# Supporting information

# -for-

## An Ab-initio Study of the Graphyne (GY) for Detection of Rare Bases in DNA

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**Table and Figure from calculation**

**Contents**:



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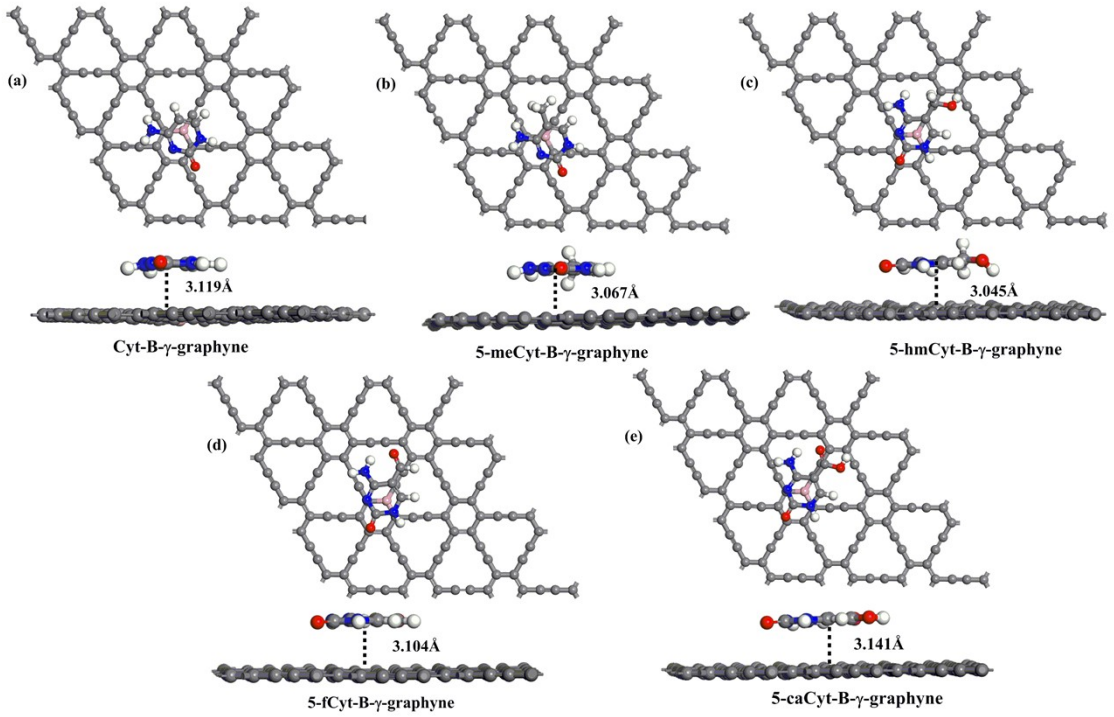
(a)
3.119Å
Cyt-B-γ-graphyne
(b)
3.067Å
5-meCyt-B-γ-graphyne
(c)
3.045Å
5-hmCyt-B-γ-graphyne
(d)
3.104Å
5-fCyt-B-γ-graphyne
(e)
3.141Å
5-caCyt-B-γ-graphyne

Fig. S1

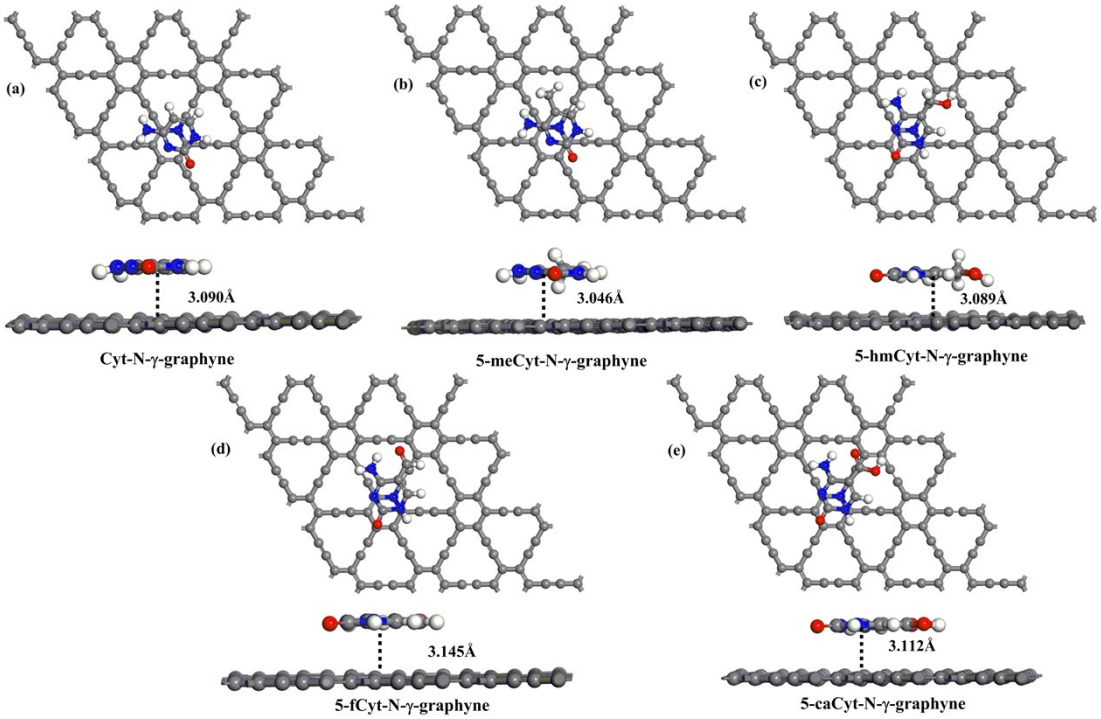
(a)
3.090Å
Cyt-N-γ-graphyne
(b)
3.046Å
5-meCyt-N-γ-graphyne
(c)
3.089Å
5-hmCyt-N-γ-graphyne
(d)
3.145Å
5-fCyt-N-γ-graphyne
(e)
3.112Å
5-caCyt-N-γ-graphyne

Fig. S2

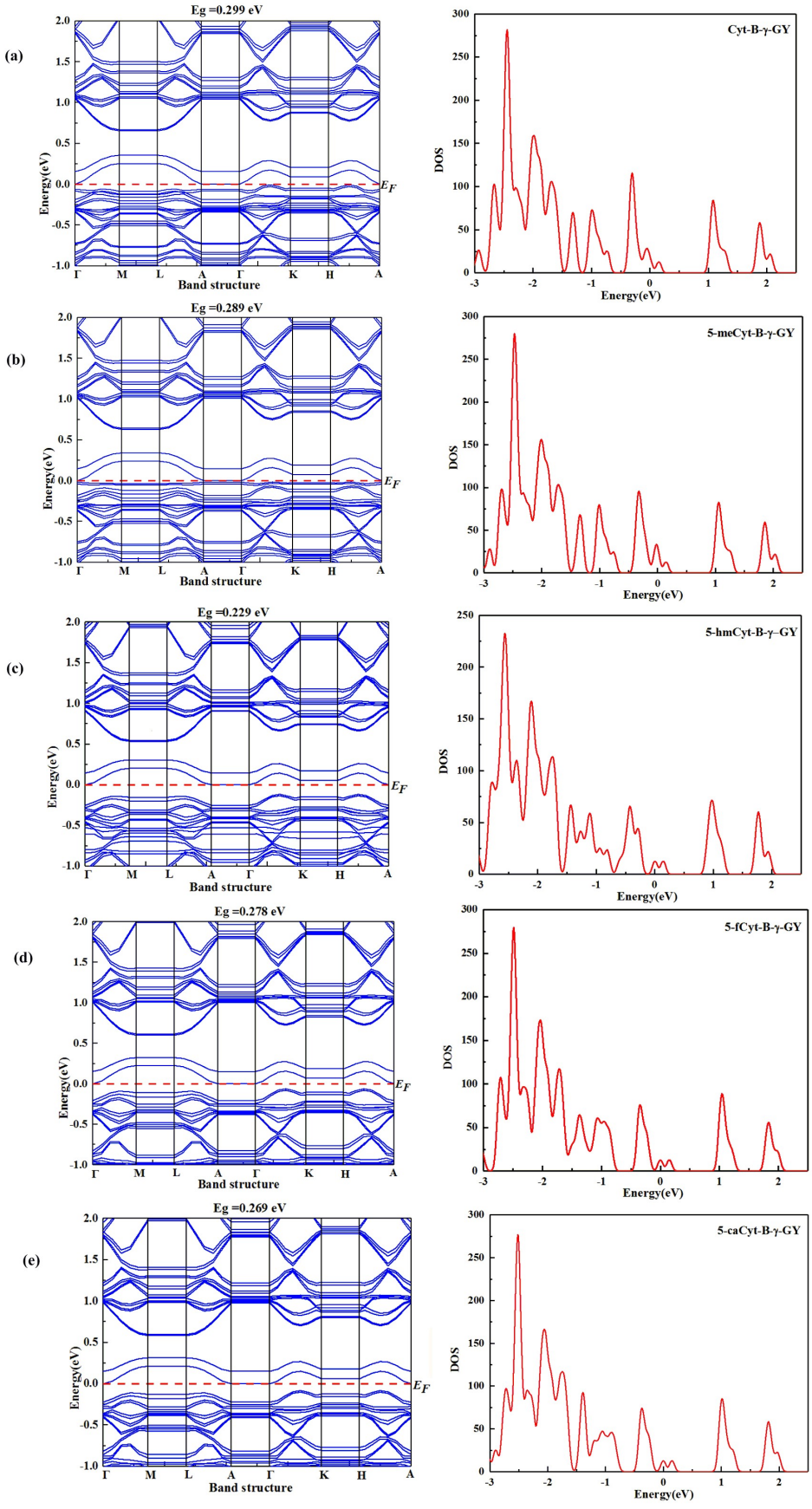
(a)
Eg =0.299 eV
Energy(eV)
Band structure
Γ M L A Γ K H A
$E_F$
DOS
Energy(eV)
Cyt-B-γ-GY
(b)
Eg =0.289 eV
5-meCyt-B-γ-GY
(c)
Eg =0.229 eV
5-hmCyt-B-γ-GY
(d)
Eg =0.278 eV
5-fCyt-B-γ-GY
(e)
Eg =0.269 eV
5-caCyt-B-γ-GY

Fig. S3

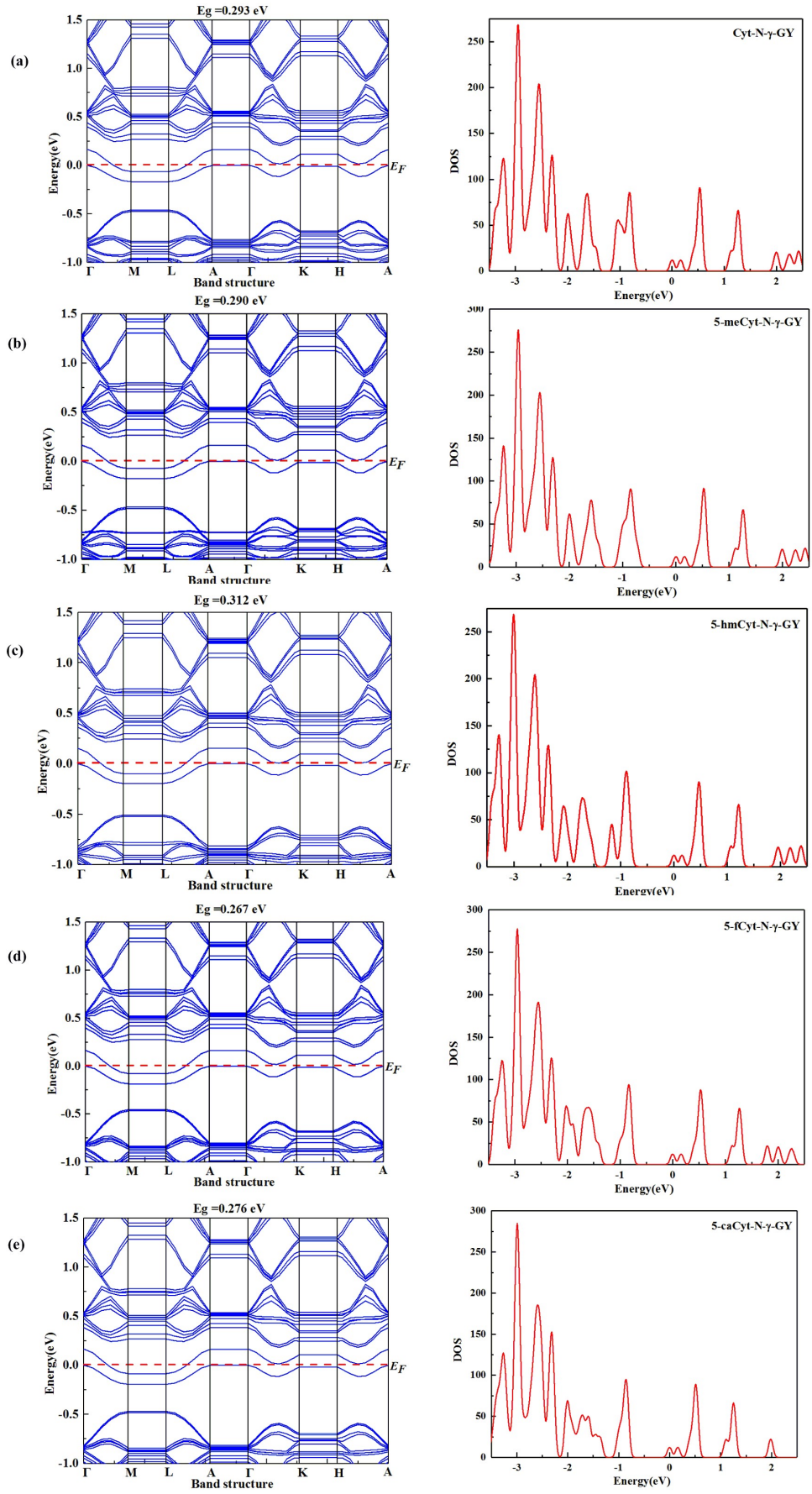
(a)
Eg =0.293 eV
Energy(eV)
Band structure
Γ M L A Γ K H A
$E_F$
Cyt-N-γ-GY
DOS
Energy(eV)
(b)
Eg =0.290 eV
5-meCyt-N-γ-GY
(c)
Eg =0.312 eV
5-hmCyt-N-γ-GY
(d)
Eg =0.267 eV
5-fCyt-N-γ-GY
(e)
Eg =0.276 eV
5-caCyt-N-γ-GY

Fig. S4

Table S1: The cohesive energies (eV) of graphene and B/N-doped grapheme, pristine, B- and N-doped γ-GY

| Nanostructure | $E_{coh}$/ eV |
|---|---|
| γ-GY | -8.79 |
| B-γ-GY | -8.78 |
| N-γ-GY | -8.74 |
| graphene | -9.35 |
| B-graphene | -9.28 |

Table S2 The adsorption energy ($E_{ad}$/eV) upon adsorption of rare base on different nanostructures

| Rare base and Nanostructure | γ-GY | B-γ-GY | N-γ-GY | graphene | B-graphene | N-graphene |
|---|---|---|---|---|---|---|
| Cyt | -0.781 | -0.986 | -0.853 | -1.156 | -1.340 | -1.298 |
| 5-meCyt | -0.814 | -1.033 | -0.905 | -1.462 | -1.633 | -1.588 |
| 5-hmCyt | -0.957 | -1.122 | -0.933 | -1.188 | -1.470 | -1.399 |
| 5-fCyt | -0.689 | -0.903 | -0.697 | -1.553 | -1.666 | -1.551 |
| 5-caCyt | -0.791 | -0.979 | -0.778 | -1.166 | -1.322 | -1.177 |