Me-N-C (Me=Fe,Cu,Co) nanosheet as a promising charged-controlled \( \text{CO}_2 \) material

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**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 nanosheet, (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 nanosheet, (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 $6.87 \times 10^{13}$ e/cm$^2$.

Fig. S5 Adsorption process (a)-(b) and desorption process (c)-(d) of CO$_2$ molecule Cu-N-C nanosheet with $17.173 \times 10^{13}$ e/cm$^2$.

Fig. S6 The adsorption energies of CO$_2$, C$_2$H$_6$, CH$_4$, H$_2$, C$_2$H$_4$ and C$_2$H$_2$ on negative
charged Fe-N-C nanomaterial as a function of negatively charge densities.

Fig. S7 The adsorption energies of C$_2$H$_6$, CH$_4$, H$_2$, C$_2$H$_4$ and C$_2$H$_2$ on negative charged Fe-N-C nanomaterial as a function of negative charge densities.

Fig. S8 The adsorption energies of CO$_2$, C$_2$H$_6$, CH$_4$, H$_2$, C$_2$H$_4$ and C$_2$H$_2$ on negative charged Co-N-C nanomaterial as a function of negative charge densities.

Fig. S9 The adsorption energies of C$_2$H$_6$, CH$_4$, H$_2$, C$_2$H$_4$ and C$_2$H$_2$ on negative charged Co-N-C nanomaterial as a function of negative charge densities.
Fig. S10 The adsorption energies of CO₂, C₂H₆, CH₄, H₂, C₂H₄ and C₂H₂ on negative charged Cu-N-C nanomaterial as a function of negative charge densities.

Fig. S11 The adsorption energies of C₂H₆, CH₄, H₂, C₂H₄ and C₂H₂ on negative charged Cu-N-C nanomaterial as a function of negative charge densities.