Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Distance Produces Beauty? Regulating the Distance of Fe Atomic Pairs to Enhance Electrocatalytic CO_2 Reduction

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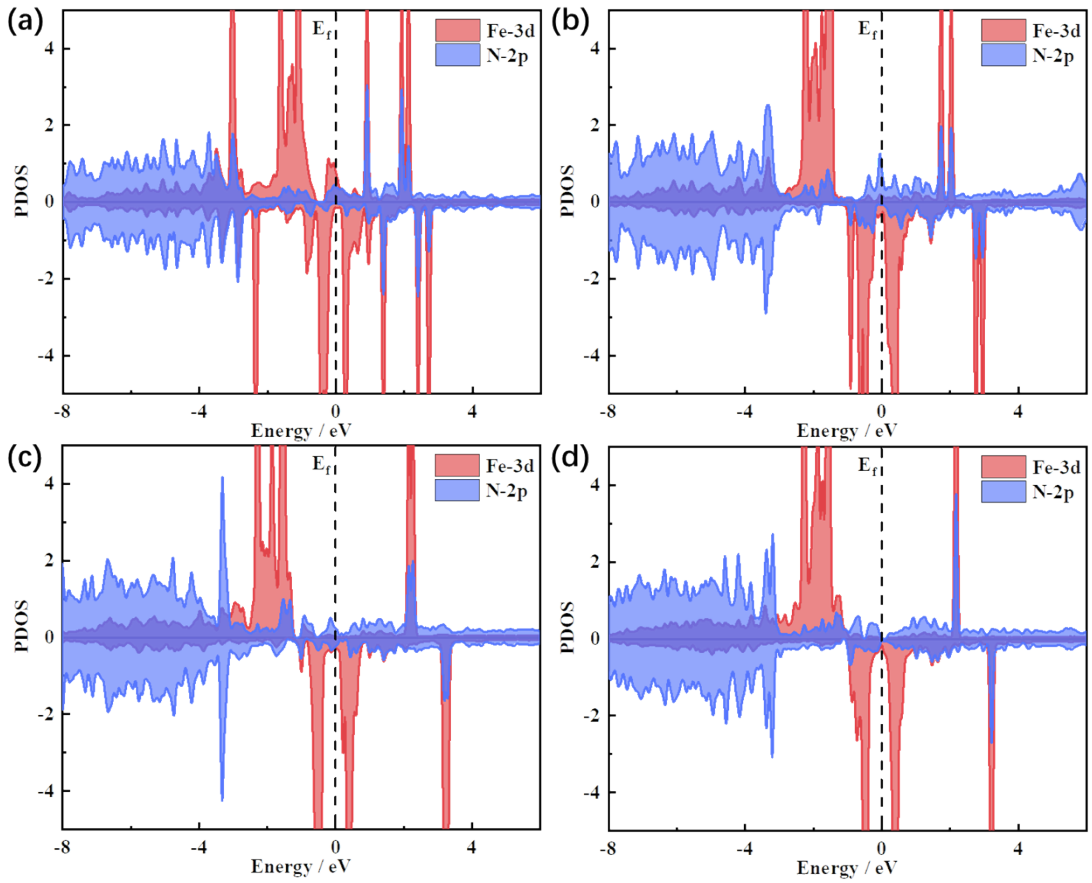


Figure S1. Partial density of states (PDOS) between N 2p-obital and Fe 3d-orbital of four catalysts, respectively.

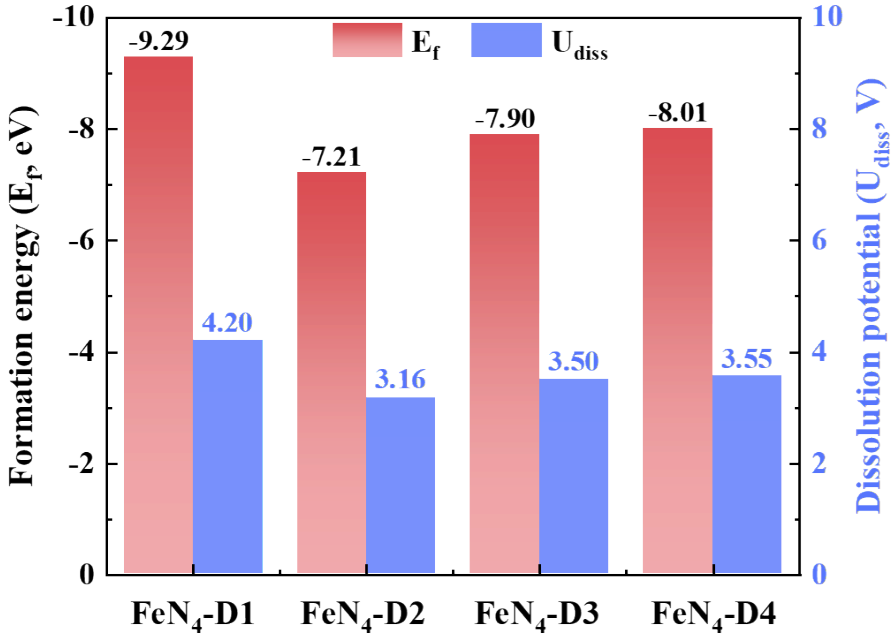


Figure S2. Forming energy (E_f, eV) and dissolution potential (U_{diss}, V) of four catalysts.

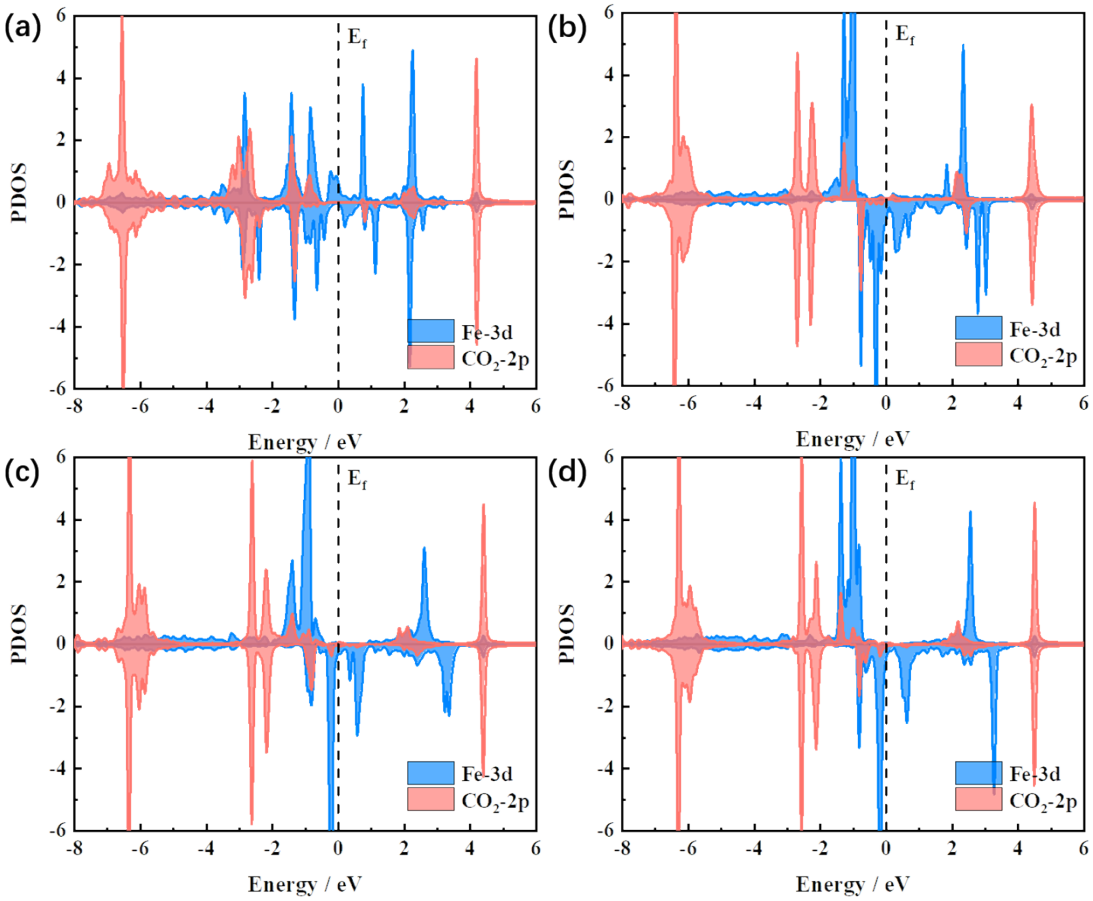


Figure S3. Partial density of states (PDOS) between CO_2 2p-obital and Fe 3d-orbital of four catalysts, respectively.

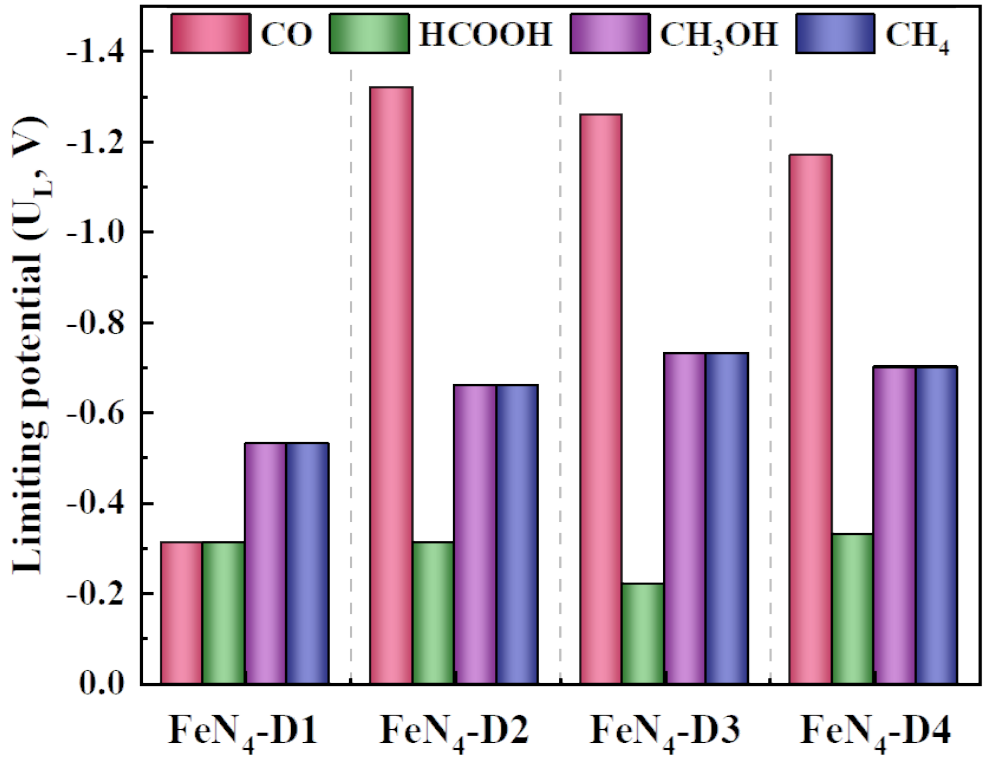


Figure S4. Summary of the limiting potential (U_L) of the products for CO, HCOOH, CH_3OH, and CH_4 on four FeN_4-Dx (x = 1, 2, 3, 4) structures.

Table S1. The bond length (D, Å), Bader charge transfer (|e|), magnetic moments (M, μ_B), and d-band center (ε_d) of four FeN_4-Dx (x = 1, 2, 3, 4) structures.

Structure	**D (Å)**		**Bader (|e|)**	**M (μ_B)**	**ε_d**	
s	Fe-Fe	Fe-N	Fe	Fe	up	down
FeN_4-D1	2.39	1.87	-1.27	3.24	-1.75	-0.78
FeN_4-D2	4.14	1.91	-1.29	3.73	-1.89	-0.19
FeN_4-D3	6.53	1.88	-1.25	4.07	-2.00	-0.20
FeN_4-D4	8.62	1.89	-1.25	4.00	-2.01	-0.20

Table S2. The C-Fe bond length, O-C-O bond angle, Bader charge transfer, adsorption energy (E_{ads}, eV) and corresponding adsorption structure of CO_2 adsorbed on four FeN_4-Dx structures.

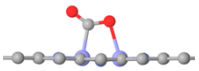
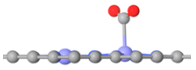
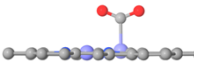
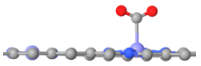
FeN_4-Dx	**C-Fe (Å)**	**∠O-C-O (°)**	**Bader (|e|)**		**E_{ads} (eV)**	**Structures**
			Fe	CO_2		
FeN_4-D1	2.02	132.99	-1.13	0.78	-0.25	
FeN_4-D2	2.11	137.75	-1.15	0.66	-0.22	
FeN_4-D3	2.05	136.54	-1.16	0.70	-0.21	
FeN_4-D4	2.05	137.50	-1.11	0.68	-0.10	

Table S3. The reaction free energy of forming different intermediates on FeN_4-Dx (x = 1, 2, 3, 4) catalysts.

Reaction steps	FeN_4-D1	FeN_4-D2	FeN_4-D3	FeN_4-D4
$* + CO_2 \rightarrow *CO_2$	0.18	0.22	0.22	0.33
$*CO_2 + H^+ + e^- \rightarrow *COOH$	0.31	-0.24	-0.03	-0.10
$*CO_2 + H^+ + e^- \rightarrow *HCOO$	0.39	-0.34	-0.09	-0.13
$*COOH + H^+ + e^- \rightarrow *HCOOH$	-0.09	0.41	0.14	0.16
$*HCOO + H^+ + e^- \rightarrow *HCOOH$	-0.17	0.31	0.20	0.20
$*HCOOH \rightarrow * + HCOOH$	-0.10	0.10	-0.03	-0.10
$*COOH + H^+ + e^- \rightarrow *CO + H_2O$	-0.15	-0.66	-0.80	-0.75
$*CO \rightarrow * + CO$	0.31	1.32	1.26	1.17
$*CO + H^+ + e^- \rightarrow *CHO$	0.02	0.66	0.73	0.70
$*CO + H^+ + e^- \rightarrow *COH$	1.79	1.96	1.84	2.22
$*CHO + H^+ + e^- \rightarrow *CH_2O$	0.53	0.50	--	--
$*CHO + H^+ + e^- \rightarrow *CHOH$	0.72	0.33	0.27	0.44
$*CH_2O + H^+ + e^- \rightarrow *CH_3O$	-0.06	-0.53	--	--
$*CH_2O + H^+ + e^- \rightarrow *CH_2OH$	-0.53	-0.40	--	--
$*CHOH + H^+ + e^- \rightarrow *CH_2OH$	-0.74	-0.23	-0.27	-0.42
$*CHOH + H^+ + e^- \rightarrow *CH + H_2O$	1.71	1.34	1.31	1.27
$*CH_2OH + H^+ + e^- \rightarrow *CH_3OH$	-0.27	-0.06	-0.13	-0.14
$*CH_3O + H^+ + e^- \rightarrow *CH_3OH$	-0.75	0.07	--	--
$*CH_3OH \rightarrow * + CH_3OH$	-0.18	-0.13	-0.09	-0.15
$*CH_3OH + H^+ + e^- \rightarrow *CH_3 + H_2O$	-0.44	-0.79	-0.62	-0.64
$*CH_2OH + H^+ + e^- \rightarrow *CH_2 + H_2O$	0.22	0.34	0.30	0.32
$*COH + H^+ + e^- \rightarrow *CHOH$	-1.05	-0.97	-0.83	-1.08
$*CH + H^+ + e^- \rightarrow *CH_2$	-2.21	-1.23	-1.29	-1.37
$*CH_2 + H^+ + e^- \rightarrow *CH_3$	-0.94	-1.19	-1.05	-1.10
$*CH_3 + H^+ + e^- \rightarrow *CH_4$	-0.72	-0.35	-0.46	-0.50
$*CH_4 \rightarrow * + CH_4$	-0.21	-0.19	-0.20	-0.20

Table S4. The reaction free energy (ΔG, eV) of CO_2RR to C_2 products (C_2H_5OH and C_2H_4) on FeN_4-D1 catalysts.

Reaction steps	FeN_4-D1
$*CO + *CO \rightarrow *COCO$	1.53
$*CO + *CHO \rightarrow *COCHO$	0.17
$*COCHO + H^+ + e^- \rightarrow *COCHOH$	-0.17
$*COCHOH + H^+ + e^- \rightarrow *COCH + H_2O$	0.33
$*COCHOH + H^+ + e^- \rightarrow *CHOCHOH$	0.08
$*COCHOH + H^+ + e^- \rightarrow *COHCHOH$	0.74
$*CHOCHOH + H^+ + e^- \rightarrow *CHOCH + H_2O$	0.34
$*CHOCHOH + H^+ + e^- \rightarrow *CH_2OCHOH$	0.90
$*CHOCH + H^+ + e^- \rightarrow *CHOHCH$	-0.56
$*CHOHCH + H^+ + e^- \rightarrow *CH_2OHCH$	0.54
$*CHOCH + H^+ + e^- \rightarrow *CHOCH_2$	-1.21
$*CHOCH + H^+ + e^- \rightarrow *CH_2OCH$	0.94
$*CHOCH_2 + H^+ + e^- \rightarrow *CH_2OCH_2$	1.21
$*CHOCH_2 + H^+ + e^- \rightarrow *CHOHCH_2$	0.06
$*CHOHCH + H^+ + e^- \rightarrow *CHOHCH_2$	-0.59
$*CHOHCH_2 + H^+ + e^- \rightarrow *CH_2OHCH_2$	-0.15
$*CH_2OHCH_2 + H^+ + e^- \rightarrow *CH_2OHCH_3$	-0.60
$*CH_2OHCH_3 \rightarrow * + C_2H_5OH$	-0.16
$*CHOHCH_2 + H^+ + e^- \rightarrow *CH_2CH_2 + H_2O$	-0.34
$*CHOHCH_2 + H^+ + e^- \rightarrow *CHCH_2 + H_2O$	-0.09
$*CHCH_2 + H^+ + e^- \rightarrow *CH_2CH_2$	-0.40
$*CH_2CH_2 \rightarrow * + C_2H_4$	-0.26

Table S5. Comparison of FeN_4-D1 structure with some reported catalysts on the PLS free energy of C_2H_5OH.

Catalysts	**PLS**	**ΔG**	**Ref.**
FeN_4-D1	*CHOCHOH + H^+ + e^- → *CHOCH + H_2O	0.34	This work
FeS(001)−V_{S1}	*CH_2COH + H^+ + e^- → *CH_2CHOH	0.86	[1]
FeFe−grafiN_6	*CO + *COH → *HOCCO	0.68	[2]
Fe/GDY	*HCOOH + H^+ + e^- → *HCO + H_2O	0.43	[3]
Fe@B-C_2N	*COCO + H^+ + e^- → *COCHO	0.45	[4]
Fe_2@6N-V_4(b)	*C_2H_5OH → * + C_2H_5OH	0.59	[5]
Cu−C_3N_4	*CO + H^+ + e^- → *CHO	0.75	[6]
T_d-Cu_4@g-C_3N_4	*CO + H^+ + e^- → *CHO	0.68	[7]
Cu_2–CuN_3	*$OHCH_3$ + *OCHO → *CH_3 + *OCHO	0.50	[8]
B@Cu(111)	*C_2H_5OH → * + C_2H_5OH	0.46	[9]
Cu@VO_2	*CO + *CO → *COCO	0.94	[10]

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Appendix

The optimized FeN_4-Dx (x = 1,2,3,4) structure details are as follows:

FeN_4-D1

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0.0000000000000000 0.0000000000000000 15.0000000000000000

C Fe N

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C N Fe

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0.1642283348135735 0.6672588726551560 0.1999908017114221

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