Heptazine-based porous graphitic carbon nitride: a visible-light driven photocatalyst for water splitting

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Fig. S1 The full of phonon dispersion of C\textsubscript{6}N\textsubscript{7} monolayer.
Fig. S2 Minimum energy path for the dissociation of a water molecule on the surface of C$_6$N$_7$ monolayer with the optimized geometries of the *H$_2$O, transition state (TS), and *OH + *H.

Fig. S3 The shift of VBM and CBM for C$_6$N$_7$ monolayer with respect to the vacuum energy, as a function of the applied strain. The linear fit of the data yields the deformation potential constant.