

Supporting information

Two-dimensional MOF-TM catalysts for electrocatalytic N₂ and CO₂ reduction: a DFT investigation

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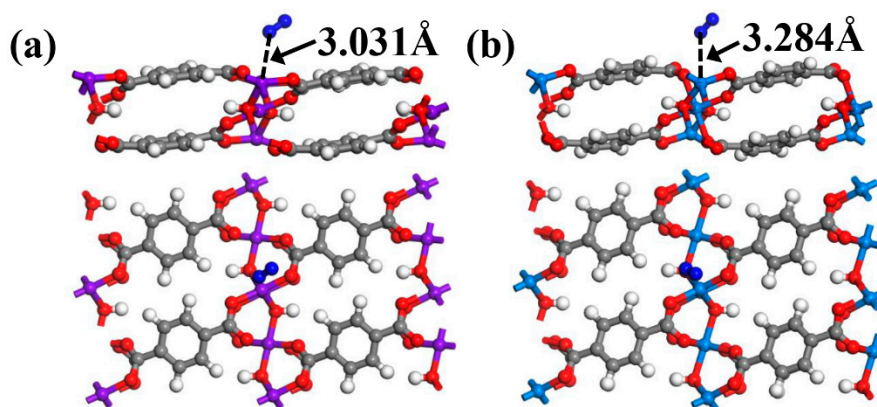


Figure S1. Side and top views of adsorption configurations for N₂ on (a) MOF-Cu, (b) MOF-Zn. Color cards: C: Grey, H: White, O: Red, Cu: Purple, Zn: Sky blue.

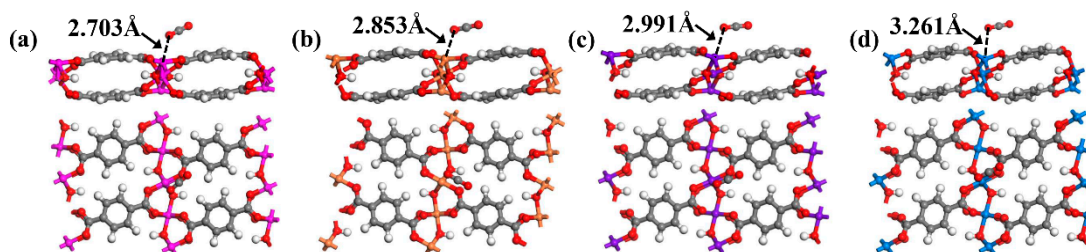
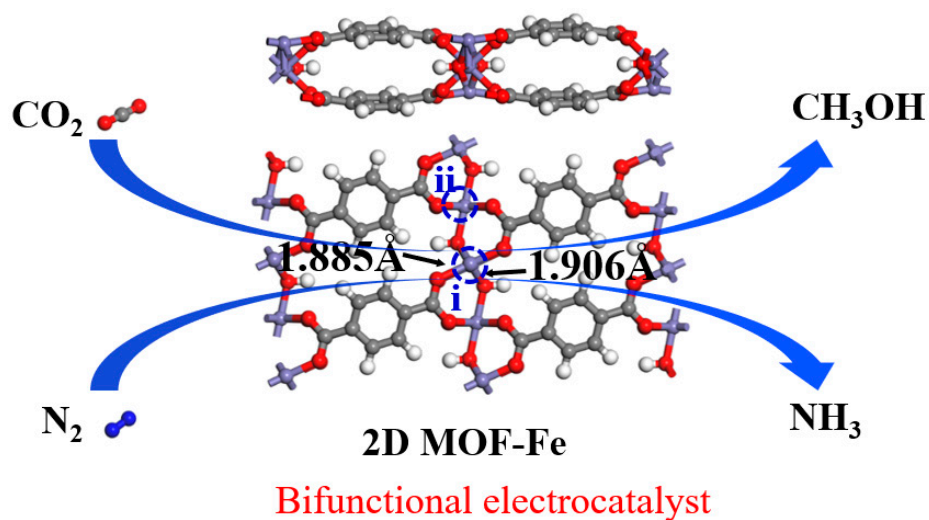


Figure S2. Side and top views of adsorption configurations for CO₂ on (a) MOF-Co, (b) MOF-Ni, (c) MOF-Cu, (d) MOF-Zn. Color cards: C: Grey, H: White, O: Red, Co: Pink, Ni: Orange, Cu: Purple, Zn: Sky blue.

2D MOF-Fe is a promising bifunctional electrocatalyst for CO₂RR to CH₃OH and NRR to NH₃.



The coordinate files of different MOF-TMs (TM = Fe, Co, Ni):

MOF-Fe

1.0

6.3337001801	0.0000000000	0.0000000000
1.2816613249	10.1269185323	0.0000000000
1.8305125602	-1.9231900066	22.3666639851

Fe	O	C	H
3	10	16	10

Direct

0.970230035	0.023870005	0.569270042
0.029769978	0.976129988	0.430729999
0.500000028	0.000000004	0.500000020
0.873099930	0.155400000	0.413000011
0.126899992	0.844600069	0.587000029
0.541470004	0.107630004	0.428529995
0.458529995	0.892370060	0.571470045
0.169429957	0.788869995	0.438669999
0.830569905	0.211130004	0.561330041
0.514699937	0.834399998	0.443300039
0.485299998	0.165600013	0.556700001
0.818769919	0.949430050	0.499030001
0.181230006	0.050570008	0.500970039
0.667469977	0.191530019	0.413330031
0.332530021	0.808470051	0.586670009
0.573399981	0.341500051	0.420000053
0.426599951	0.658499971	0.579999988
0.355129982	0.393370028	0.421670021

0.644869950	0.606629995	0.578330020
0.291399970	0.530500007	0.425000021
0.708599957	0.469500039	0.575000019
0.457629991	0.609270022	0.424670002
0.542369941	0.390730001	0.575330039
0.675330021	0.564470053	0.411670041
0.324669977	0.435530016	0.588330000
0.728670001	0.426930001	0.410330007
0.271330006	0.573070022	0.589670033
0.372869981	0.757629990	0.432330040
0.627129955	0.242370009	0.567670000
0.835129958	0.852830030	0.501559981
0.164869980	0.147170019	0.498440016
0.763989948	0.675490019	0.575970038
0.236009979	0.324510027	0.424030002
0.874670059	0.425480040	0.567640026
0.125330023	0.574519982	0.432360014
0.207649972	0.366809996	0.593030009
0.792350031	0.633190050	0.406970032
0.105109952	0.618380042	0.597710020
0.894889971	0.381620027	0.402290020

MOF-Co

1.0

6.3337001801	0.0000000000	0.0000000000
1.2816613249	10.1269185323	0.0000000000
1.8305125602	-1.9231900066	22.3666639851

Co O C H
3 10 16 10

Direct

0.970230035	0.023870005	0.569270042
0.029769978	0.976129988	0.430729999
0.500000028	0.000000004	0.500000020
0.873099930	0.155400000	0.413000011
0.126899992	0.844600069	0.587000029
0.541470004	0.107630004	0.428529995
0.458529995	0.892370060	0.571470045
0.169429957	0.788869995	0.438669999
0.830569905	0.211130004	0.561330041
0.514699937	0.834399998	0.443300039
0.485299998	0.165600013	0.556700001
0.818769919	0.949430050	0.499030001

0.181230006	0.050570008	0.500970039
0.667469977	0.191530019	0.413330031
0.332530021	0.808470051	0.586670009
0.573399981	0.341500051	0.420000053
0.426599951	0.658499971	0.579999988
0.355129982	0.393370028	0.421670021
0.644869950	0.606629995	0.578330020
0.291399970	0.530500007	0.425000021
0.708599957	0.469500039	0.575000019
0.457629991	0.609270022	0.424670002
0.542369941	0.390730001	0.575330039
0.675330021	0.564470053	0.411670041
0.324669977	0.435530016	0.588330000
0.728670001	0.426930001	0.410330007
0.271330006	0.573070022	0.589670033
0.372869981	0.757629990	0.432330040
0.627129955	0.242370009	0.567670000
0.835129958	0.852830030	0.501559981
0.164869980	0.147170019	0.498440016
0.763989948	0.675490019	0.575970038
0.236009979	0.324510027	0.424030002
0.874670059	0.425480040	0.567640026
0.125330023	0.574519982	0.432360014
0.207649972	0.366809996	0.593030009
0.792350031	0.633190050	0.406970032
0.105109952	0.618380042	0.597710020
0.894889971	0.381620027	0.402290020

MOF-Ni

1.0

6.3337001801	0.0000000000	0.0000000000
1.2816613249	10.1269185323	0.0000000000
1.8305125602	-1.9231900066	22.3666639851

Ni	O	C	H
3	10	16	10

Direct

0.970230035	0.023870005	0.569270042
0.029769978	0.976129988	0.430729999
0.500000028	0.000000004	0.500000020
0.873099930	0.155400000	0.413000011
0.126899992	0.844600069	0.587000029
0.541470004	0.107630004	0.428529995

0.458529995	0.892370060	0.571470045
0.169429957	0.788869995	0.438669999
0.830569905	0.211130004	0.561330041
0.514699937	0.834399998	0.443300039
0.485299998	0.165600013	0.556700001
0.818769919	0.949430050	0.499030001
0.181230006	0.050570008	0.500970039
0.667469977	0.191530019	0.413330031
0.332530021	0.808470051	0.586670009
0.573399981	0.341500051	0.420000053
0.426599951	0.658499971	0.579999988
0.355129982	0.393370028	0.421670021
0.644869950	0.606629995	0.578330020
0.291399970	0.530500007	0.425000021
0.708599957	0.469500039	0.575000019
0.457629991	0.609270022	0.424670002
0.542369941	0.390730001	0.575330039
0.675330021	0.564470053	0.411670041
0.324669977	0.435530016	0.588330000
0.728670001	0.426930001	0.410330007
0.271330006	0.573070022	0.589670033
0.372869981	0.757629990	0.432330040
0.627129955	0.242370009	0.567670000
0.835129958	0.852830030	0.501559981
0.164869980	0.147170019	0.498440016
0.763989948	0.675490019	0.575970038
0.236009979	0.324510027	0.424030002
0.874670059	0.425480040	0.567640026
0.125330023	0.574519982	0.432360014
0.207649972	0.366809996	0.593030009
0.792350031	0.633190050	0.406970032
0.105109952	0.618380042	0.597710020
0.894889971	0.381620027	0.402290020