Electronic Supplementary Information

Origin of photoactivity in graphitic carbon nitride and strategies for enhancement of photocatalytic efficiency: Insights from first-principles computations

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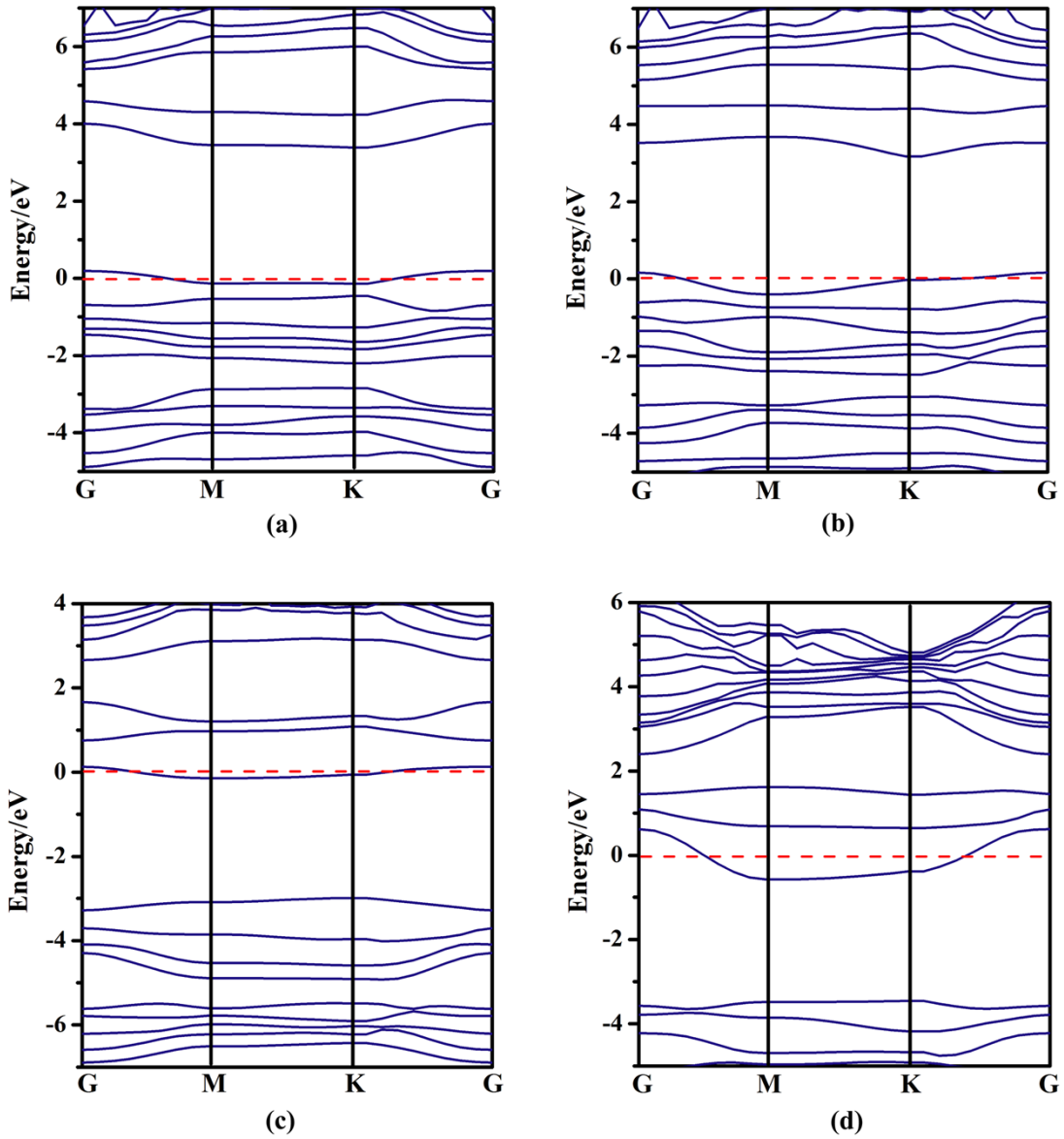

Fig. S1 Band structures of H-g-CNML with H absorbed on (a) C1, (b) C2, (c) N1 and (d) N2 atoms, computed by HSE06. Red dashed lines present the Fermi level at 0 eV.

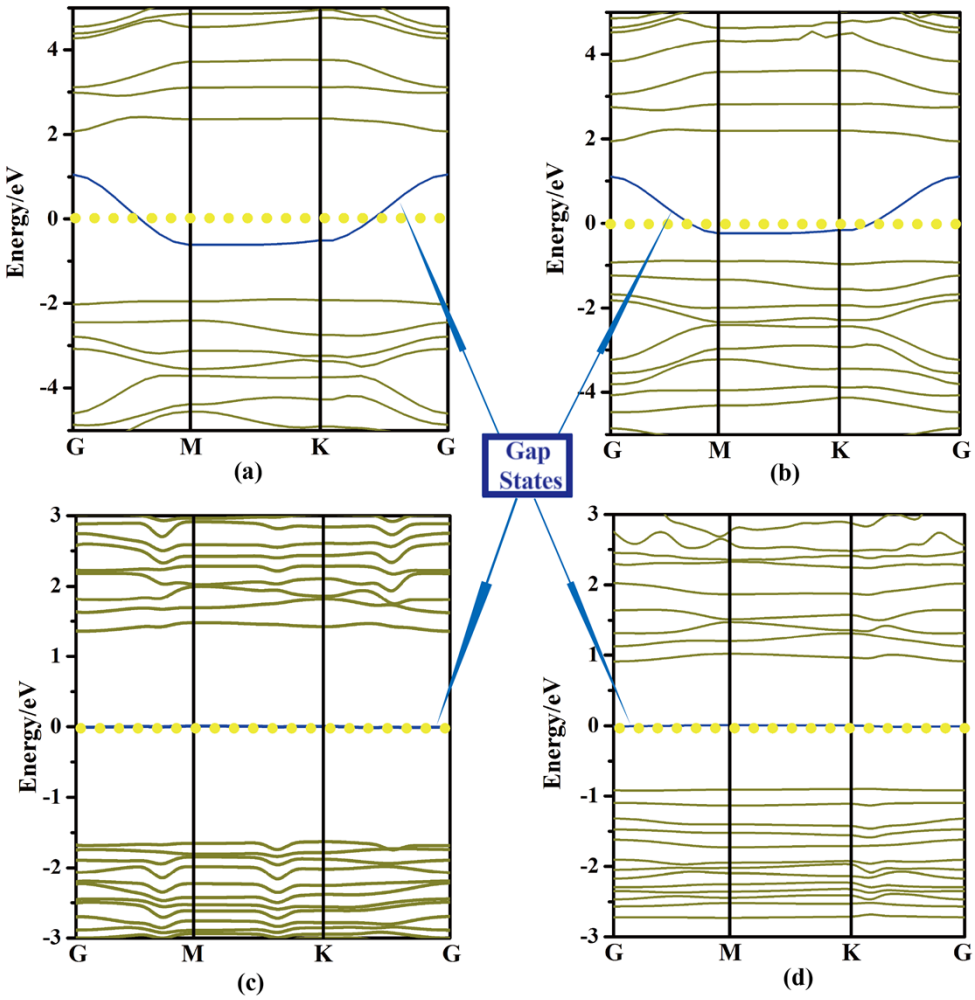

Fig. S2 Band structures of g-CNML with (a,b) N3-position hydrogenation, and (c d) N2 vacancy, computed by (a,c) HSE06 and (b,d) SDFT, respectively. Yellow dotted lines present the Fermi level at 0 eV. Blues lines around the Fermi level denote gap states.

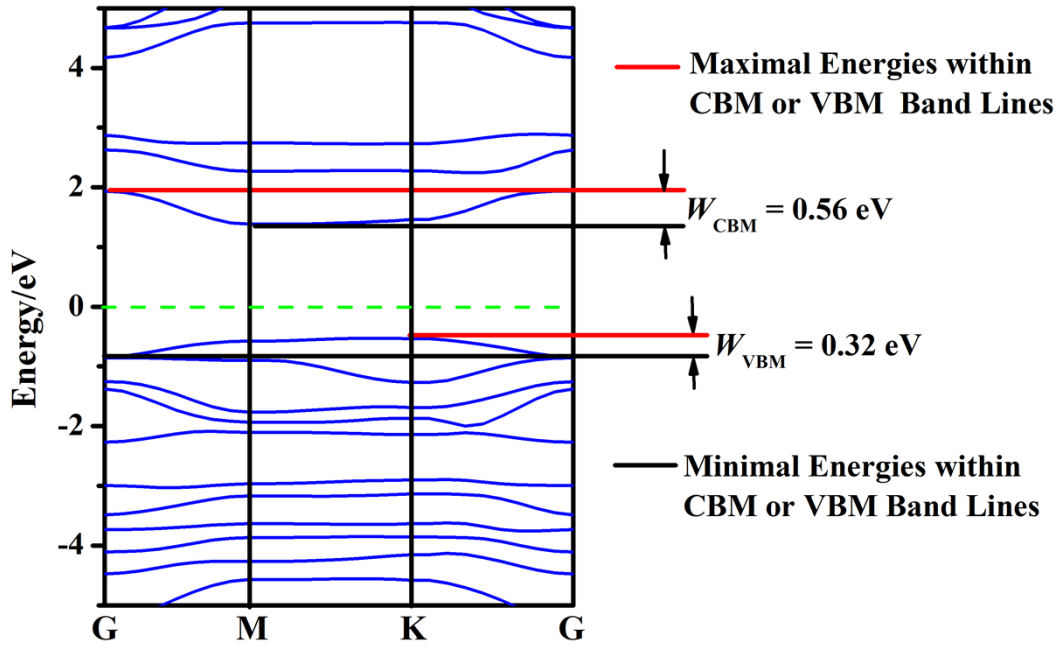

Fig. S3 Band structure and band widths of the CBM (W_{CBM}) and VBM (W_{VBM}) for g-CN1ML, computed by PBE functional. The band widths are determined by the largest energy differences within the CBM and VBM band lines, respectively. Green dashed line presented the Fermi level at 0 eV.

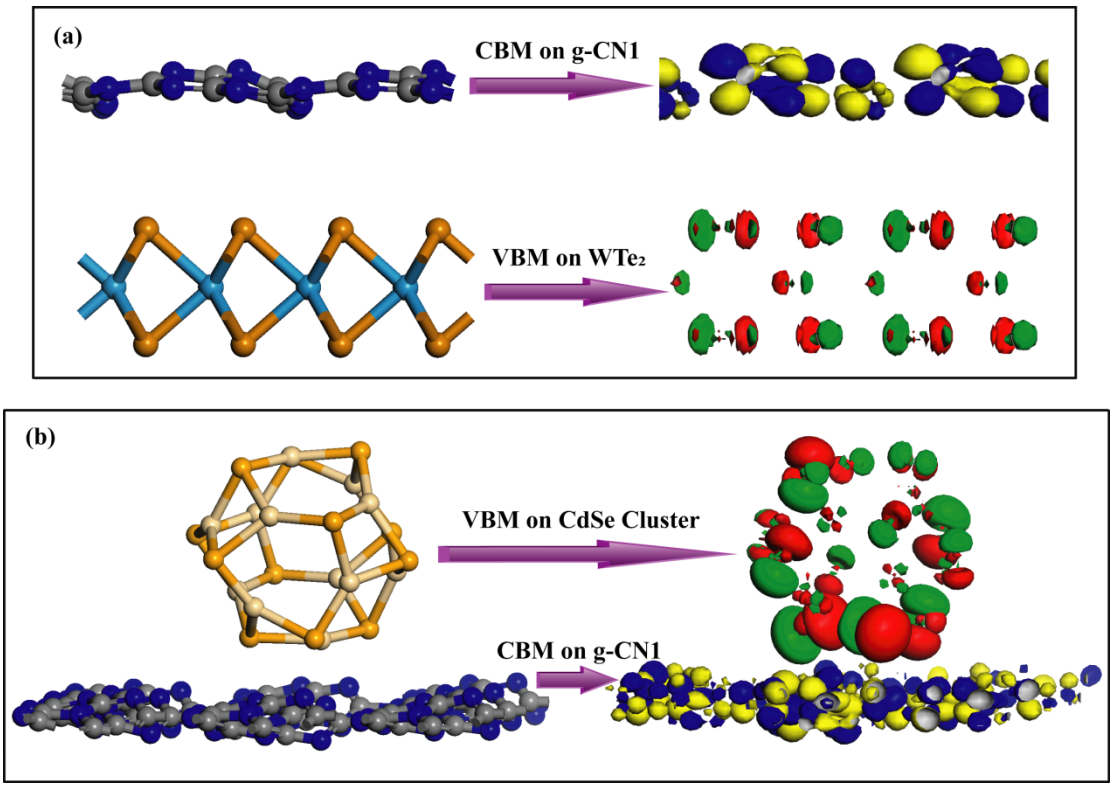

Fig. S4 Spatial distributions of the VBM (red/green isosurface) and CBM (blue/yellow isosurface) states at the Γ point (right) for the (a) WT-g-CN1ML and (b) CS-g-CN1ML nanosheets. Optimized geometries are also given on the left.