

Electronic Supplementary Information

***Polymeric heptazine imide by doping O and
constructing van der Waals heterostructures
for photocatalytic water splitting: a theoretical
perspective from transition dipole moment
analyses***

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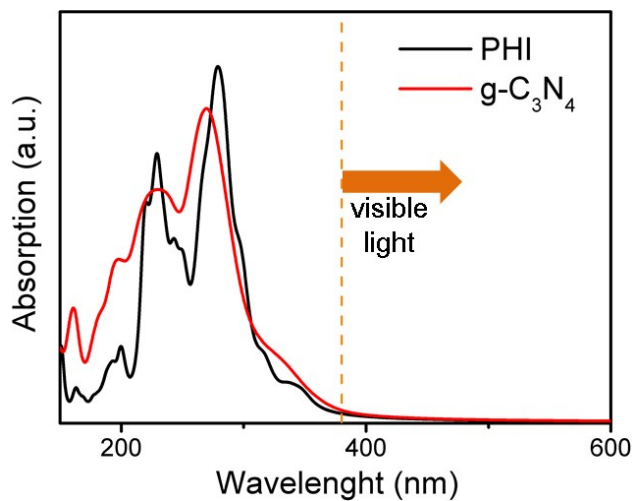


Fig. S1 Light absorption of PHI and g-C₃N₄. They both lack visible light absorption.

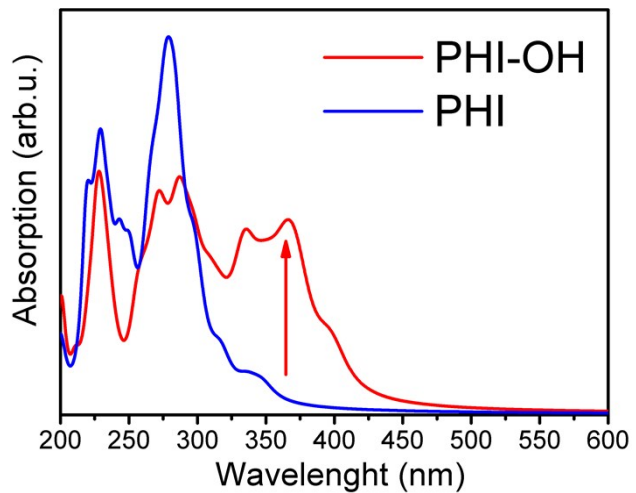


Fig. S2 Light absorption of PHI and PHI-OH. PHI-OH has an absorption peak around 370 nm.

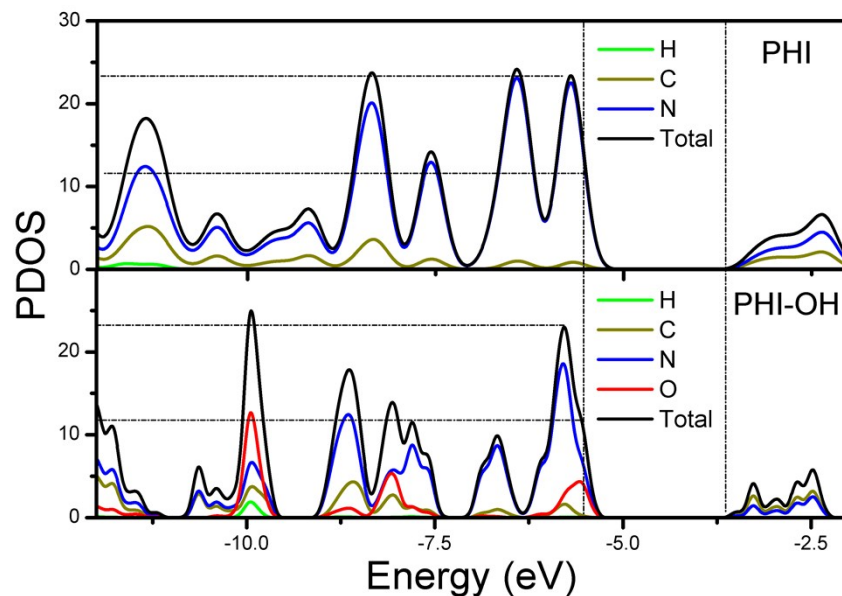


Fig. S3 PDOS of PHI and PHI-OH. O atoms has a contribution around $-5\sim-6$ eV in PHI-OH DOS, yet the total DOS doesn't increase near Fermi energy.

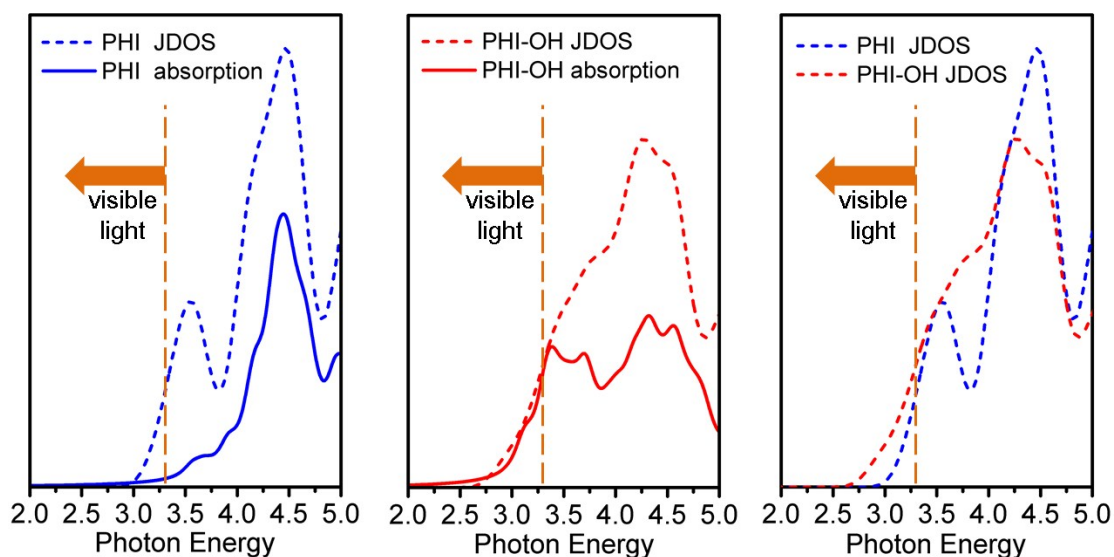


Fig. S4 JDOS of PHI and PHI-OH comparing with their light absorptions. JDOS of PHI and PHI-OH has similar value around $3\sim3.5$ photon energy. However, because of significant difference in TDM, PHI and PHI-OH has very different light absorption this energy range.

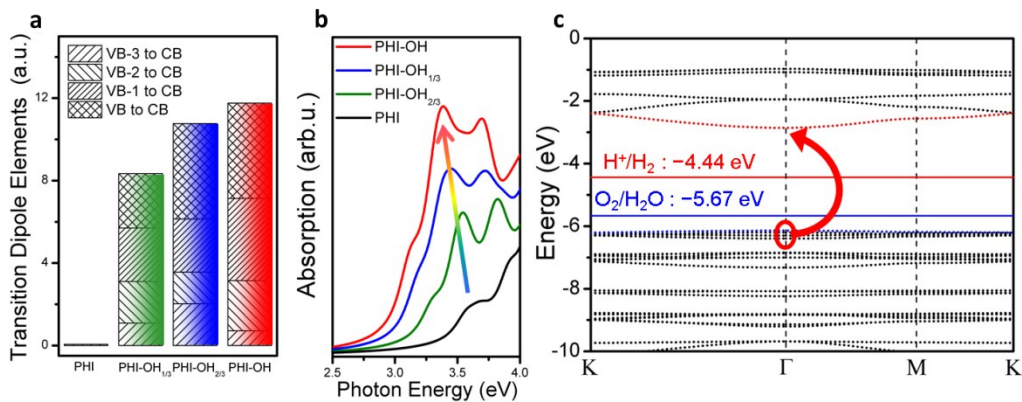


Fig. S5 TDM of Γ point of PHI, PHI-OH_{1/3}, PHI-OH_{2/3} and PHI-OH and their light absorption. Visible light absorptions are improved while TDMs becoming bigger.

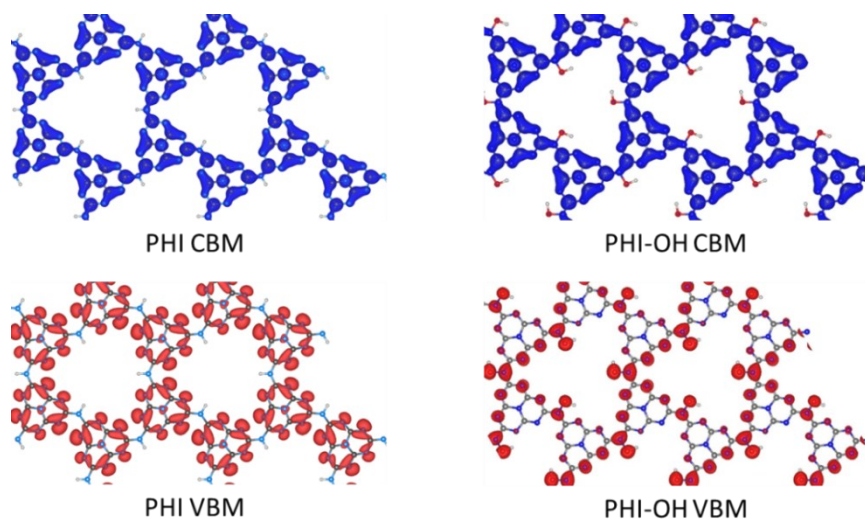


Fig. S6 The charge densities of the CBM (red) and VBM (blue) for PHI and PHI-OH.

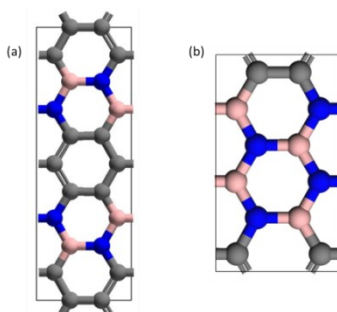


Fig. S7 Structures of BC₃N and BCN. Pink, blue and dark grey spheres represent B, N and C atoms, respectively.