225207719   0.3228346739383312   0.2113867482381977
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0.5008458511522136    0.1620883082493307    0.2462841218506142
0.3365858417151415    0.9963447877950316    0.1300534799376223
0.3333064421910876    0.1651795537079082    0.1796801991074872
0.4981078031559960    0.5001085390598305    0.1985285981589371
0.1752102568249114    0.4989943201013531    0.2329005706467910
0.4986753346047550    0.8228564679397650    0.1830356262089055
0.5009154058765404    0.6621435420208712    0.1479443078893823
0.3363830365468345    0.4962981992768860    0.2642504503787677
0.3332508662687488    0.6652235284651269    0.2149291078850268
0.9981091495508920    0.0001080280015984    0.1985218277768510
0.6752139366865677    0.9990007879974314    0.2328928984600296
0.9986695316138139    0.3228522215451761    0.1830406841904590
0.0009125107654313    0.1621392229330070    0.1479406007523707
0.8363836741081627    0.9962981885072466    0.2642427025323144
0.8332508271134671    0.1652186253429875    0.2149271945568785
0.8977900049920109    0.6463954598522506    0.6895172215347998
0.5753417123798670    0.6453858902018439    0.6766042895530902
0.8978830935686375    0.9681022122420657    0.7264669663242884
0.9014849992258007    0.8077560344394143    0.7516754058489283
0.7365299590686618    0.6446735513540105    0.6302819447368933
0.7320184166383754    0.8106334052917532    0.7070063033932570
0.3977890180618573    0.1463936565946042    0.6895082991844674
0.0753414047085954    0.1453865846975404    0.6765998698553091
0.3978812475052962    0.4681014003255868    0.7264646293794215
0.4014831683761386    0.3077507056604176    0.7516672033124365
0.2365290532365947    0.1446726693872264    0.6302731439602169
0.2320122469278232    0.3106271909046185    0.7070014816642143
0.3977629441646968    0.6464288868044576    0.7051486485355127
0.0753814826213954    0.6455177546193553    0.7182057504708510
0.3980933800088167    0.9682176809763803    0.6682839374948344
0.4016886470831196    0.8078857674185329    0.6429629666432035
0.2364349638289269    0.6447299808318050    0.7644220114544567
0.2321605909432236    0.8107851450275518    0.6879782741630294
0.8977631961905956    0.1464285247354979    0.7051485194673361
0.5753802640133685    0.1455127762116462    0.7182083460025694
0.8980957148109638    0.4682192596966956    0.6682992989774519
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