Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Heteroatom–Doped C_3N as a Promising Metal–Free Catalyst for High–Efficiency Carbon Dioxide Reduction Reaction

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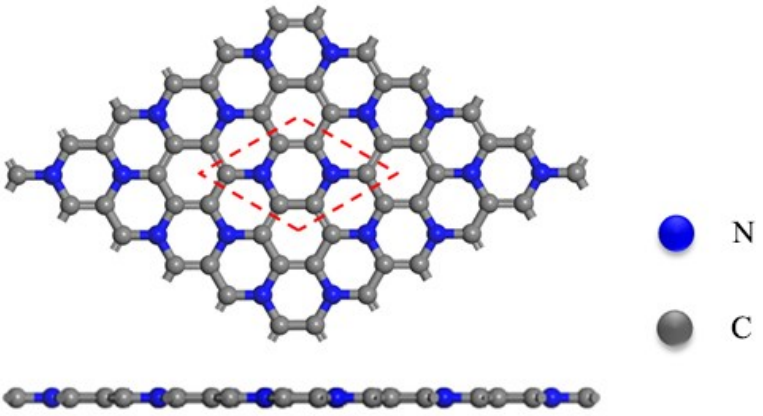

Fig. S1 Top and side views of the C_3N.

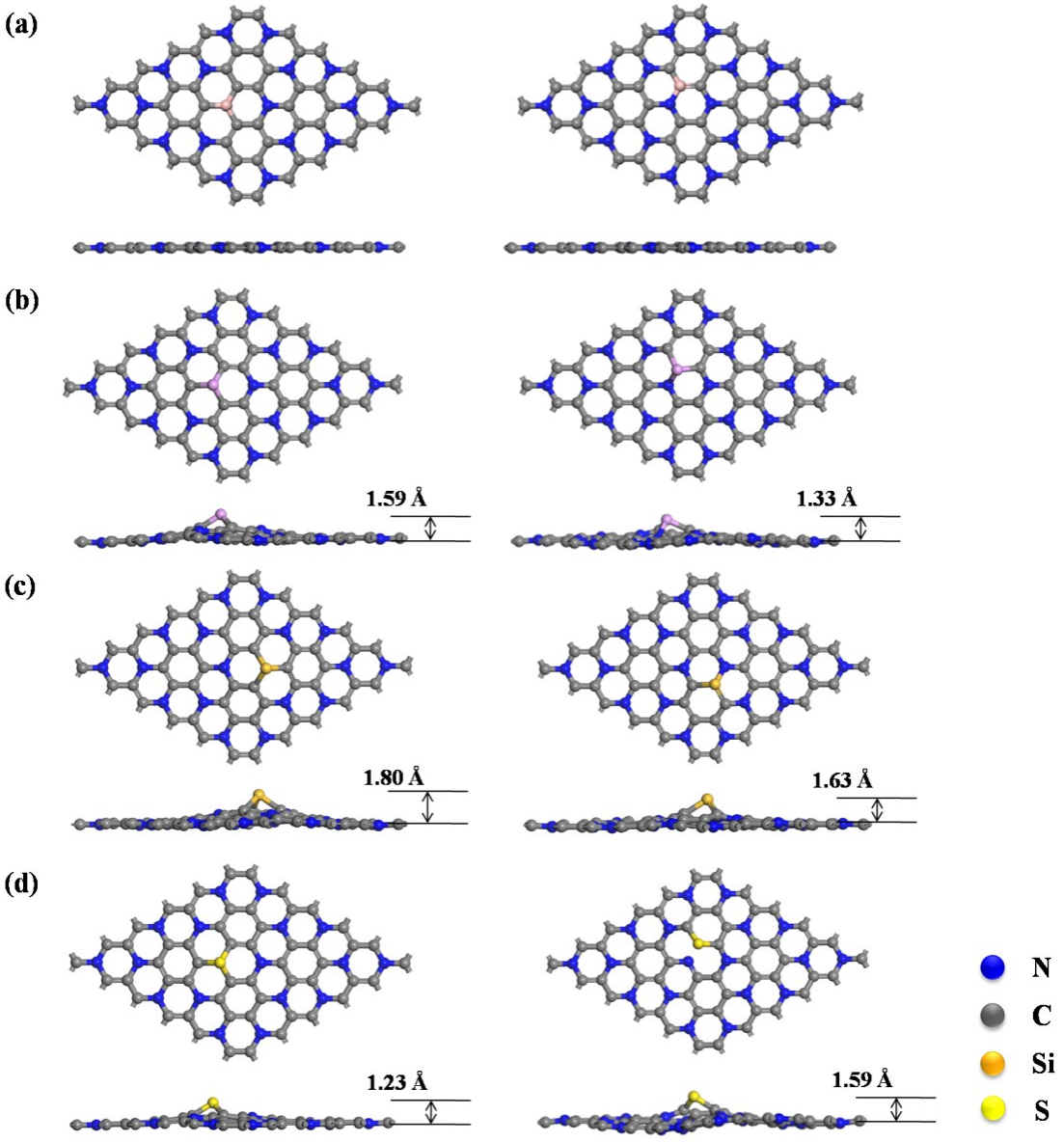

Fig. S2 Top and side views of B (a), P (b), Si (c), S (d)–doped C_3N, and the corresponding formation energies.

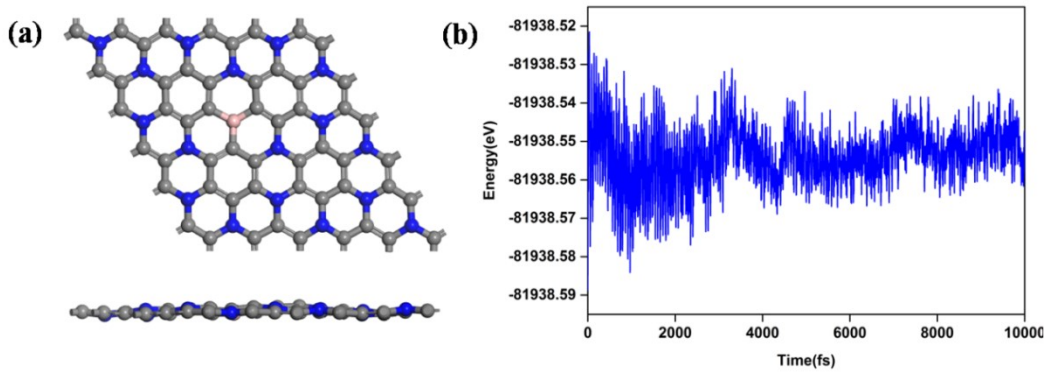

Fig. S3 Geometry snapshot (a) and variations of energy (b) against time for MD simulations of B_N–doped C_3N, and the simulation is run at 500 K for 10 ps with a time step of 1 fs.

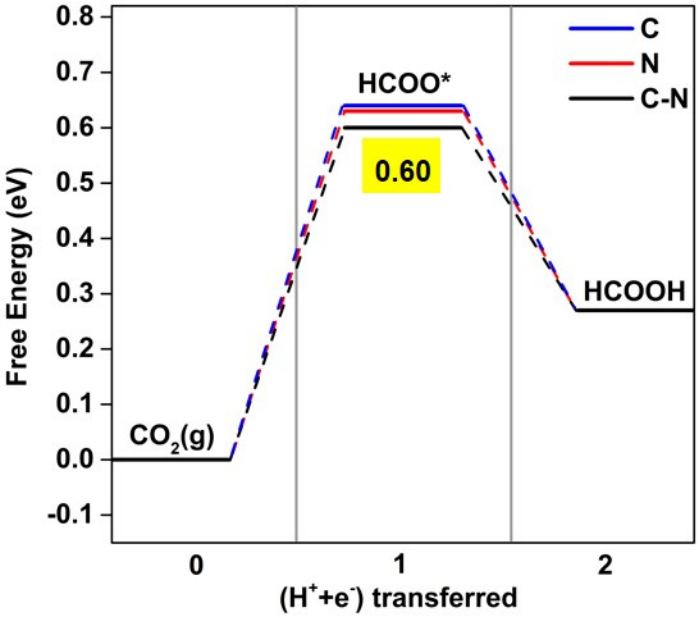

Fig. S4 The free energy diagram for CO_2ER on C_3N.

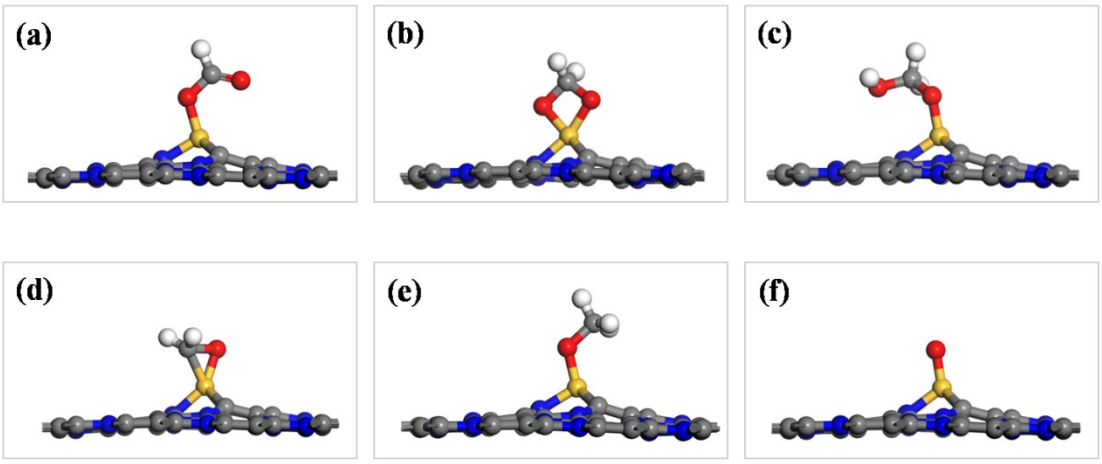

Fig. S5 The optimized geometric structures of HCOO* (a), H_2COO* (b), H_2COOH* (c), H_2CO* (d), H_3CO* (e), and O* (d), along the most favorable reaction path of CO_2ER proceeded on Si_C–doped C_3N.

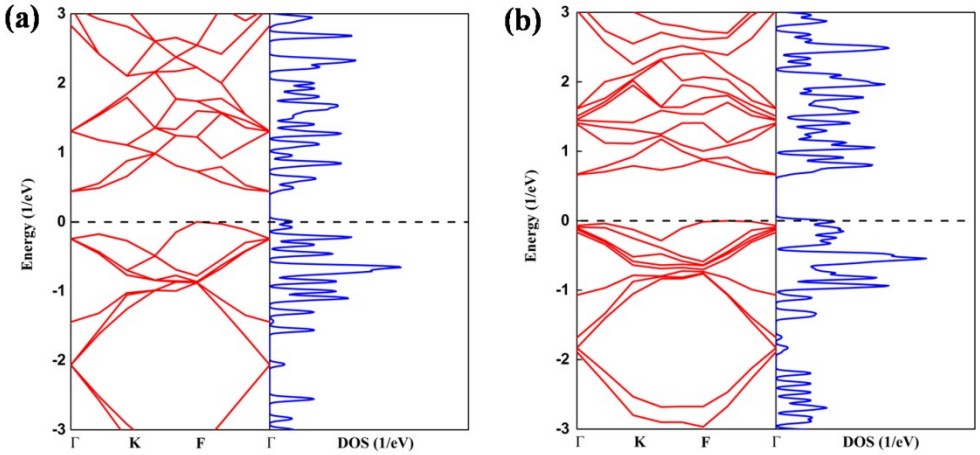

Fig. S6 Band structures and DOS for C_3N (a) and B_N−doped C_3N (b).