Supporting Information

Theoretical insight into the mechanism of photoreduction CO_2 to CO by graphitic carbon nitride

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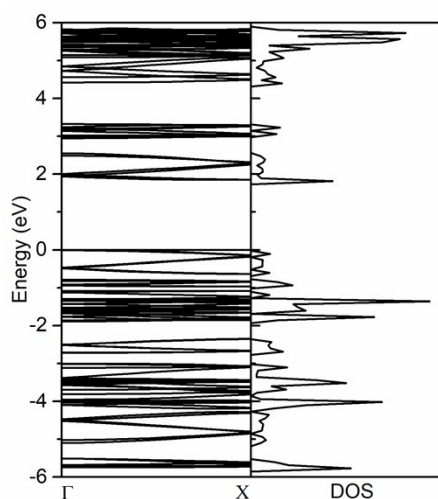
Fig. S1 Band dispersions and electronic density of state of g-C_3N_4 with ideal edges. The underestimation of energy gap with standard functional PBE has been verified in our previous results.[1]
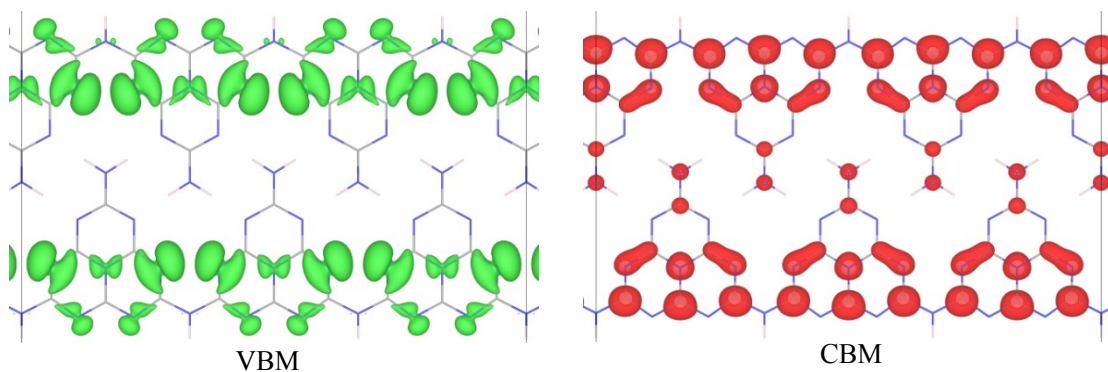

VBM   CBM

Fig. S2 Charge density of the valence band maximum (VBM) (green isosurface, isosurface = 0.001) and conductive band minimum (CBM) (red isosurface, isosurface = 0.001) of g-C_3N_4 with ideal edges.
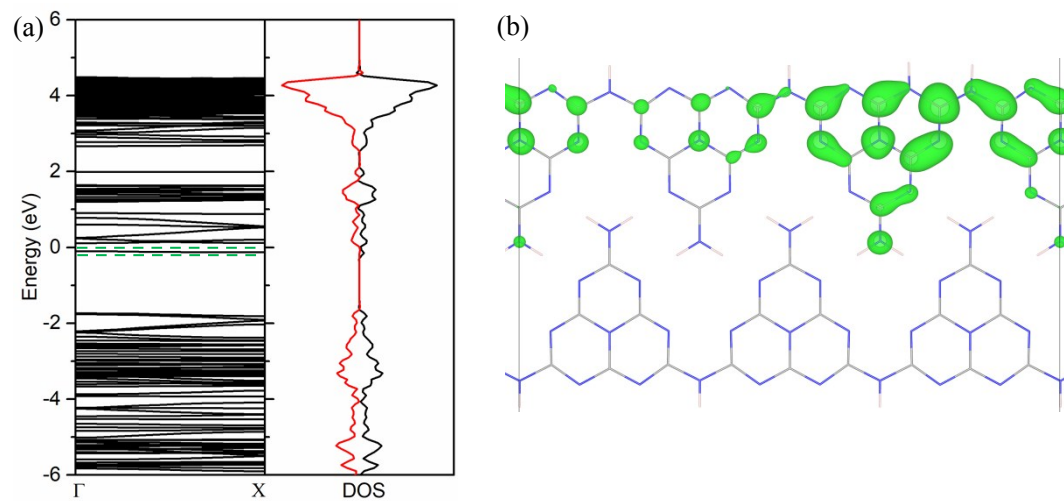

Fig. S3 (a) Band dispersions and electronic density of state of g-C_3N_4 with a proton, (b) Charge density of g-C_3N_4 with a proton at an energy range from -0.05 to 0 eV (corresponding to green dash line in (a)).
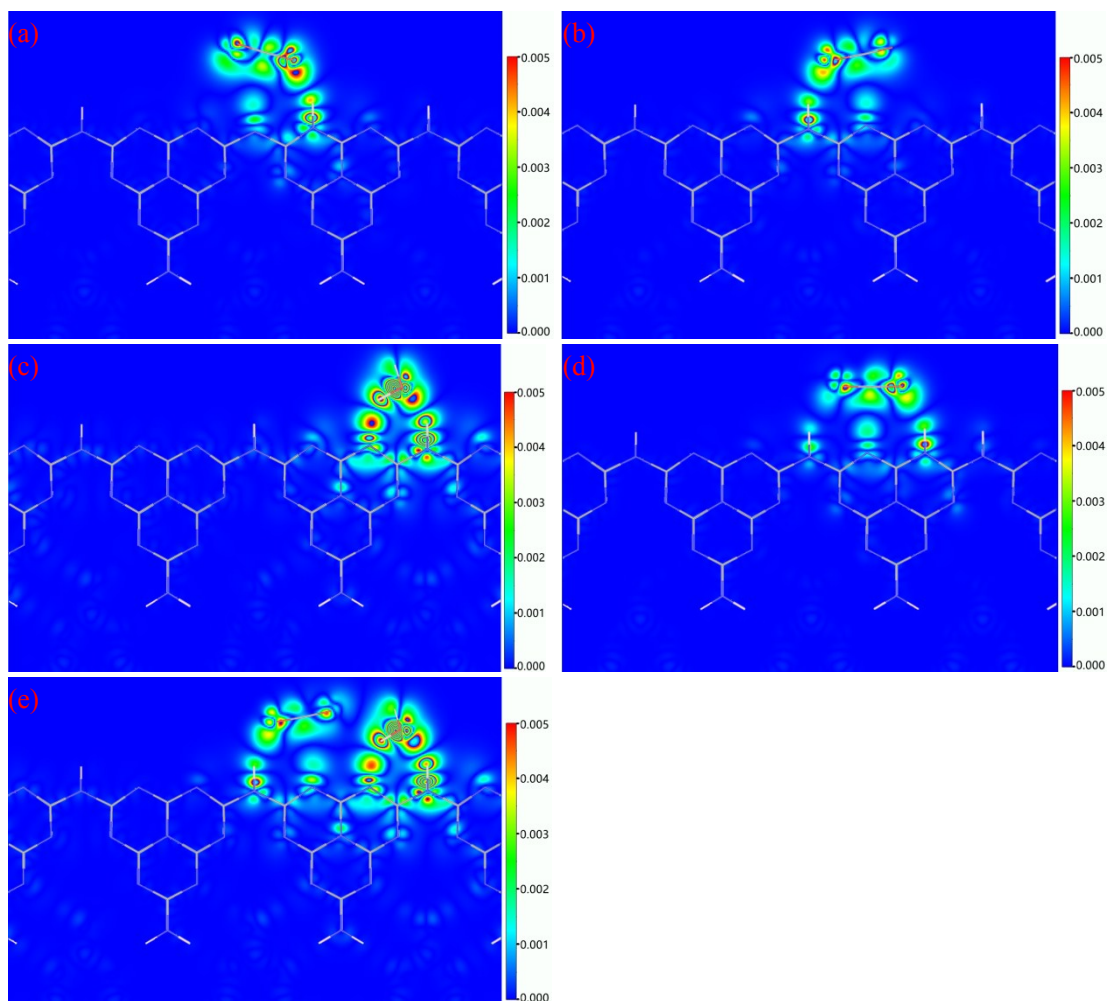
Fig. S4 Isosurface of the charge density difference resulting from adsorption of (a) CO_2 at N1 site, (b) CO_2 at N2 site, (c) H_2O at edge, (d) CO_2 at N1 site with proton assistance, (e) and coadsorption of CO_2 and H_2O at edge, respectively.

1   H.-Z. Wu, Q.-H. Zhong, S. Bandaru, J. Liu, W. M. Lau, L.-L. Li and Z. Wang, *J. Phys.: Condens. Matter.*, 2018, **30**, 155303.