

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

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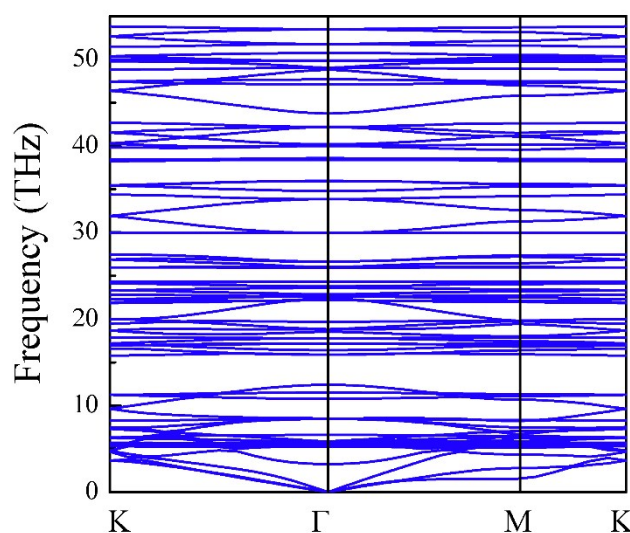


Fig. S1 The full of phonon dispersion of C₆N₇ monolayer.

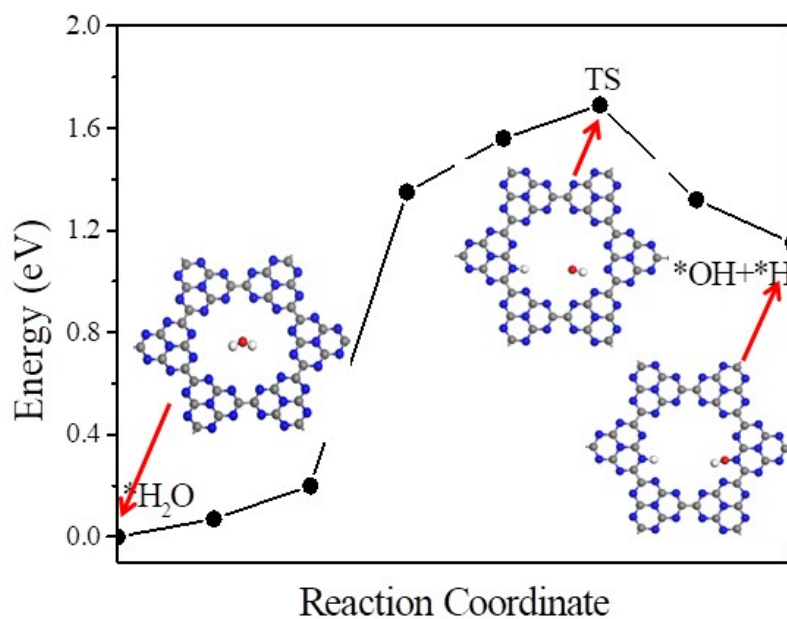


Fig. S2 Minimum energy path for the dissociation of a water molecule on the surface of C_6N_7 monolayer with the optimized geometries of the $*H_2O$, transition state (TS), and $*OH + *H$.

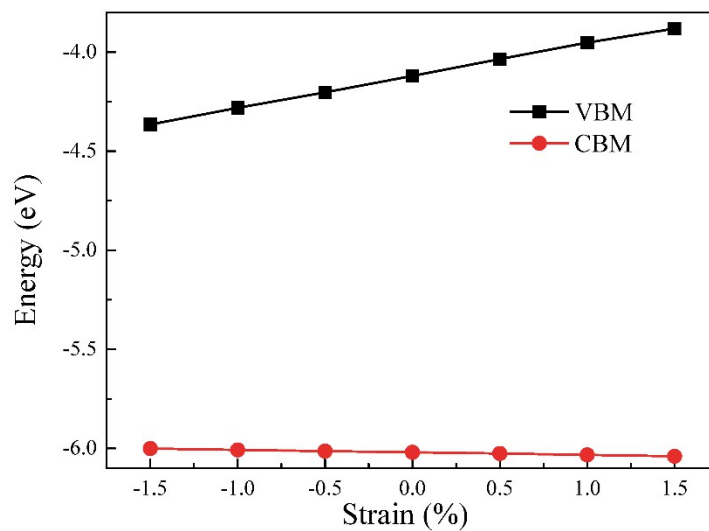


Fig. S3 The shift of VBM and CBM for C_6N_7 monolayer with respect to the vacuum energy, as a function of the applied strain. The linear fit of the data yields the deformation potential constant.