

Supporting information

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Table S1. E_{HOMO} and E_{LUMO} of the intermediates in CO₂RR to methanol

intermediate	HOMO (Ha)	LUMO (Ha)	intermediate	HOMO (Ha)	LUMO (Ha)
CO ₂	-0.3860	-0.0197	TS5	0.0329	0.1267
COOH ⁻	0.0122	0.1395	H ₃ CO	0.0329	0.1267
CO	-0.3875	-0.0424	CH ₃ OH	-0.2843	-0.0132
HCO	0.0627	0.1452	HCOOH	-0.3102	-0.0257
TS4	-0.2819	-0.0643	H ₂ COOH ⁻	0.0059	0.1200
H ₂ CO	-0.2819	-0.0642	CH ₂ OOH ⁻	-0.3391	-0.1889

Table S2. Gibbs free energy of the intermediates in CO₂RR to methanol

intermediate	ΔG (Ha)
CO ₂	-188.6559
COOH	-189.2200
CO	-113.3630
HCO	-113.9150
TS4	-114.5370
H ₂ CO	-114.5360
TS5	-115.1345
H ₃ CO	-115.1350
CH ₃ OH	-115.7370
H ⁺	-0.1746
H ₂ O	-76.4549
H	-0.5129

Table S3. E_{HOMO} and E_{LUMO} of the intermediates in CO₂RR to ethanol

intermediate	HOMO (Ha)	LUMO (Ha)	intermediate	HOMO (Ha)	LUMO (Ha)
CO ₂	-0.3860	-0.0197	CH ₃ CO	-0.1243	-0.0584
COOH-	0.0122	0.1395	CH ₃ CHO	-0.1739	-0.0579
CO	-0.3875	-0.0424	CH ₃ CH ₂ OH	-0.1895	0.0542
CO-	0.0626	0.2654	OCHCH ₂	-0.1556	-0.0588
OCCO	-0.1991	-0.1703	HOCH ₂ CH ₂	-0.1176	0.0506
OCHCO	-0.2357	-0.1673	OCHCH ₃	-0.1707	-0.0797

Table S4. Gibbs free energy of the intermediates in CO₂RR to ethanol

intermediate	ΔG (Ha)
CO ₂	-188.6600
COOH-	-189.2200
CO	-113.3600
OCCO	-226.5900
OCHCO	-227.1800
CH ₃ CO	-153.2100
CH ₃ CHO	-153.8500
CH ₃ CH ₂ OH	-155.0400
OCHCH ₂	-153.2100
HOCH ₂ CH ₂	-154.3800