

Supporting Information

A novel C_6N_2 monolayer as a potential material

for charge-controlled CO_2 capture

C. He¹, M. Zhang¹, T.T. Li¹, W.X. Zhang^{2*}

¹ State Key Laboratory for Mechanical Behavior of Materials, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China

² School of Materials Science and Engineering, Chang'an University, Xi'an 710064, China

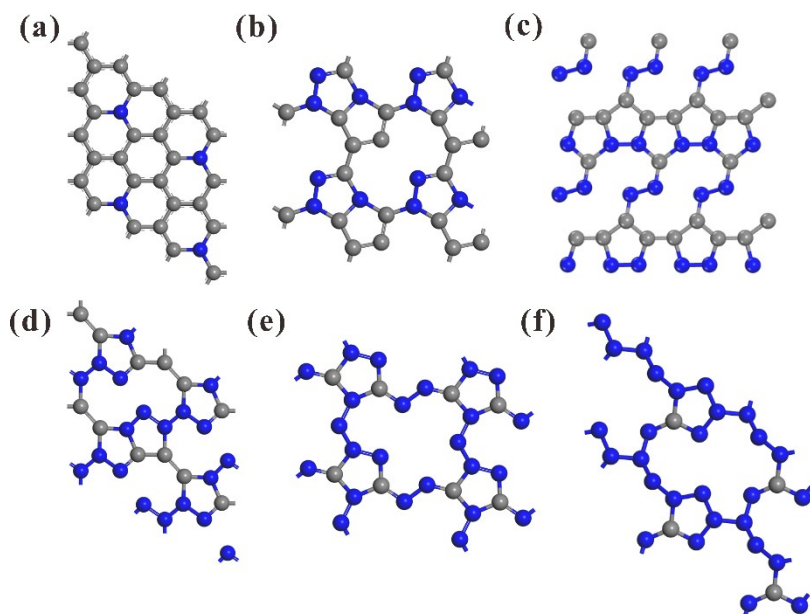


Fig. S1 (a)-(f) the structure of C_7N , C_5N_3 , C_4N_4 , C_3N_5 , C_2N_6 and CN_7 monolayers.

*Corresponding Author: W. X. Zhang (wxzhang@chd.edu.cn)

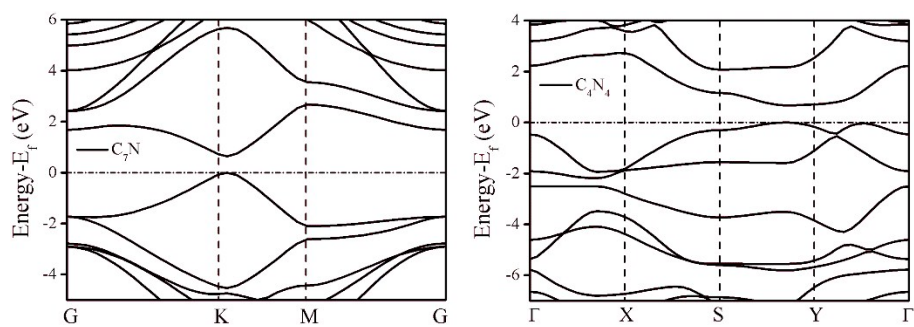


Fig. S2 Band structures of C_7N and C_4N_4 .

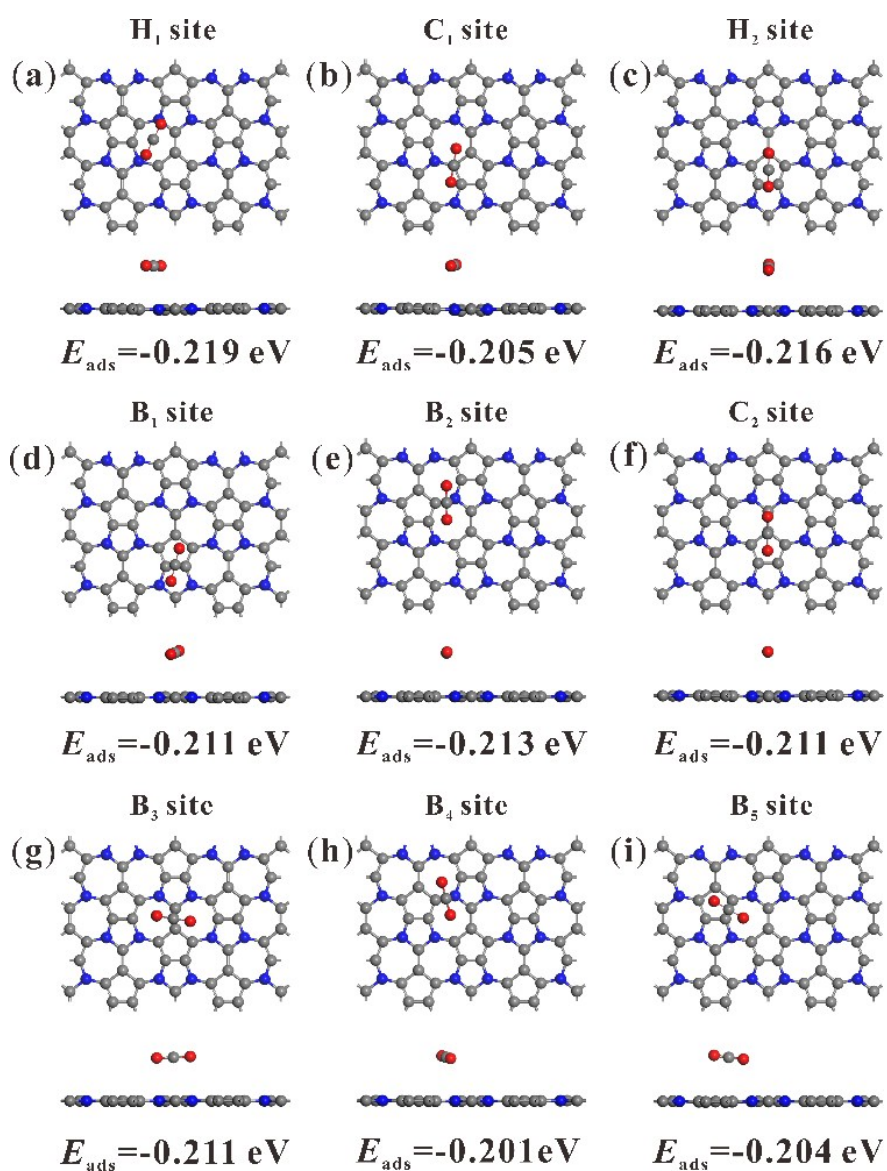


Fig. S3 The stable configurations of CO_2 on neutral C_6N_2 nanosheet with different adsorption sites.

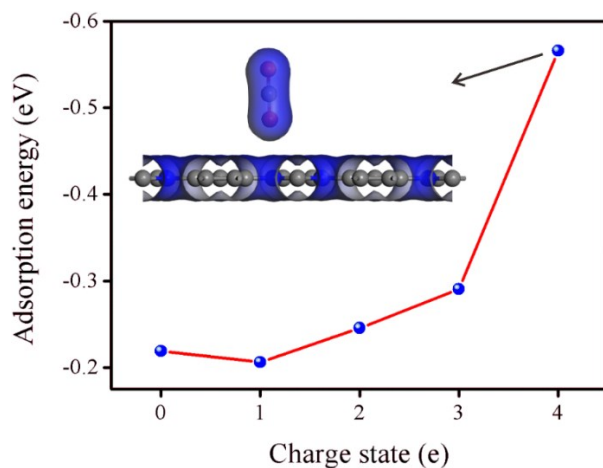


Fig. S4 Adsorption energy of CO₂ as a function of the positively charged C₆N₂ monolayer. Internally, the charge density distribution under four positive charges is shown.

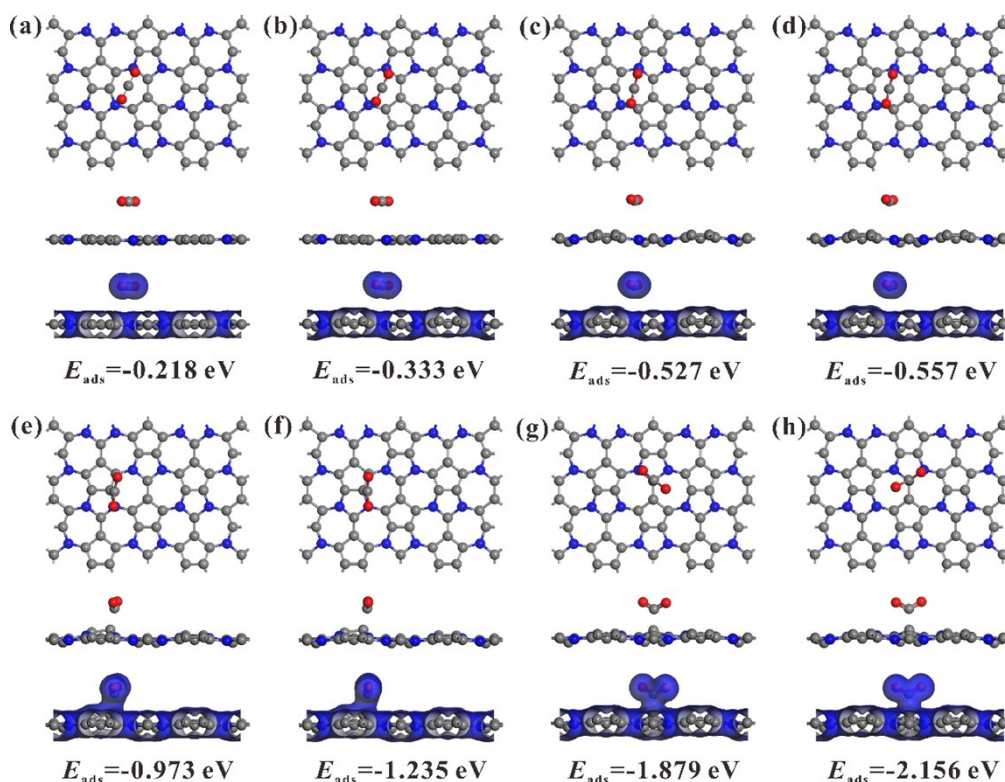


Fig. S5 The stable configurations and total charge density distribution of CO₂ on (a) 0 e⁻, (b) 1 e⁻, (c) 2 e⁻, (d) 2.1 e⁻, (e) 2.2 e⁻, (f) 2.5 e⁻, (g) 2.7 e⁻ and (h) 3 e⁻ charged C₆N₂ monolayer.

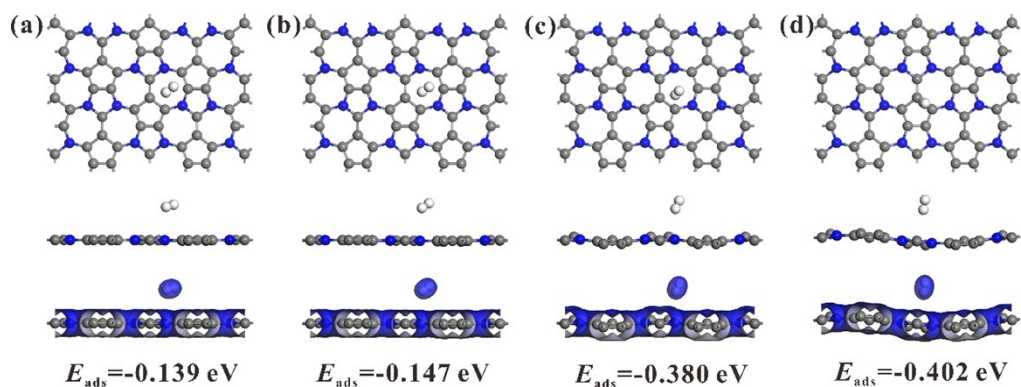


Fig. S6 The stable configurations and total charge density distribution of H_2 on (a) $0 e^-$, (b) $1 e^-$, (c) $2 e^-$, (d) $3 e^-$ charged C_6N_2 monolayer.

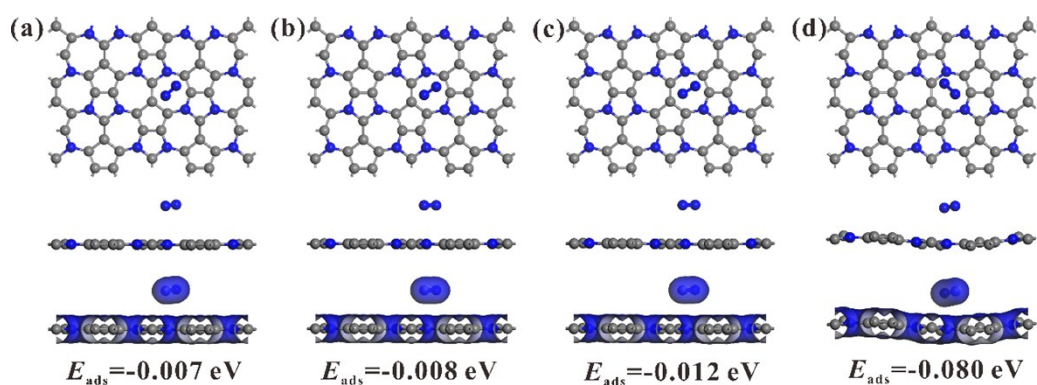


Fig. S7 The stable configurations and total charge density distribution of N_2 on (a) $0 e^-$, (b) $1 e^-$, (c) $2 e^-$, (d) $3 e^-$ charged C_6N_2 monolayer.

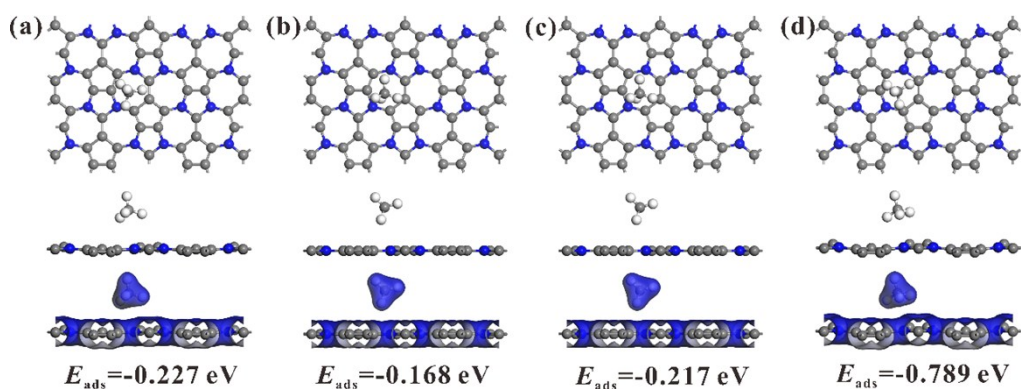


Fig. S8 The stable configurations and total charge density distribution of CH_4 on (a) $0 e^-$, (b) $1 e^-$, (c) $2 e^-$, (d) $3 e^-$ charged C_6N_2 monolayer.

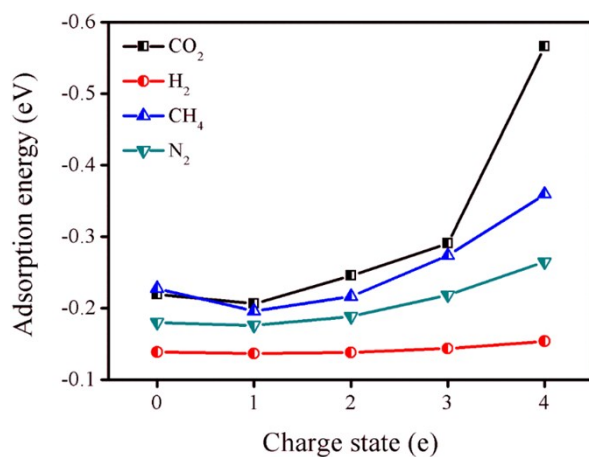


Fig. S9 Adsorption energy of CO₂, H₂, CH₄ and N₂ as a function of positively charged C₆N₂ monolayer.

Table S1 The *G* values crossing the Fermi level for the absorption systems of CO₂, H₂, CH₄, or N₂ on C₆N₂ monolayer with different negatively charges state.

	0	1	2	3
CO₂	2	10	10	6
H₂	2	10	10	12
CH₄	6	10	10	8
N₂	2	10	10	10