Supporting Information

Mechanistic insight into electroreduction of carbon dioxide on FeN_x(x = 0 – 4) embedded graphene

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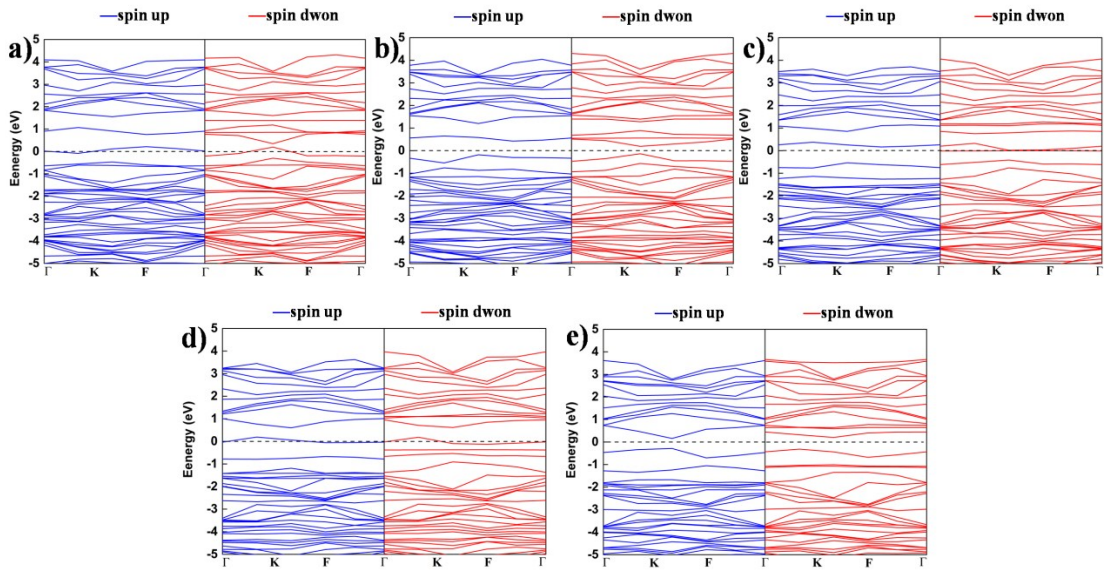

Fig. S1 The band structure of FeN_0–gra (a), FeN_1–gra(b), FeN_2–gra (c),FeN_3–gra (d), and FeN_4–gra (e).

Table S1 The computed band gap (eV), spin magnetic moment (μ_B) and *d* band center (ε_d) of FeN_x–gra (x = 0 – 4).

	FeN_0–gra	FeN_1–gra	FeN_2–gra	FeN_3–gra	FeN_4–gra
band gap	—	0.33	0.02	—	0.44
spin	2.80	2.85	2.31	2.02	1.94
ε_d	–1.49	–1.42	–1.36	–1.14	–1.28

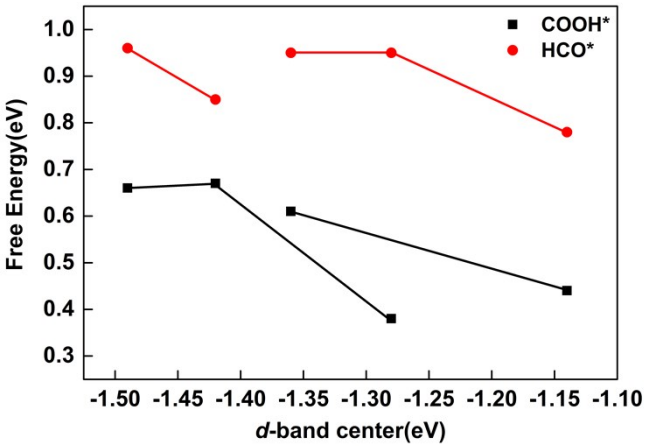

Fig.S2 Gibbs free energy of adsorbates corresponding to *d* band center ε_d.

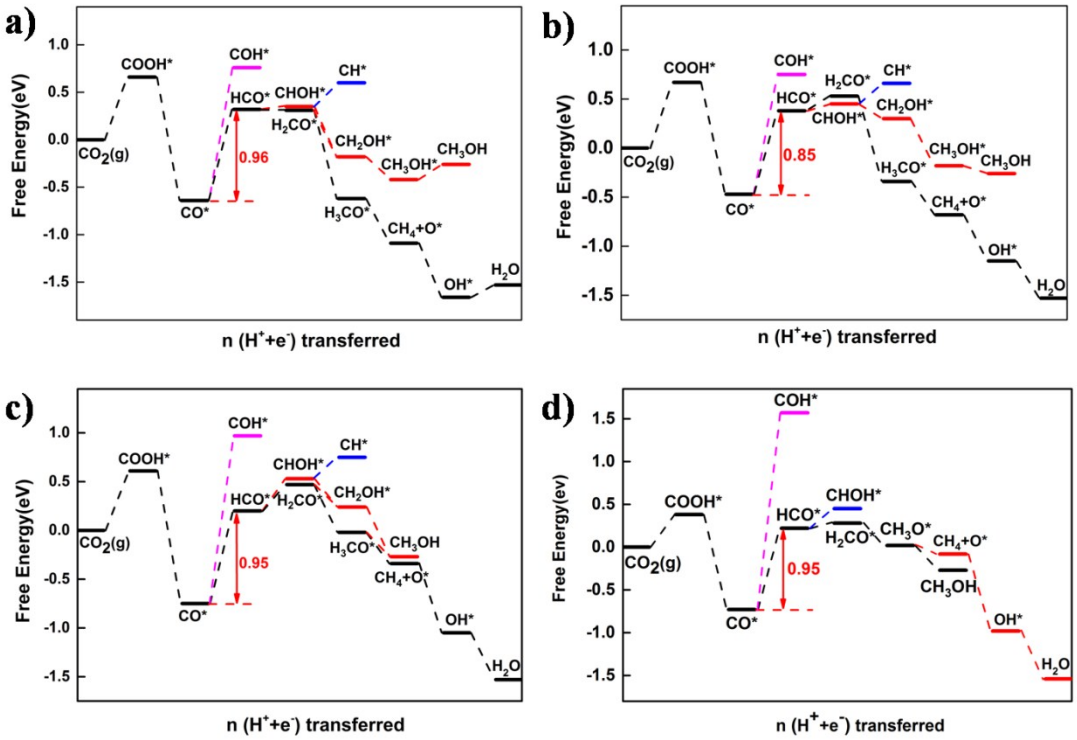

Fig. S3 Free energy profiles for CO_2ER on FeN_0–gra (a), FeN_1–gra (b), FeN_2–gra (c), and FeN_4–gra(d).

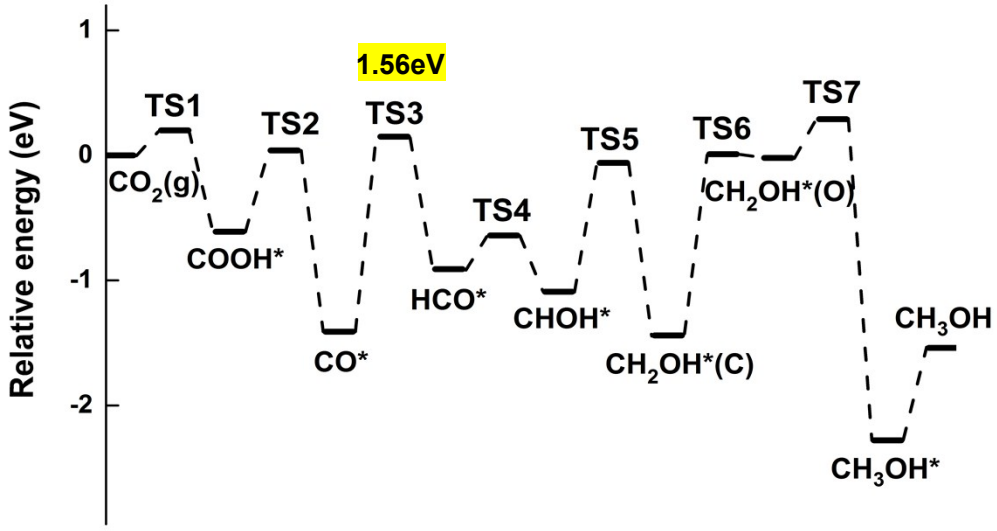

Fig. S4 Relative energy diagram for CO_2 reduction to CH_3OH on FeN_3–gra.

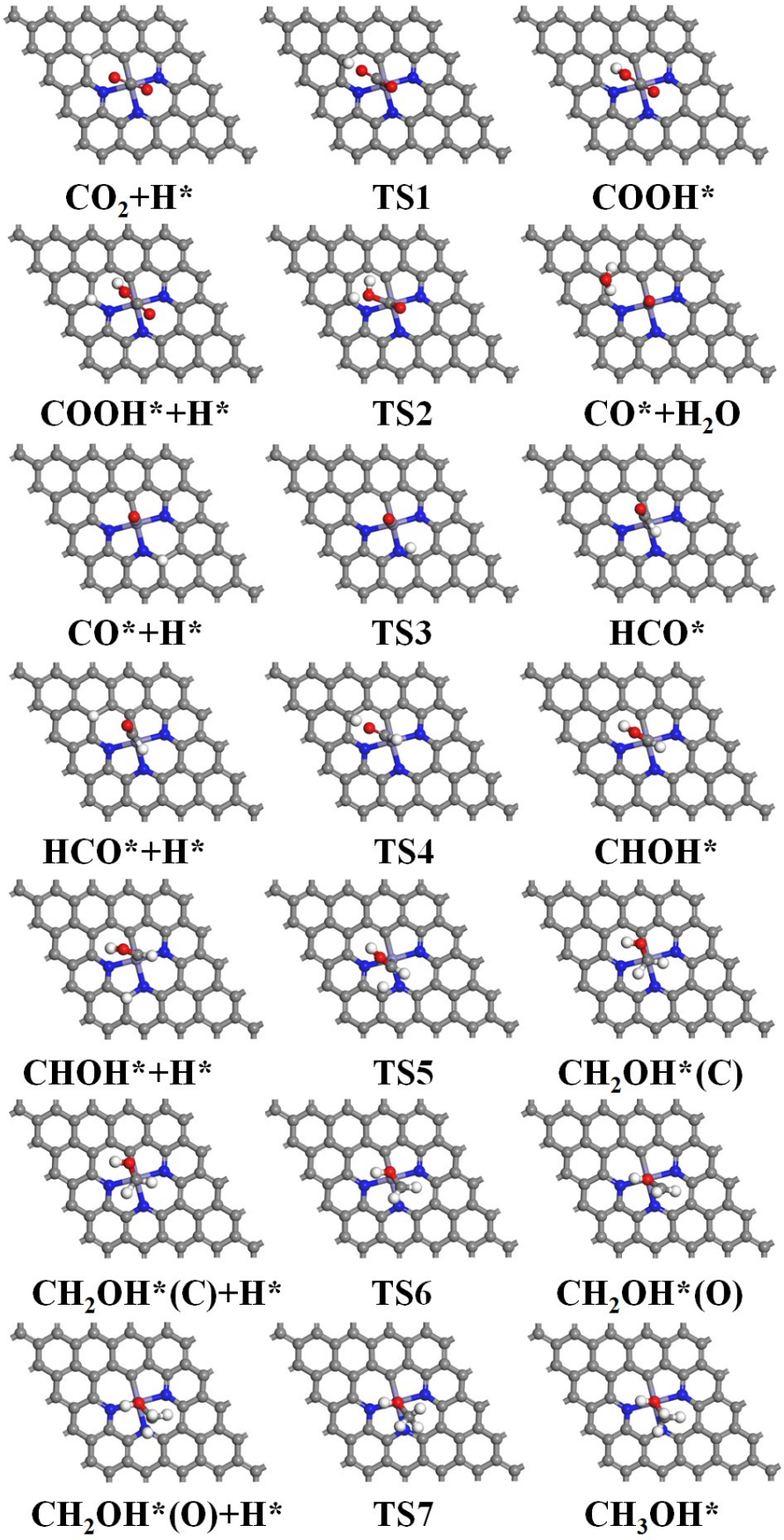

Fig. S5 The optimized geometric structures of initial states, transition states, and final states involved in the optimal reaction path for CH_3OH formation.

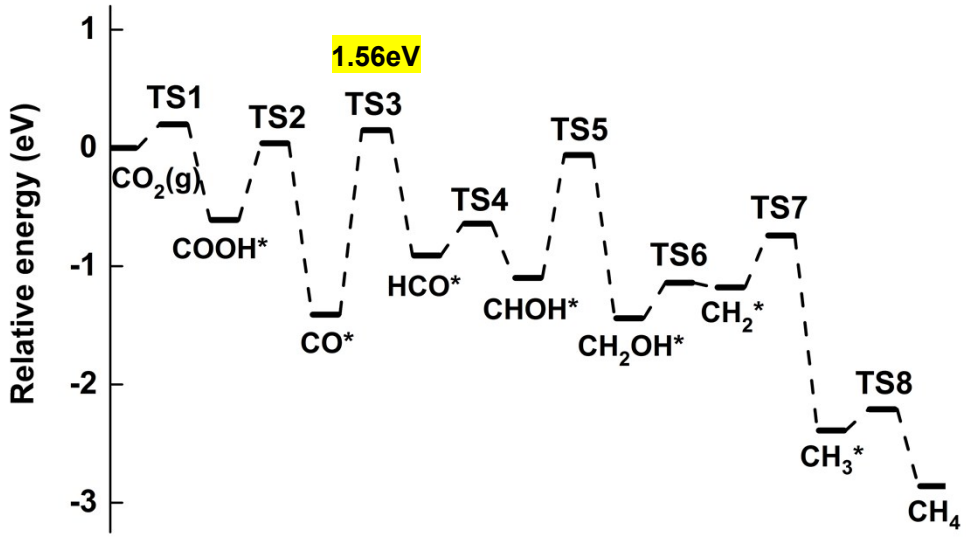

Fig. S6 Potential energy profiles for CO_2reduction to CH_4 on FeN_3–gra.

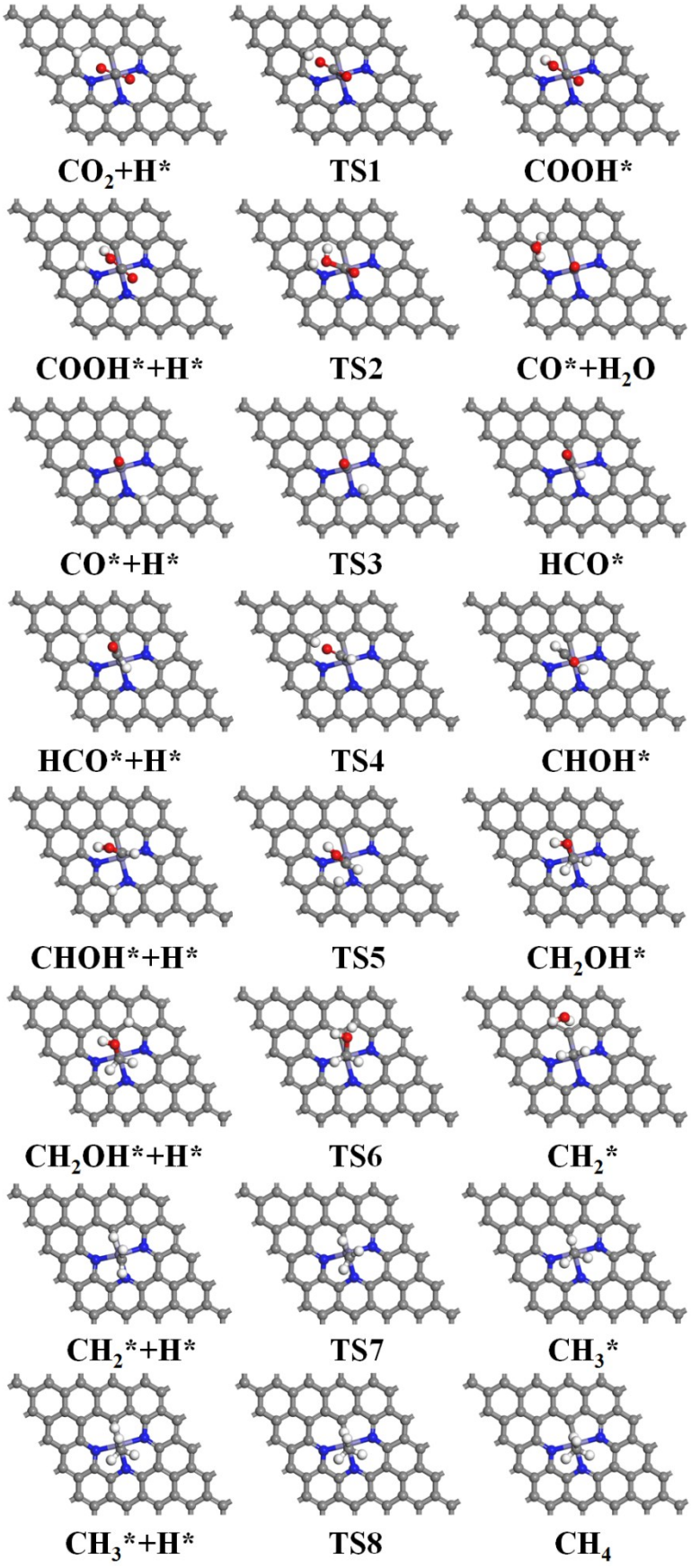

Fig. S7 The optimized geometric structures of initial states, transition states, and final states involved in the optimal reaction path for CH_4 formation.