Me-N-C (Me=Fe,Cu,Co) nanosheet as a promising charged-controlled CO₂ material

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Charge density= 0 e^{-1}/cm^{2} Charge density = 22. 90×10¹³ e^{-1}/cm^{2} Fig. S1 The total charge density distribution of a single CO₂ 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.

E <i>ad</i> = -0.497 eV	Ead = -1.685 eV	Ead = -1.184 eV	Ead = -0.337 eV
000	6 0 0	6 0 0	000
O-COCINCIRCIPCIES CENERATIO	-0-00000000000000000-0-	<	0-00000000000000000-0
$6.87 \times 10^{13} \text{ e}^{-}/\text{ cm}^{2}$	$6.87 \times 10^{13} \text{ e}^{-}/\text{cm}^{2}$	Without charge	Without charge
(a)	(b)	(c)	(d)

Fig. S4 Adsorption process (a)-(b) and desorption process (c)-(d) of CO₂ molecule Co-N-C nanosheet with 6.87×10^{13} e⁻/cm².

Ead = -0.386 eV	Ead = -2.999 eV	Ead = -1.161 eV	Ead = -0.263 eV
000	••	0 0 ⁰	000
0-030303030303030300-0	0-000000000000000000000000	0-01000000000000000-0	0-010103032362362500-0
17. $173 \times 10^{13} \text{ e}^{-}/\text{ cm}^{2}$	$17.173 \times 10^{13} \text{ e}^{-1} \text{ cm}^{2}$	Without charge	Without charge
(a)	(b)	(c)	(d)

Fig. S5 Adsorption process (a)-(b) and desorption process (c)-(d) of CO₂ molecule Cu-N-C nanosheet with $17.173 \times 10^{13} \text{ e-/cm}^2$.



Fig. S6 The adsorption energies of CO₂, C_2H_6 , CH_4 , H_2 , C_2H_4 and C_2H_2 on negative S-3



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.