Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

P- or S-Doped Graphdiyne as a Superior *Metal-Free* Electrocatalyst for Hydrogen Evolution Reaction: A Computational Study

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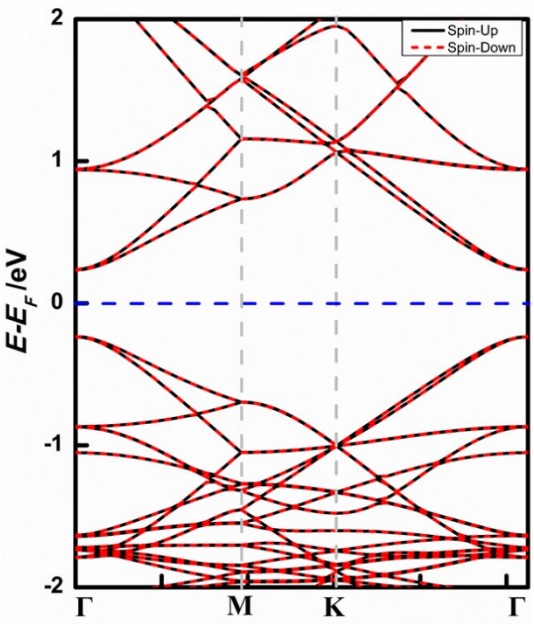
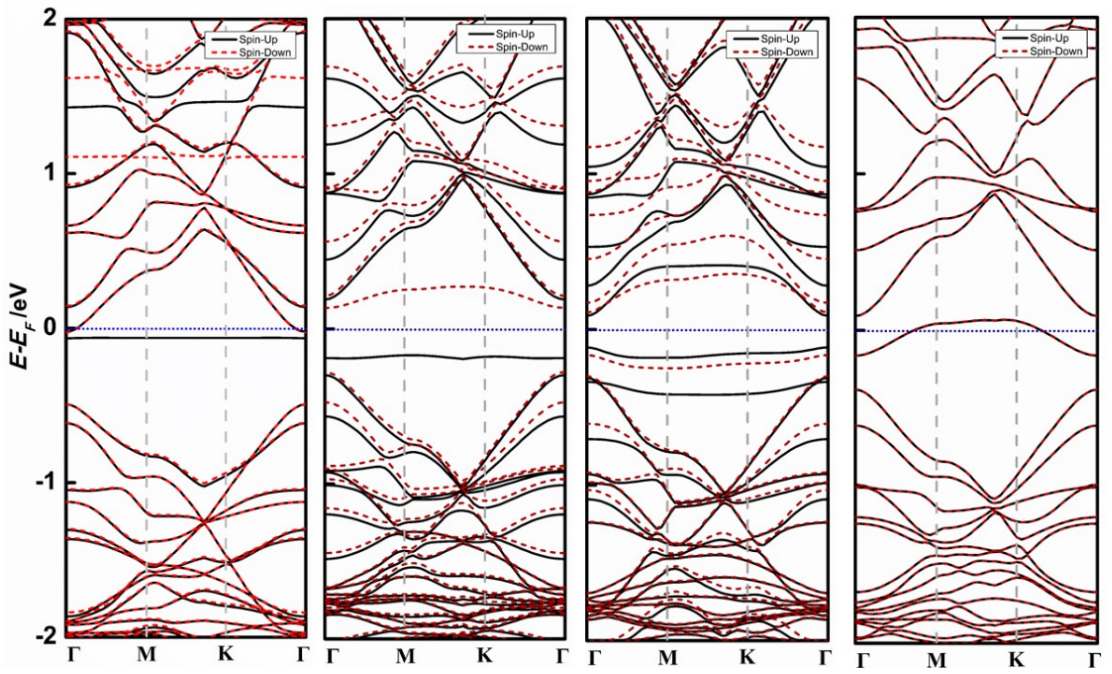
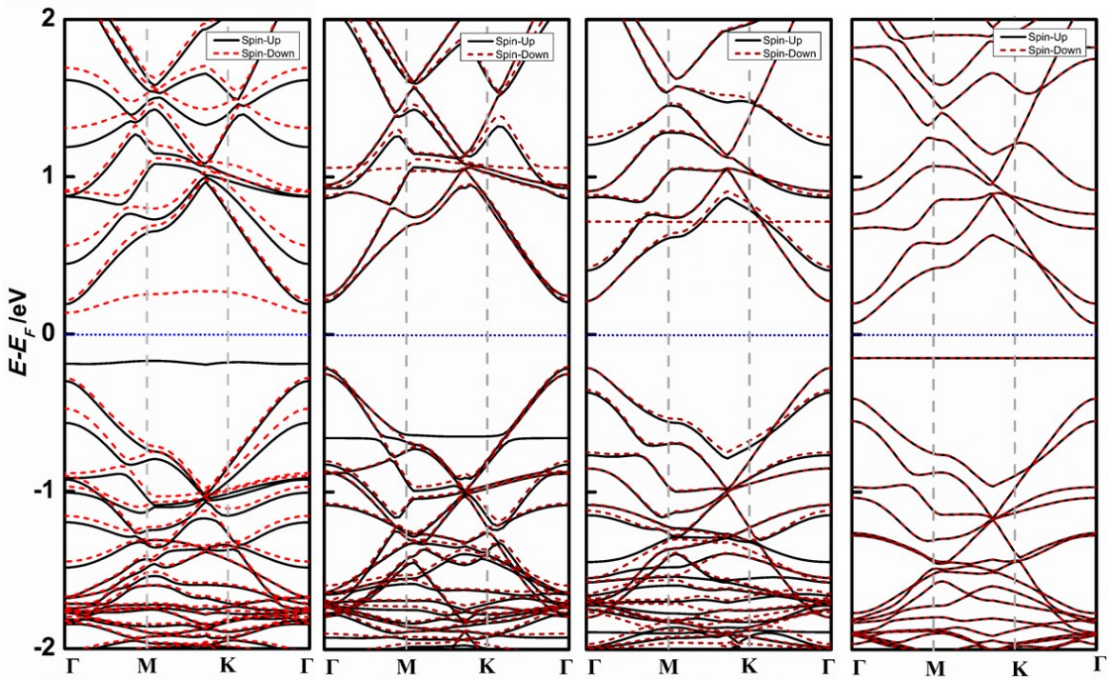


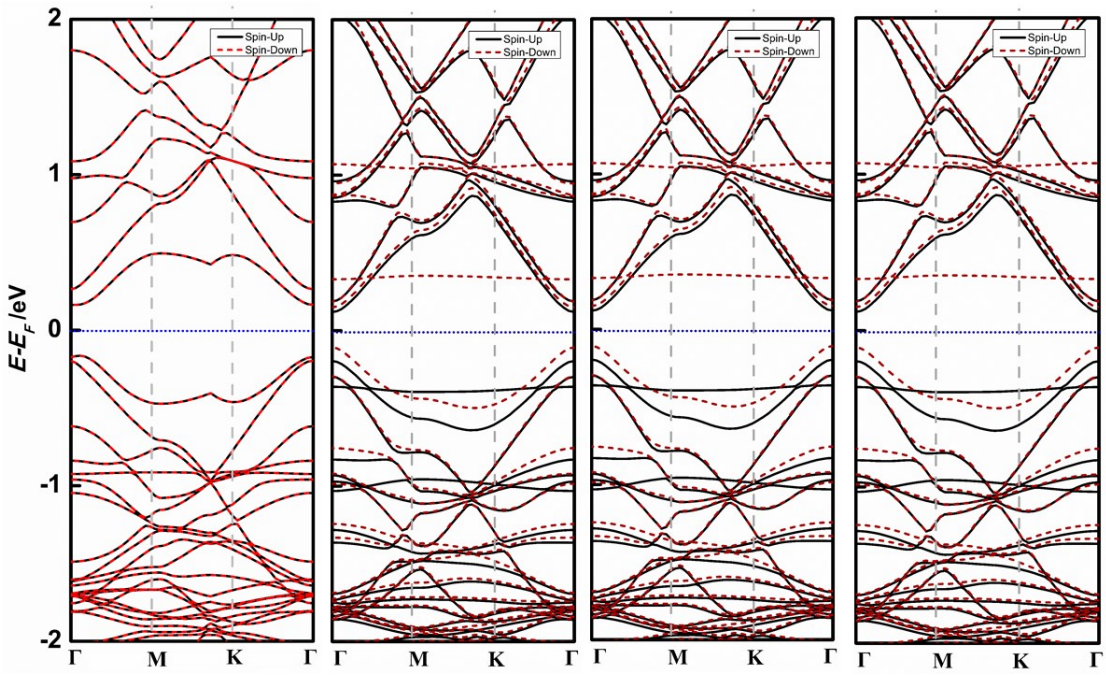
Fig. S1. The computed band structure of pristine graphydine. The Fermi level was set to zero in bule dashed line.


E-E_F /eV
2
1
0
-1
-2
Spin-Up
Spin-Down
Γ M K Γ

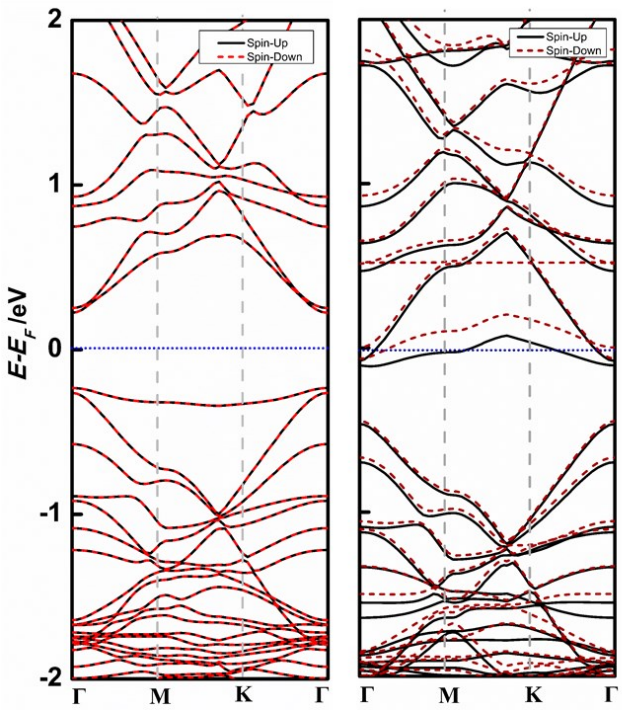
(a) (b) (c) (d)


E-E_F /eV
2
1
0
-1
-2
Spin-Up
Spin-Down
Γ M K Γ

(e) (f) (g) (h)



(i) (j) (k) (l)



(m) (n)

Fig. S2. The obtained band structures of doped GDY systems with (a) I_{P1}, (b) I_{P2}, (c) I_{P3}, (d) S_{P1}, (e) S_{P2}, (f) S_{P3}, (g) S_{P4}, (h) I_{S1}, (i) I_{S2}, (j) I_{S3}, (k) S_{S1}, (l) S_{S2}, (m) S_{S3}, and (n) S_{S4}. The Fermi level was set to zero in blue dotted line.

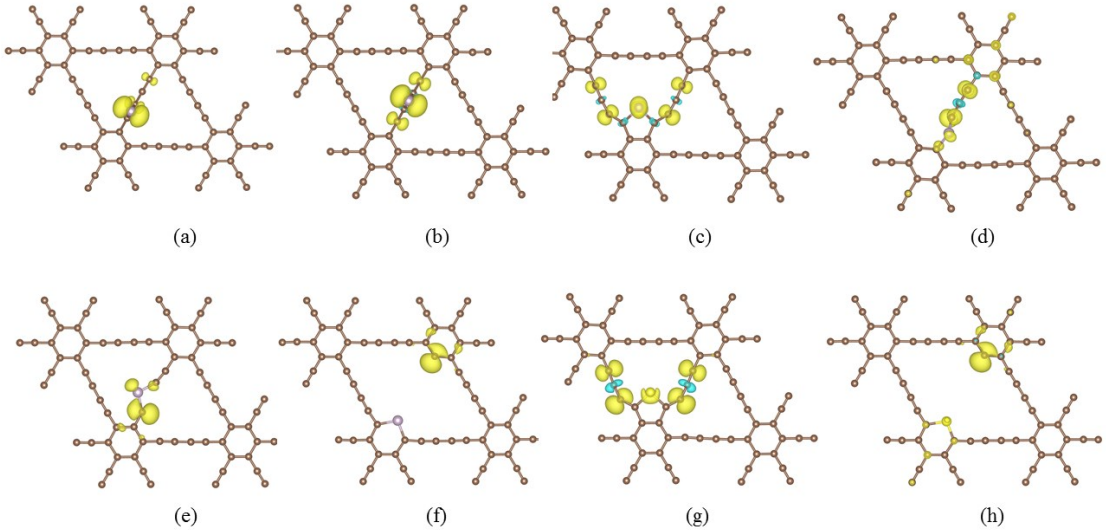
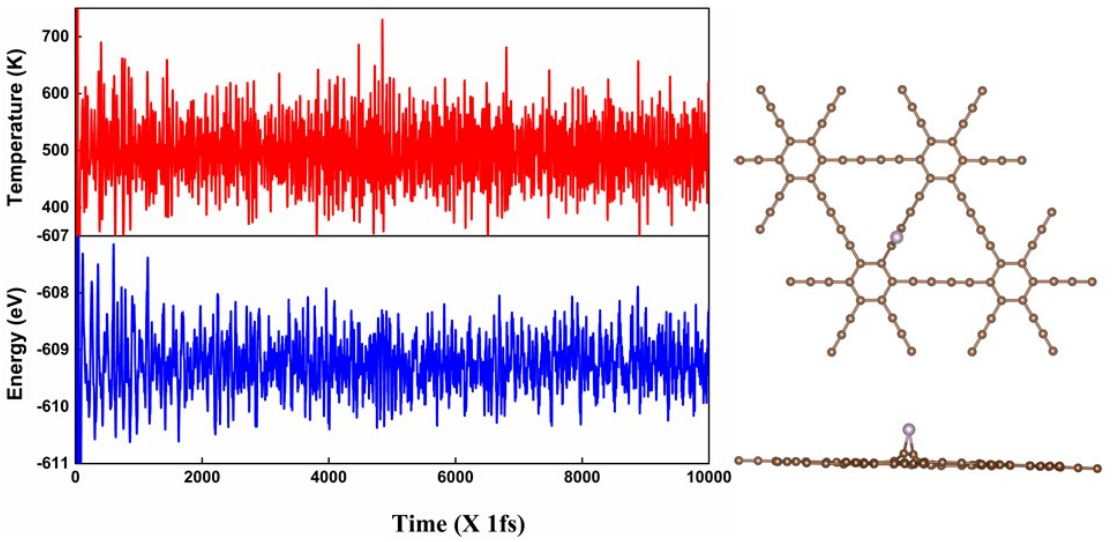
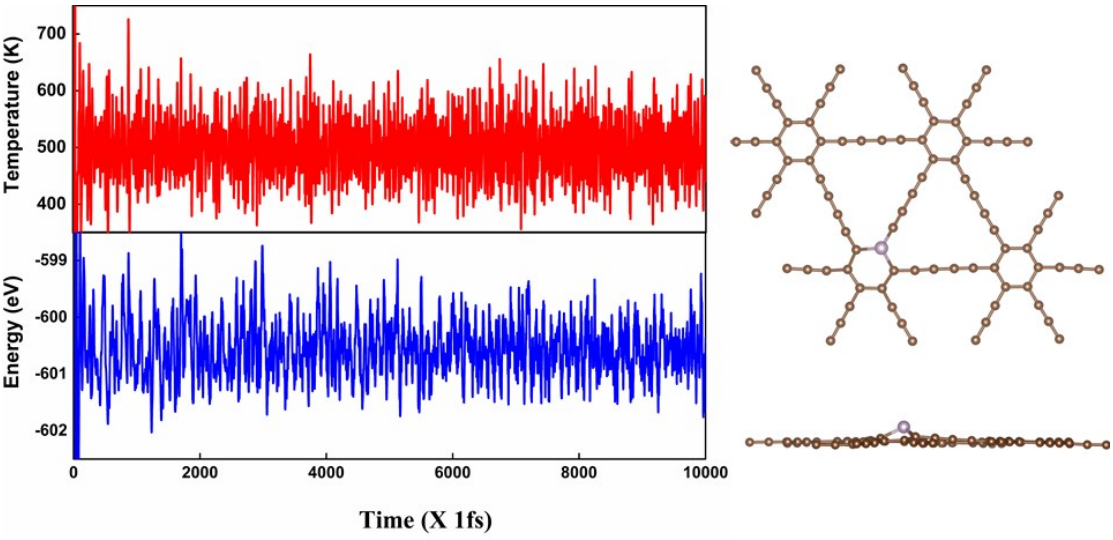


Fig. S3. The computed isosurfaces of spin density for (a) I_{P1}, (b) I_{P2}, (c) I_{P3}, (d) S_{P2}, (e) S_{P3}, (f) S_{P4}, (g) I_{S3}, and (h) S_{S4}.



(a)



(b)

Fig. S4. Variations of temperature and energy versus the time for AIMD simulations under 500 K for 10 ps with a time step of 1 fs and the corresponding schematic diagrams of the atomic configurations after dynamics simulation (top and side views) for (a) I_{P1} and (b) S_{P1}.

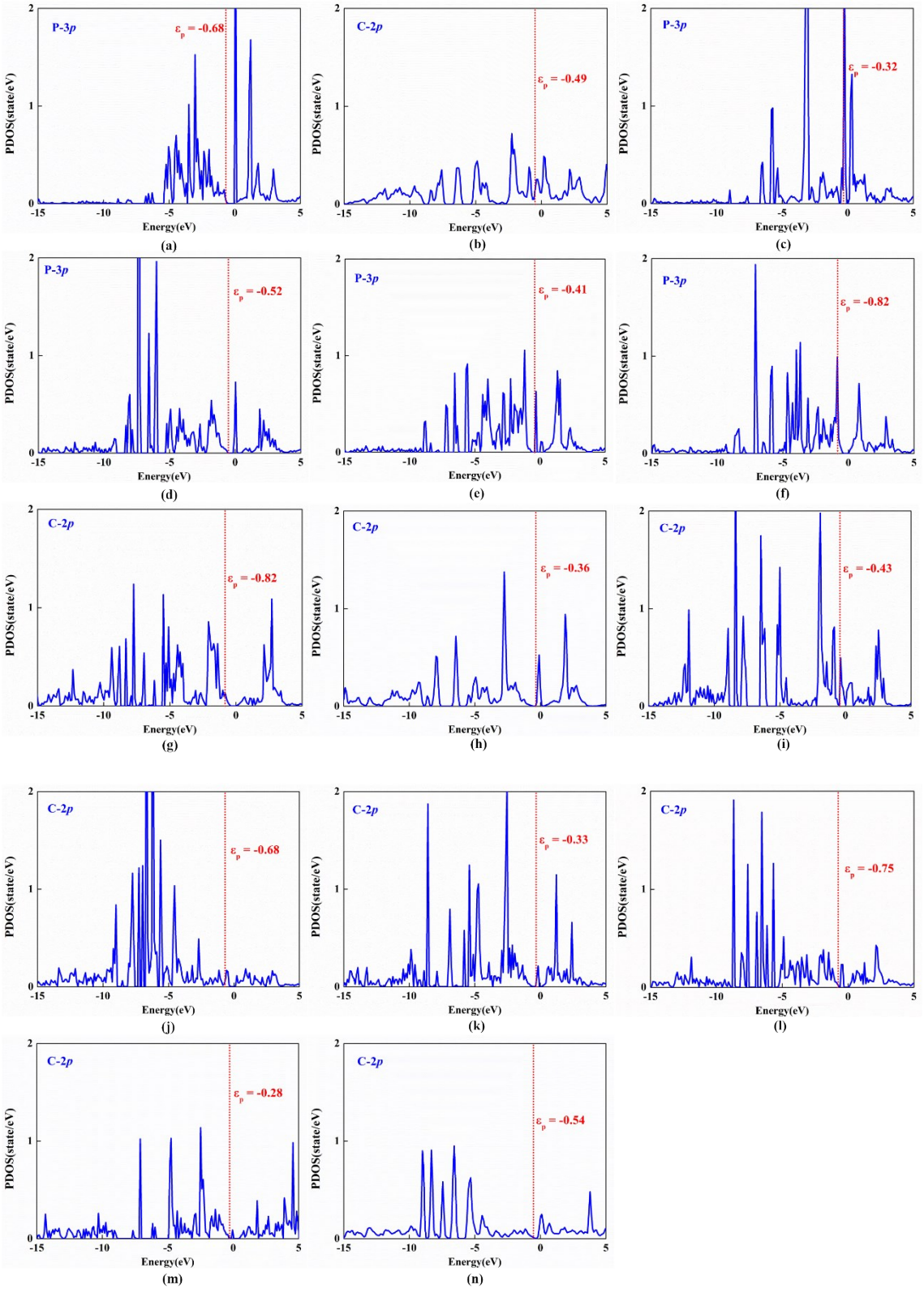


Fig. S5. The computed p-projected density of states of (a) I_{P1}, (b) I_{P2}, (c) I_{P3}, (d) S_{P1}, (e) S_{P2}, (f) S_{P3}, (g) S_{P4}, (h) I_{S1}, (i) I_{S2}, (j) I_{S3}, (k) S_{S1}, (l) S_{S2}, (m) S_{S3}, and (n) S_{S4}. The Fermi level was set to zero in red dotted line.