

Supplementary information

Theoretical study of *p*-block metal single atom loaded carbon nitride catalyst for photocatalytic water splitting

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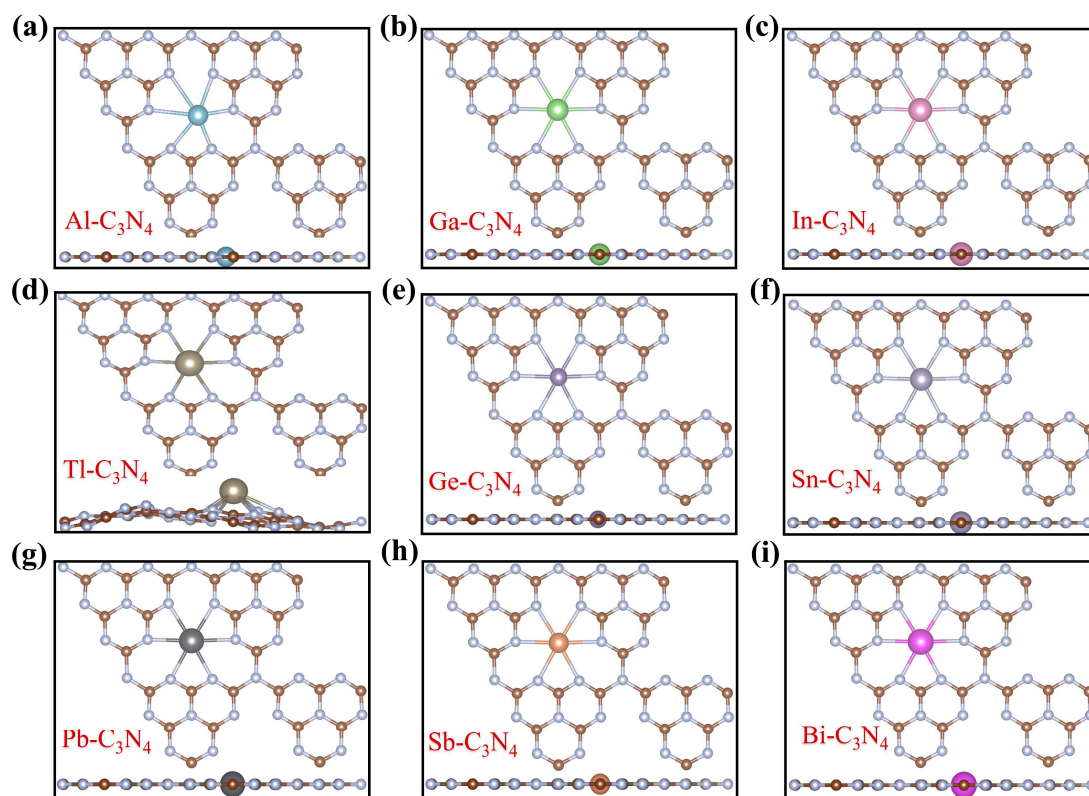


Figure S1. Optimized structures of $\text{PM-C}_3\text{N}_4$ (PM = Al, Ga, In, Tl, Ge, Sn, Pb, Sb, Bi). Color scheme: brown, carbon; greyish-white, nitrogen.

Table S1. The average bond length between the PM and nitrogen atoms in PM-C₃N₄.

p-block metal (PM)		L(PM-N) (Å)
The IIIA group	Al	2.39
	Ga	2.40
	In	2.42
The IVA group	Ge	2.35
	Sn	2.42
	Pb	2.44
The VA group	Sb	2.40
	Bi	2.43

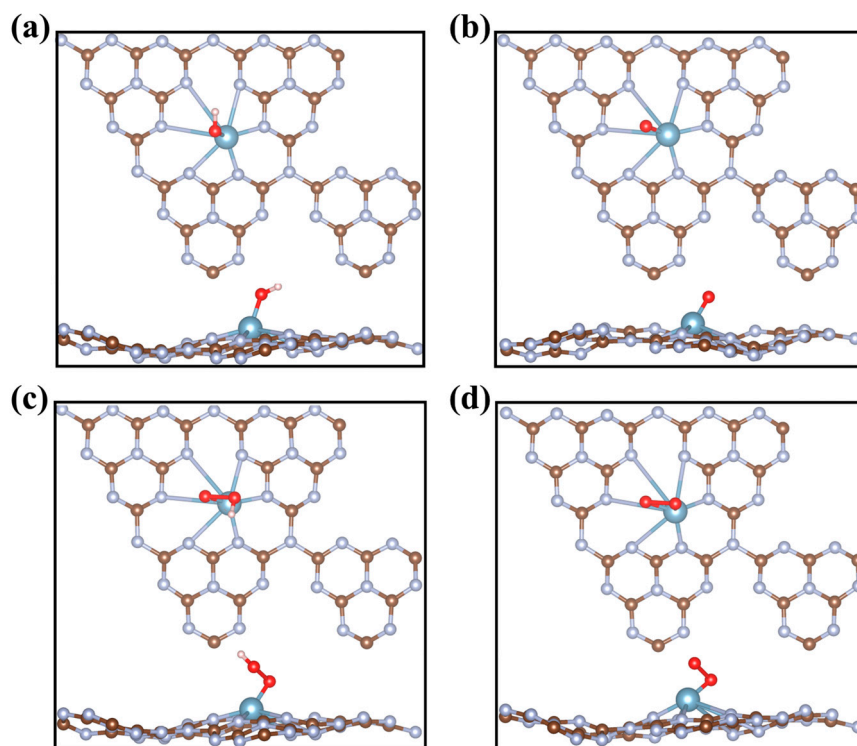


Figure S2. Optimized structures for intermediates during OER catalyzed by Al-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates. Color scheme: red, oxygen.

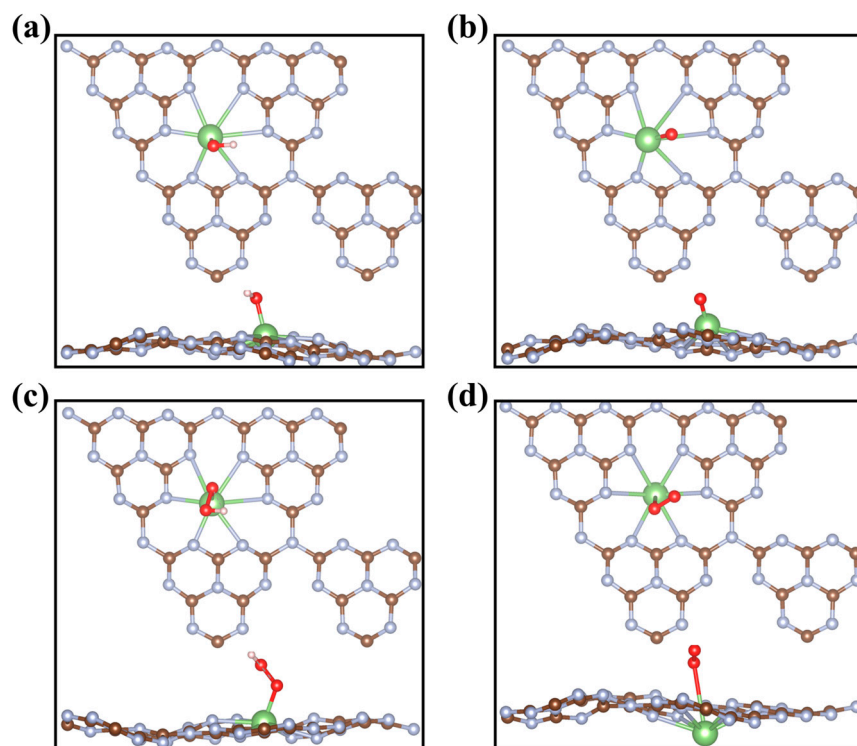


Figure S3. Optimized structures for intermediates during OER catalyzed by Ga-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

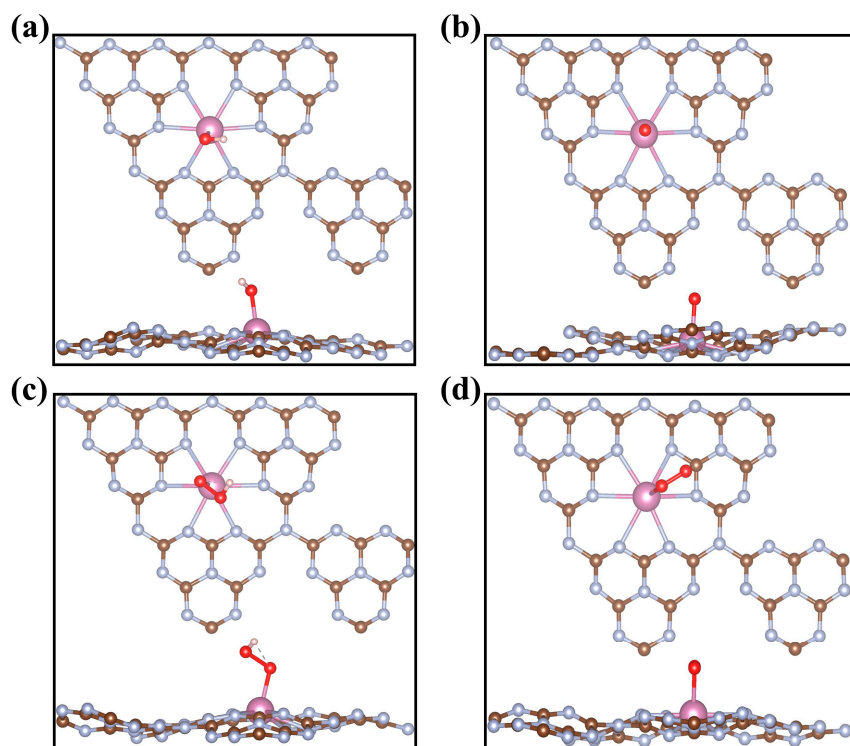


Figure S4. Optimized structures for intermediates during OER catalyzed by In-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

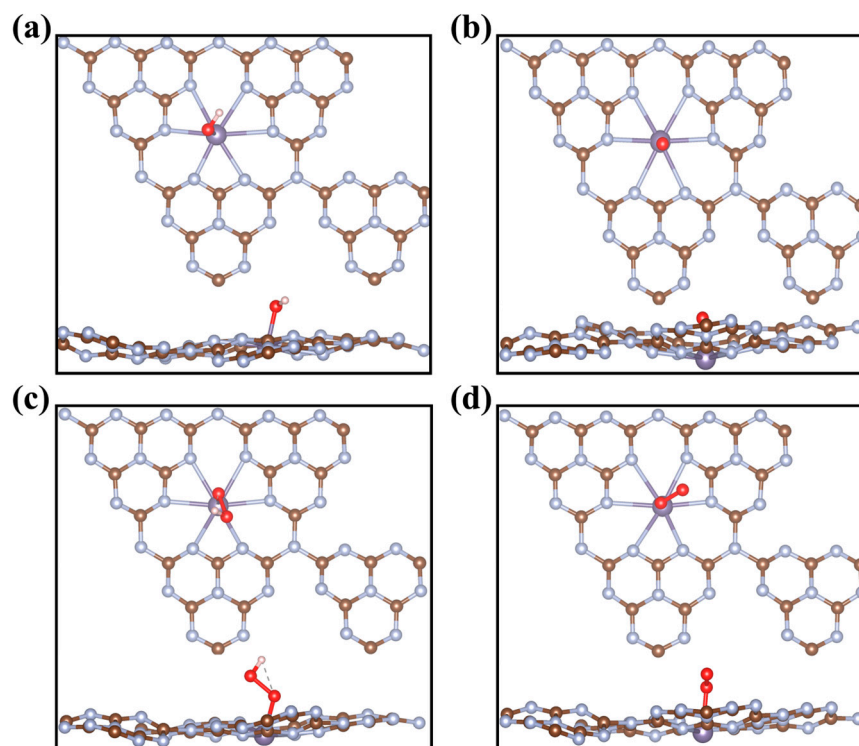


Figure S5. Optimized structures for intermediates during OER catalyzed by Ge-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

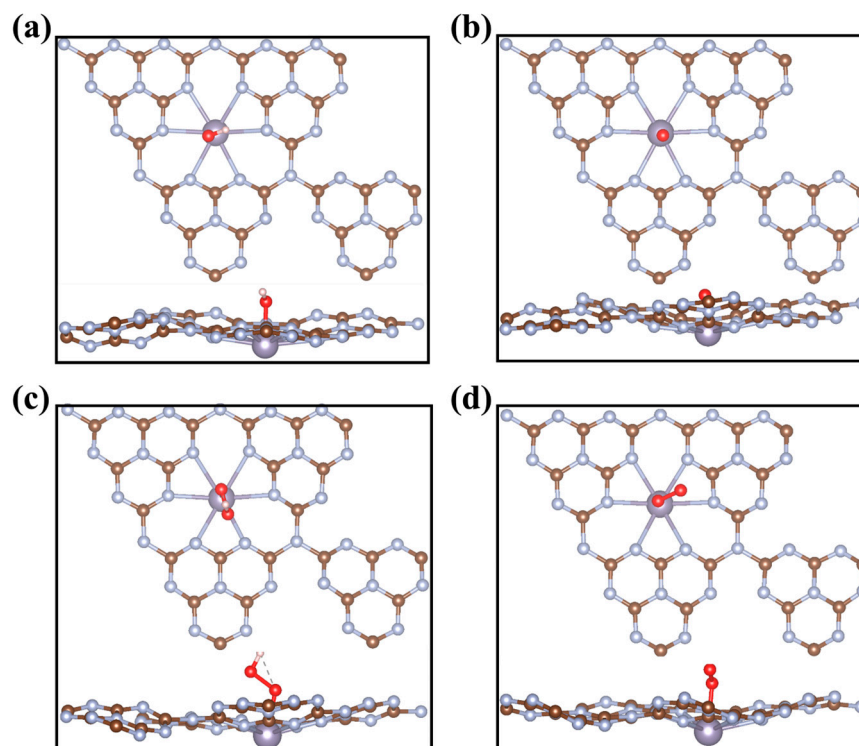


Figure S6. Optimized structures for intermediates during OER catalyzed by Sn-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

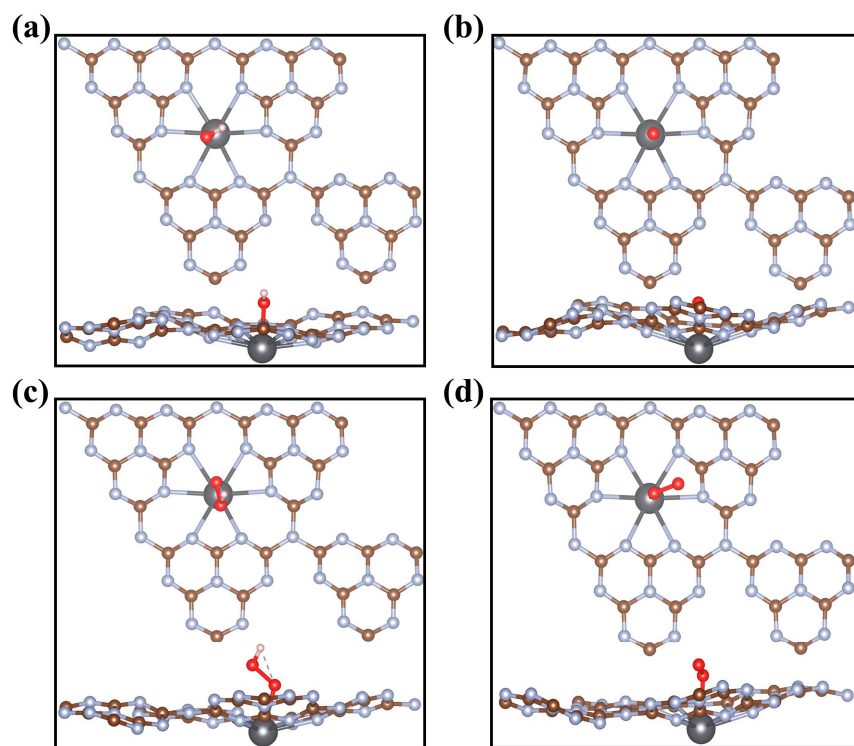


Figure S7. Optimized structures for intermediates during OER catalyzed by Pb-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

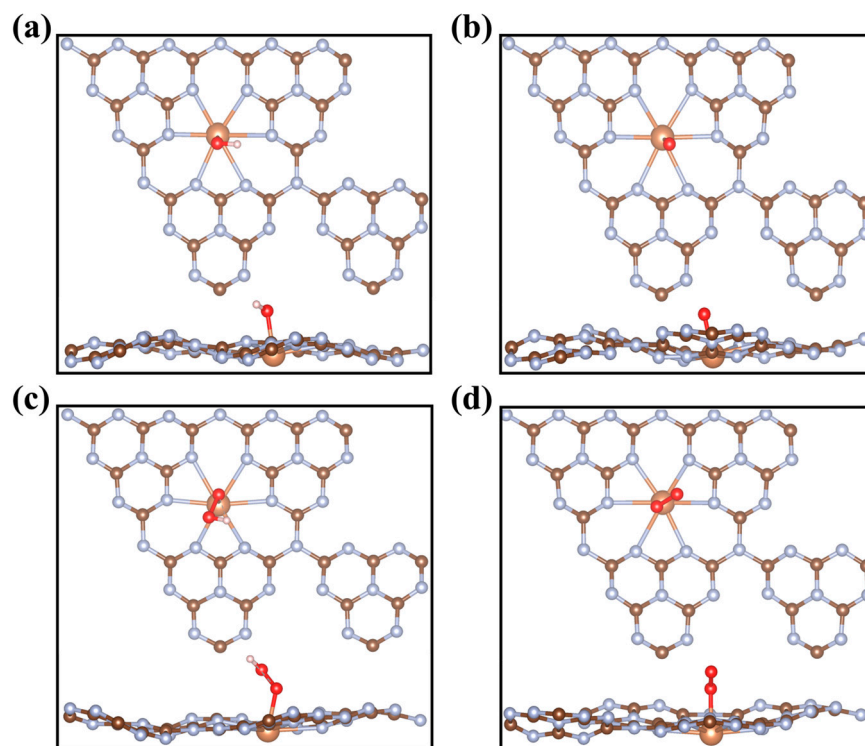


Figure S8. Optimized structures for intermediates during OER catalyzed by Sb-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

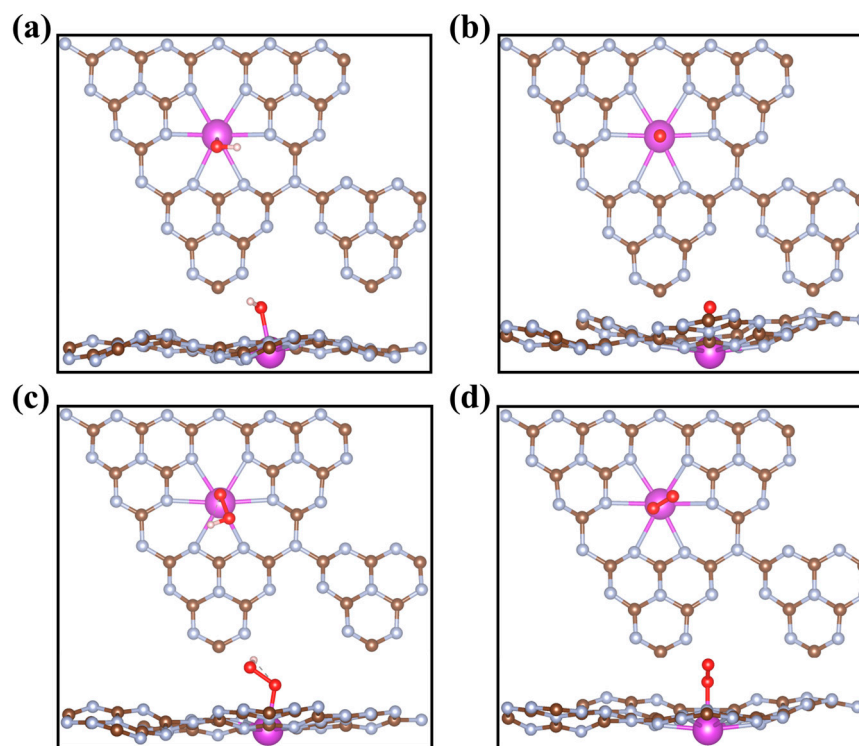


Figure S9. Optimized structures for intermediates during OER catalyzed by Bi-C₃N₄. (a) *OH; (b) *O; (c) *OOH; (d) *OO intermediates.

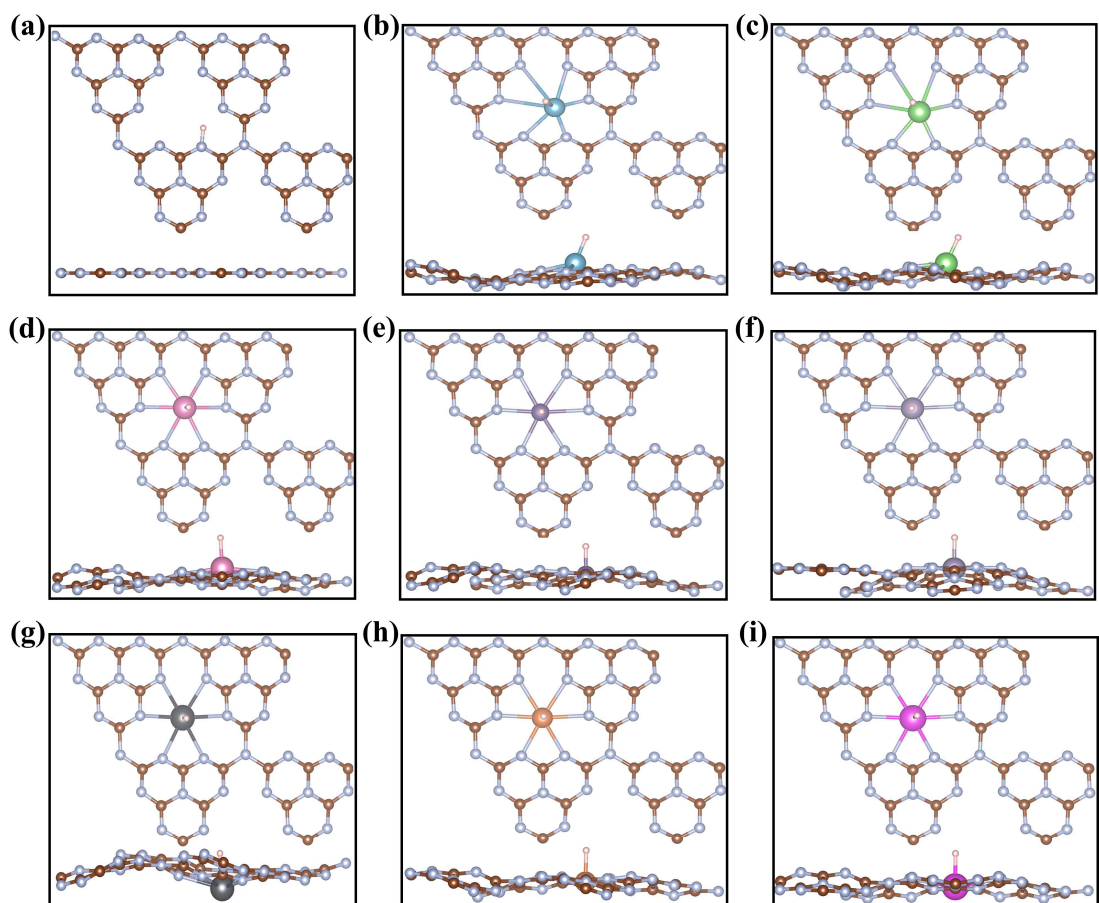


Figure S10. Optimized structures for $^*\text{H}$ on $g\text{-C}_3\text{N}_4$ and $\text{PM-C}_3\text{N}_4$. (a) $g\text{-C}_3\text{N}_4$; (b) $\text{Al-C}_3\text{N}_4$; (c) $\text{Ga-C}_3\text{N}_4$; (d) $\text{In-C}_3\text{N}_4$; (e) $\text{Ge-C}_3\text{N}_4$; (f) $\text{Sn-C}_3\text{N}_4$; (g) $\text{Pb-C}_3\text{N}_4$; (h) $\text{Sb-C}_3\text{N}_4$ and (i) $\text{Bi-C}_3\text{N}_4$.

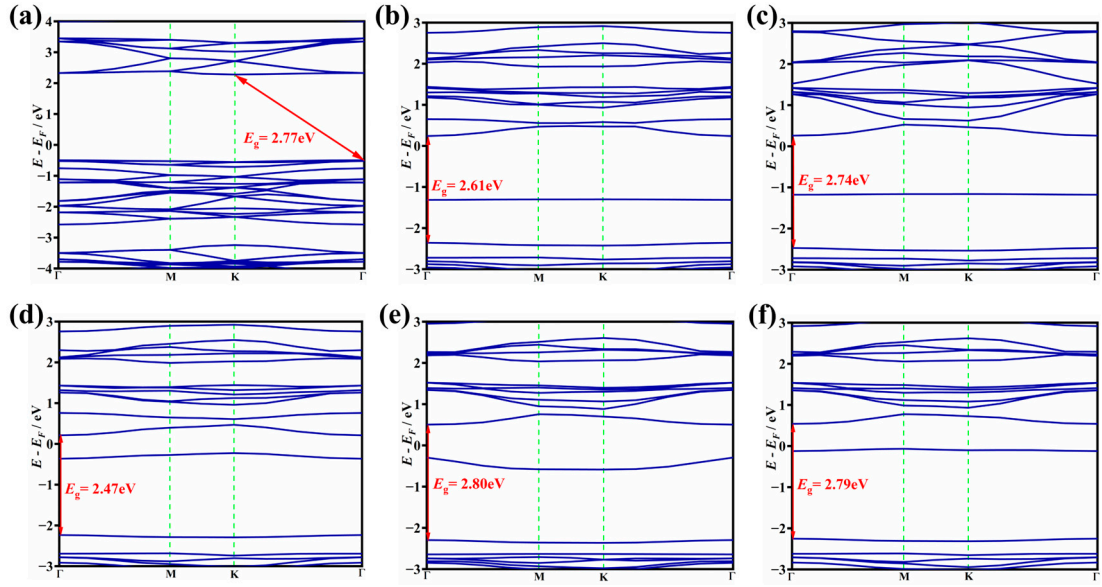


Figure S11. The electronic band structures of $g\text{-C}_3\text{N}_4$ and $\text{PM-C}_3\text{N}_4$. (a) $g\text{-C}_3\text{N}_4$; (b) $\text{Al-C}_3\text{N}_4$; (c) $\text{Ga-C}_3\text{N}_4$; (d) $\text{In-C}_3\text{N}_4$; (e) $\text{Sb-C}_3\text{N}_4$ and (f) $\text{Bi-C}_3\text{N}_4$.

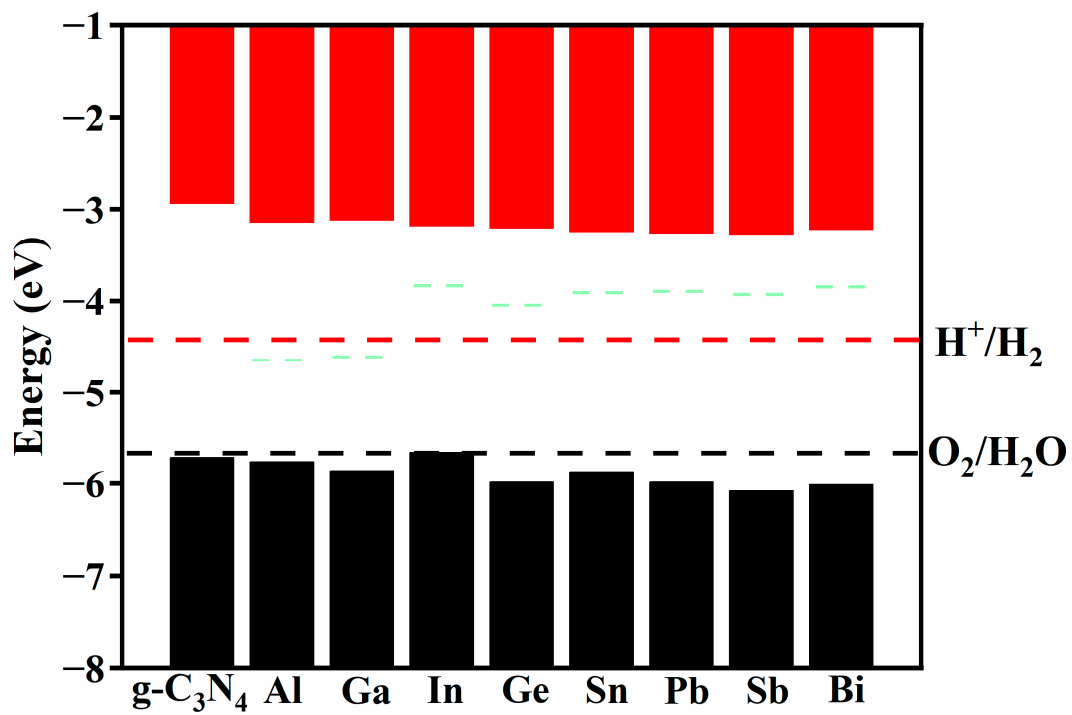


Figure S12. Band edges (i.e., VBM and CBM) alignment of *g*-C₃N₄ and PM-C₃N₄ corresponding to the redox potential for water splitting. The green dash-lines represent the doping energy level.

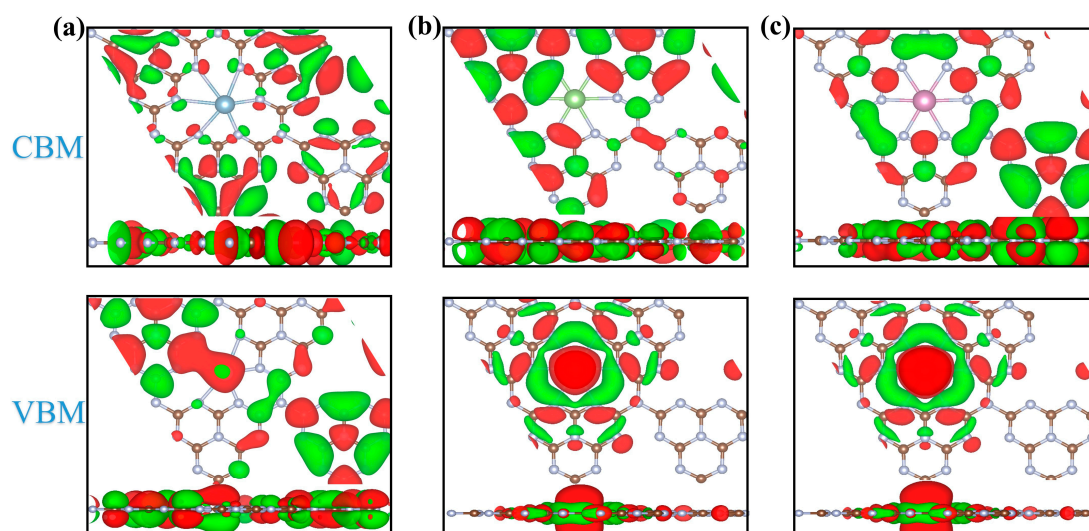


Figure S13. The isosurface (isolevel: $0.008 \text{ e}/\text{\AA}^3$) of band-decomposed electron density for the CBM (upper) and VBM (bottom) of PM- C_3N_4 (PM=Al, Ga, In). (a) Al- C_3N_4 ; (b) Ga- C_3N_4 and (c) In- C_3N_4 .

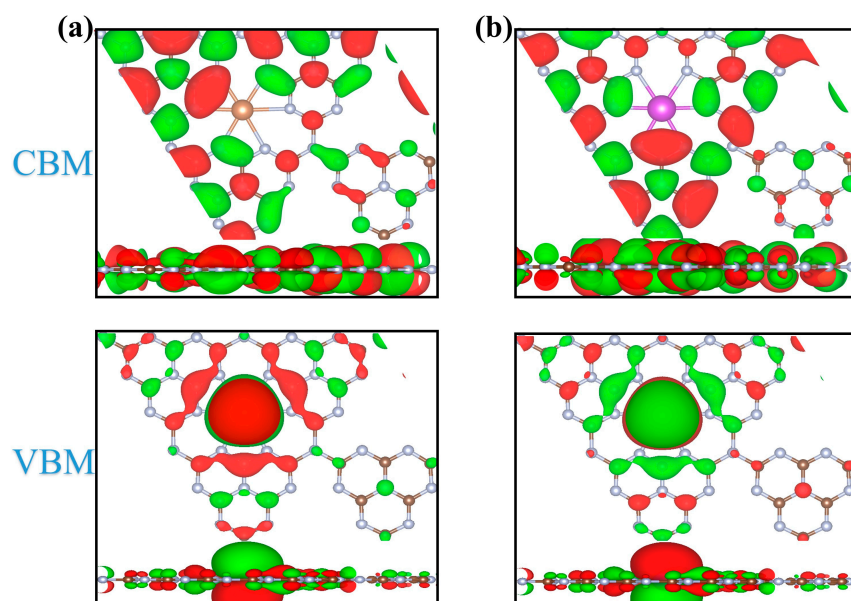


Figure S14. The isosurface (isolevel: $0.008 \text{ e}/\text{\AA}^3$) of band-decomposed electron density for the CBM (upper) and VBM (bottom) of PM- C_3N_4 (PM=Sn, Bi). (a) Sn- C_3N_4 and (b) Bi- C_3N_4 .