Me-N-C (Me=Fe,Cu,Co) nanosheet as a promising charged-controlled CO_2 material

Xiaofang Li,[a,b] Lei Zhu,[a,*] Xiao Chang,[a] Daliang He,[a] Qingzhong Xue, [a,*] Wei Xing[a]

[a]State Key Laboratory of Heavy Oil Processing, College of Science, China University of Petroleum, Qingdao 266555, Shandong, P. R. China

[b]Research School Physics and Engineering, College of Physical & Mathematical Sciences, The Australian National University, 60 Mills Road, Acton ACT 2601 Australia

*Corresponding author:

Tel: 86-532-86981169. E-mail: xueqingzhong@tsinghua.org.cn; (Prof. Q. Z. Xue)

E-mail: zhuleiupc@126.com (L. Zhu)

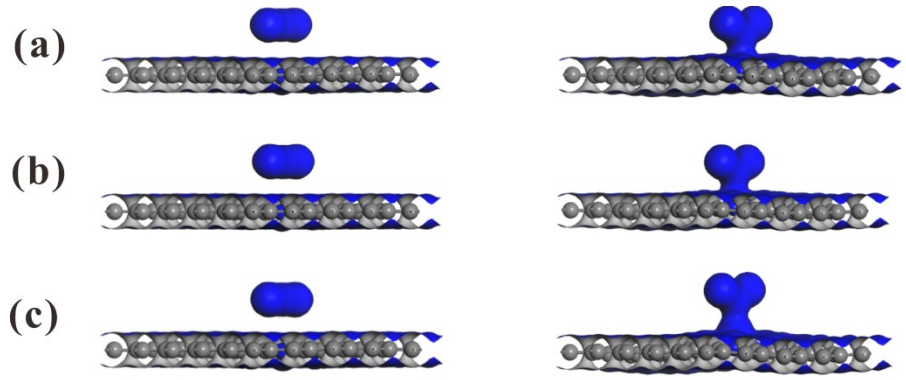

Fig. S1 The total charge density distribution of a single CO_2 molecule on (a) Fe-N-C nanosheet, (b) Co-N-C nanosheet, (c) Cu-N-C nanosheet with different charge densities.

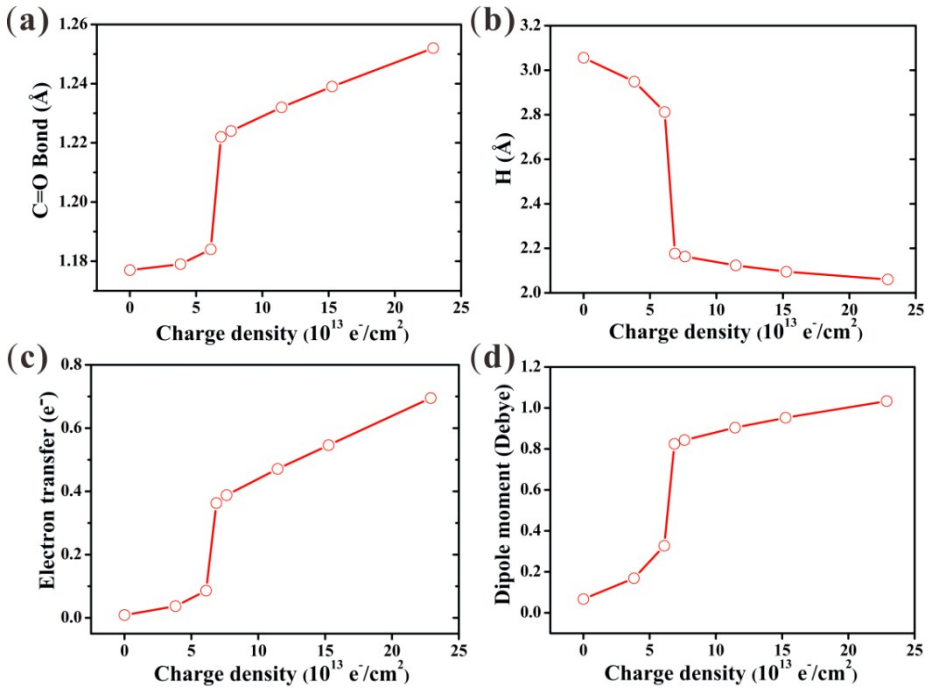

Fig. S2 (a) C=O length, (b) Co-C distance, (c) electron transfer between CO_2 molecule and Co-N-C nosheet, (d) induced dipole moment of CO_2 molecule as a function of different charge densities.

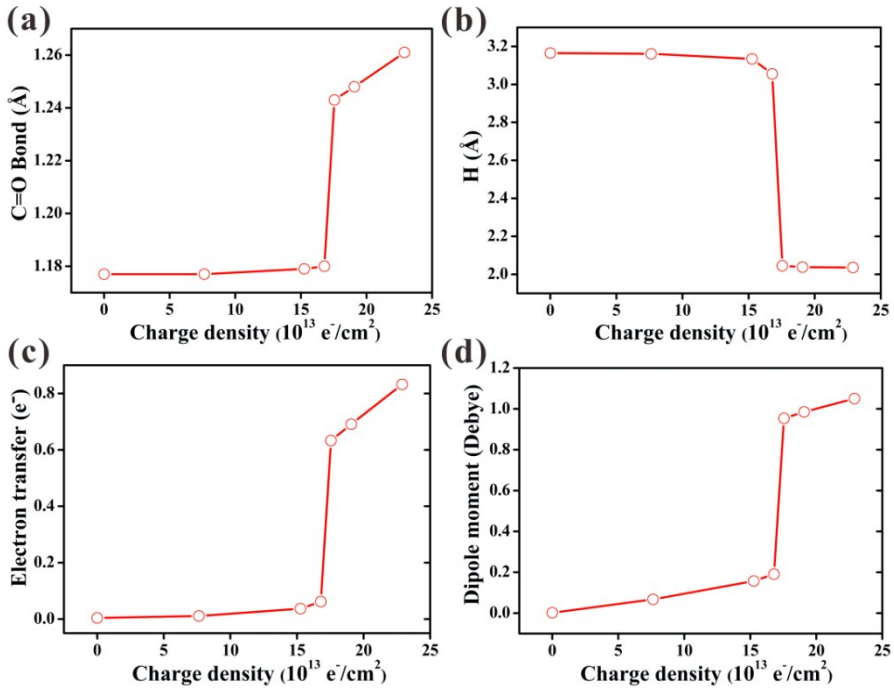

Fig. S3 (a) C=O length, (b) Cu-C distance, (c) electron transfer between CO_2 molecule and Cu-N-C nosheet, (d) induced dipole moment of CO_2 molecule as a function of different charge densities.

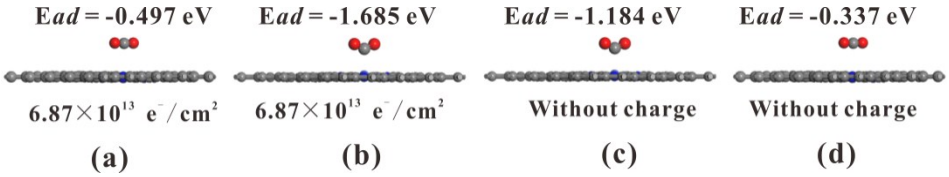

Fig. S4 Adsorption process (a)-(b) and desorption process (c)-(d) of CO_2 molecule Co-N-C nanosheet with 6.87 × 10^{13} e$^-$/cm^2.

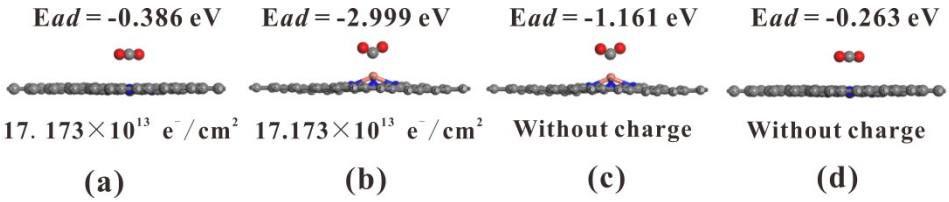

Fig. S5 Adsorption process (a)-(b) and desorption process (c)-(d) of CO_2 molecule Cu-N-C nanosheet with 17.173 × 10^{13} e$^-$/cm^2.

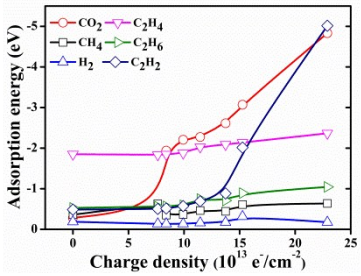

Fig. S6 The adsorption energies of CO_2, C_2H_6, CH_4, H_2, C_2H_4 and C_2H_2 on negative

charged Fe-N-C nanomaterial as a function of negatively charge densities.

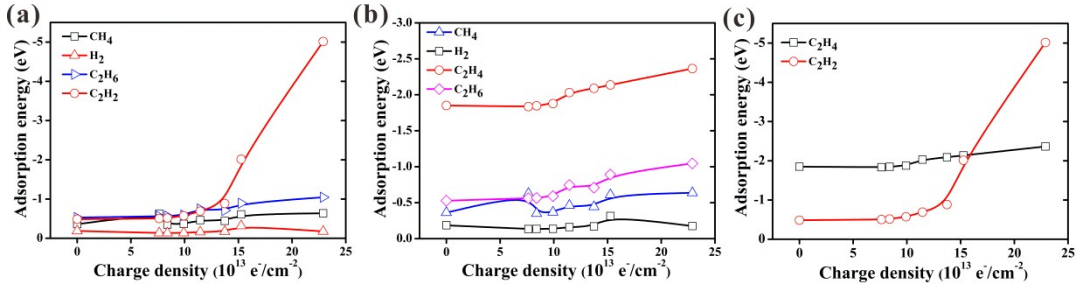

Fig. S7 The adsorption energies of C_2H_6, CH_4, H_2, C_2H_4 and C_2H_2 on negative charged Fe-N-C nanomaterial as a function of negative charge densities.

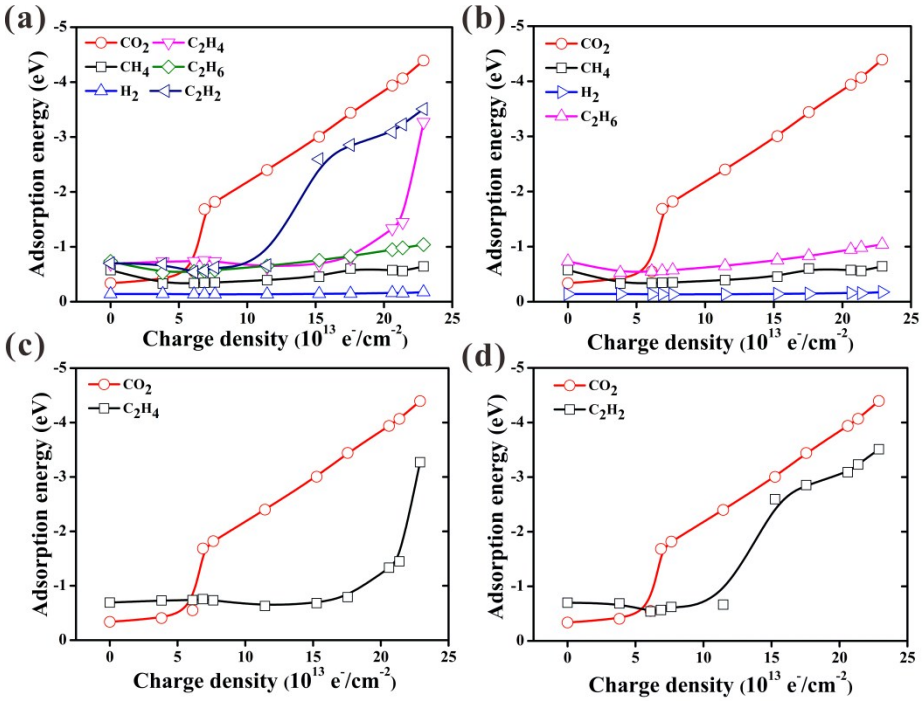

Fig. S8 The adsorption energies of CO_2, C_2H_6, CH_4 H_2, C_2H_4 and C_2H_2 on negative charged Co-N-C nanomaterial as a function of negative charge densities.

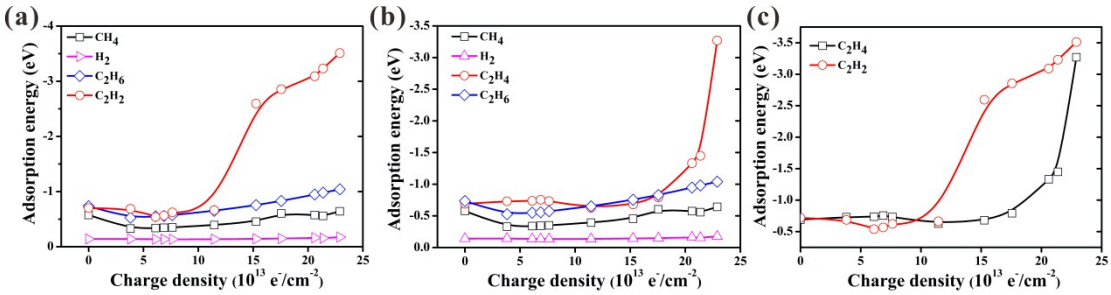

Fig. S9 The adsorption energies of C_2H_6, CH_4, H_2, C_2H_4 and C_2H_2 on negative charged Co-N-C nanomaterial as a function of negative charge densities.

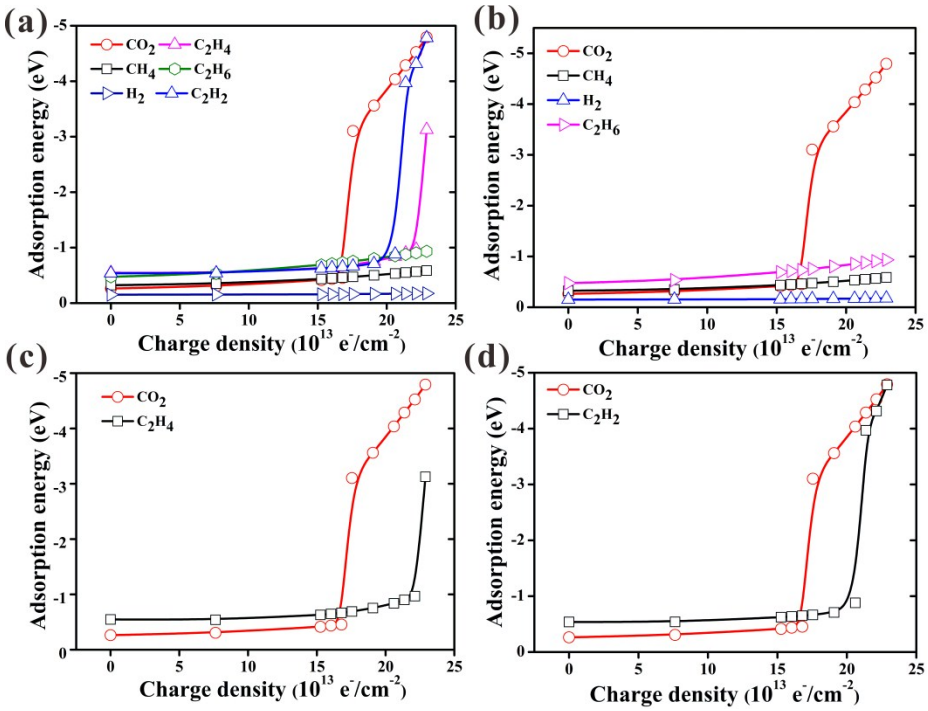

Fig. S10 The adsorption energies of CO_2, C_2H_6, CH_4, H_2, C_2H_4 and C_2H_2 on negative charged Cu-N-C nanomaterial as a function of negative charge densities.

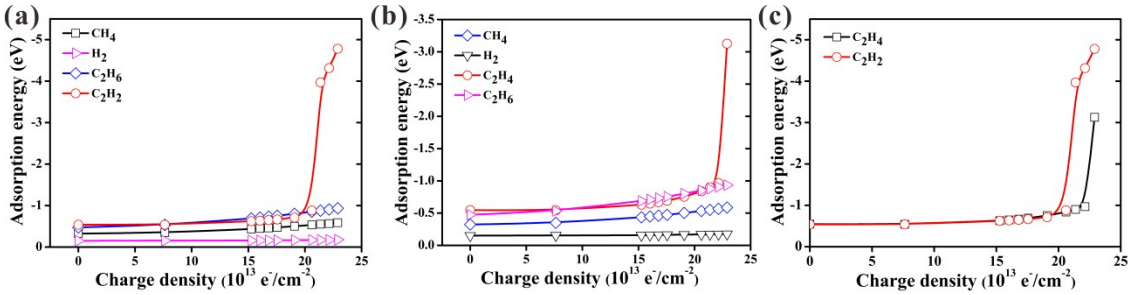

Fig. S11 The adsorption energies of C_2H_6, CH_4, H_2, C_2H_4 and C_2H_2 on negative charged Cu-N-C nanomaterial as a function of negative charge densities.