Supporting Information

Ca-embedded C_2N: An efficient adsorbent for CO_2 capture

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Table S1. The relative values of energies (in eV) of the other optimized configurations to those of the most stable configurations for the metal single atom adsorption on C_2N. Same as shown in Figure 1 in the main text, h1, h2, h3, B1, B2, B3, H1, and H2 represent the considered sites for metal adsorption on C_2N. Metal atoms embedded at B2 and B3 sites will move to the sites with the lowest energy and the structures for metal embedded at B1 site are identical to those at H2 site after optimization.

	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
h1	0.00	0.20	0.40	0.69	0.46	0.31	0.62	1.65	1.06	0.43	0.47
h2	4.88	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
h3	4.91	0.00	-	0.04	0.04	0.02	0.04	0.07	0.14	0.05	0.08
H1	6.75	6.02	5.19	4.23	4.98	5.12	4.54	4.43	3.28	3.98	2.45
H2	5.67	4.59	3.86	3.02	3.65	3.80	3.19	2.99	2.06	2.49	1.01

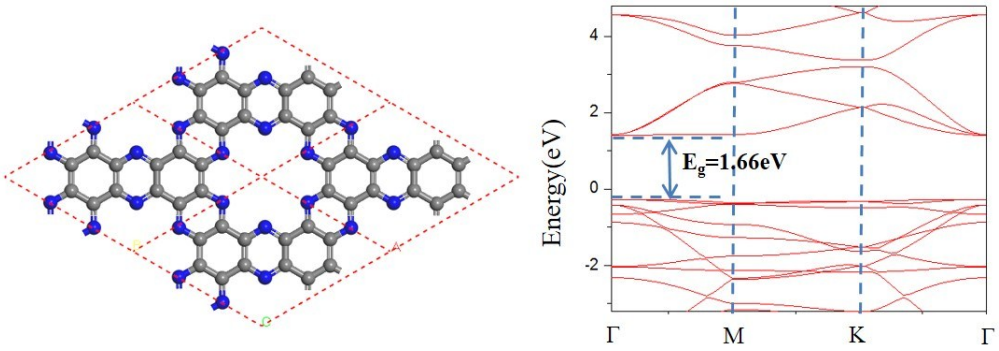

Fig. S1 The geometric structure and the calculated band dispersion of pristine C_2N nanosheet based on Perdew–Burke–Ernzerhof functional. The lattice constant is optimized to be 8.33 Å. The C and N atoms are represented by grey and blue spheres, respectively. The primitive cell of C_2N is enclosed by the red dashed line.

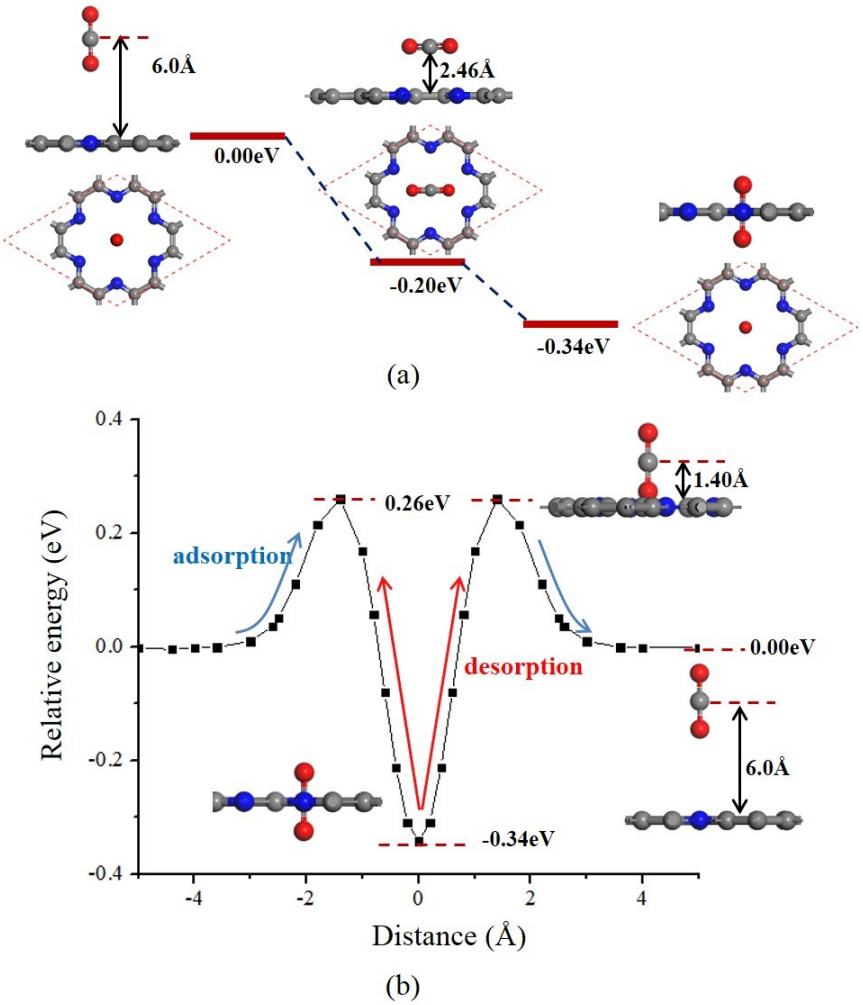

Fig. S2 (a) The optimized stable structures and the relative energies to the left-most geometry which stands for isolated CO_2 molecule and C_2N. (b) The adsorption and desorption diagram for CO_2 molecule capture inside the cavity of C_2N. Grey, blue, and red balls represent C, N, and O atoms, respectively.

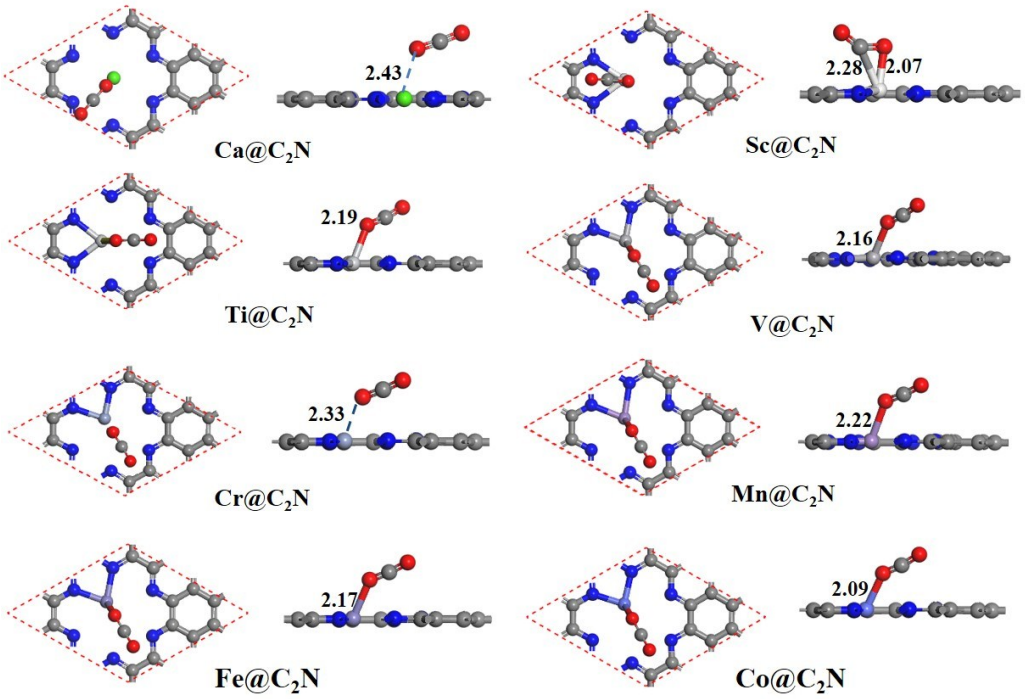

Fig. S3 Top and side views of one CO_2 molecule adsorbed on Ca and transition metals (Sc, Ti, V, Cr, Mn, Fe, Co) embedded C_2N nanosheets, as well as the distances between metal atom and the nearest O atom of CO_2 molecule in unit of Å. Grey, blue, red, and green balls represent C, N, O, and Ca metal atoms, respectively. Other balls off cavity center of C_2N sheet and binding to two N atoms represent the transition metal atoms.

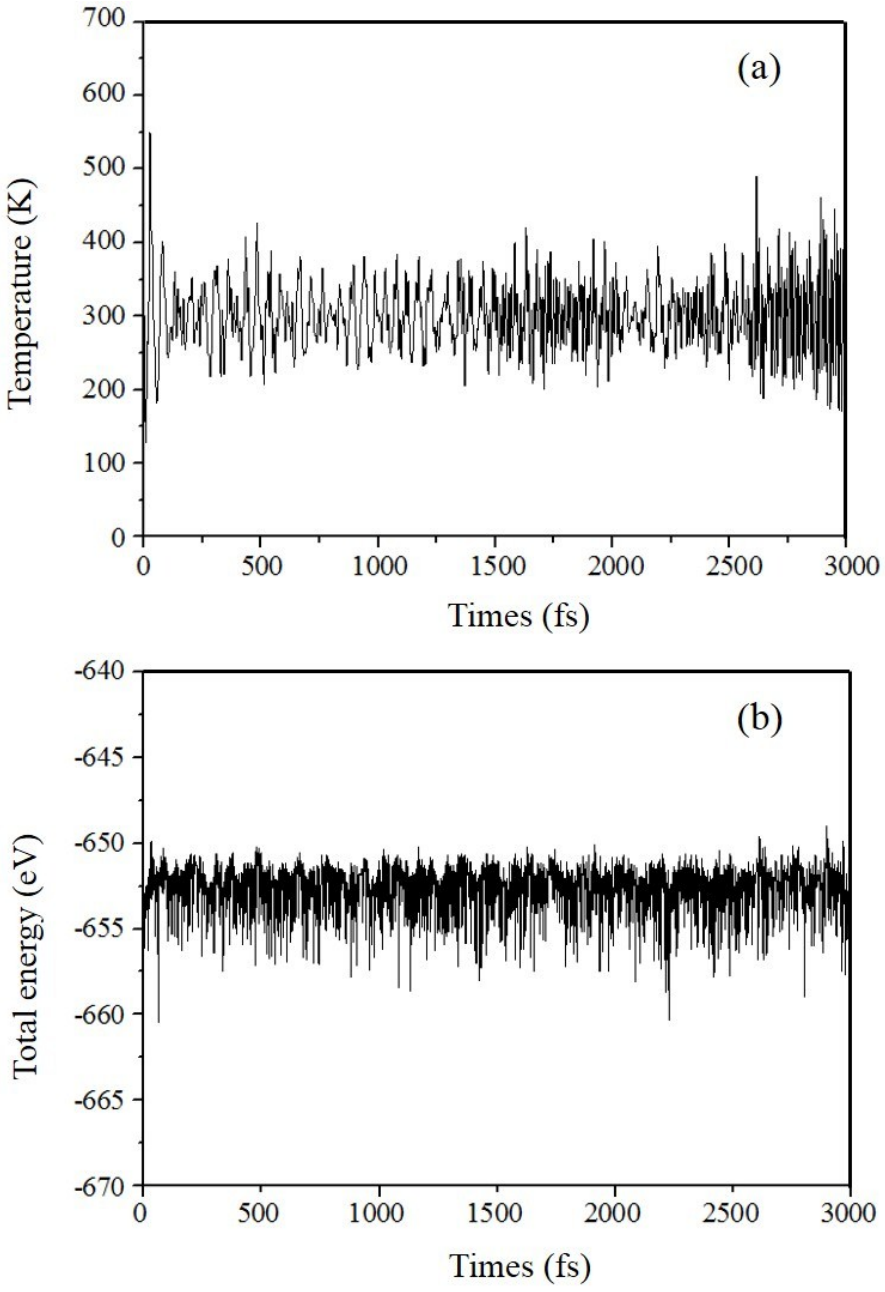

Fig. S4 Fluctuations of (a) temperature and (b) total energy of Ca embedded C_2N as a function of molecular dynamics simulation time.