

Supporting Information

Two-dimensional metal-organic frameworks $\text{TM}_3\text{C}_{12}\text{O}_{12}$ (TM= Mn, Co, Fe, Ni) as high-efficiency bifunctional electrocatalysts for water splitting

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Supplementary Figures

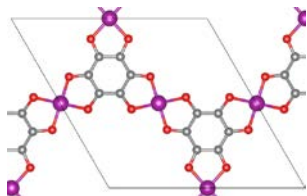
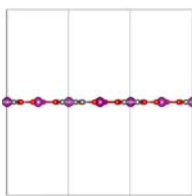
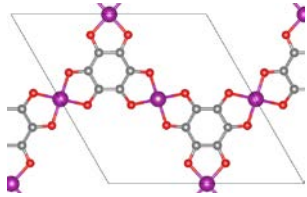
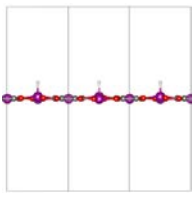
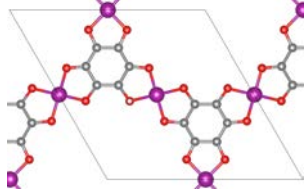
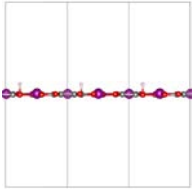
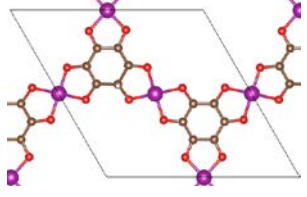
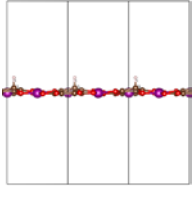
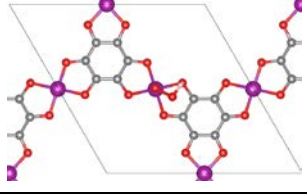
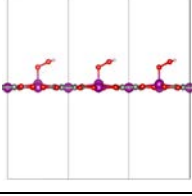
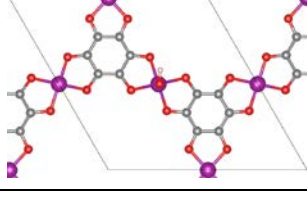
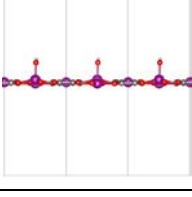
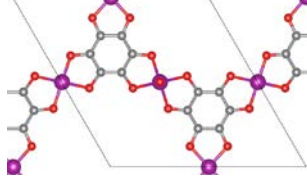
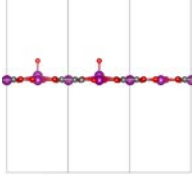
Materials	Adsorbate/ site	Top view	Side view
Mn-O-MOF	-		
Mn-O-MOF	H/ Mn		
Mn-O-MOF	H/ O		
Mn-O-MOF	H/ C		
Mn-O-MOF	OOH/Mn		
Mn-O-MOF	OH/Mn		
Mn-O-MOF	O/Mn		

Figure S1. The optimized top and side views of H, OOH, O, and OH on Mn-O MOF monolayer.

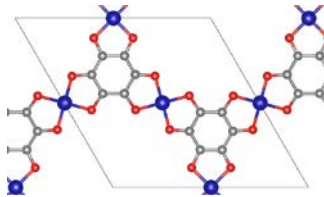
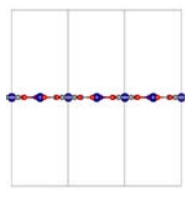
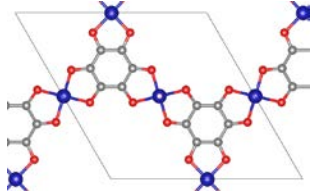
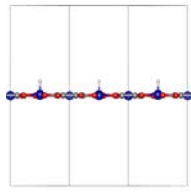
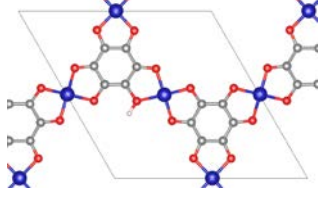
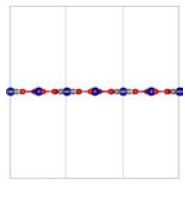
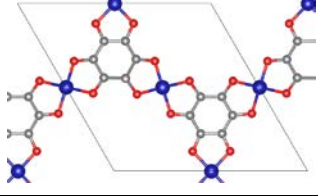
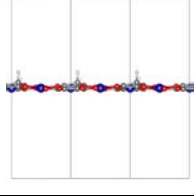
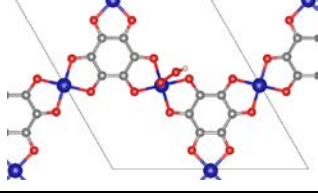
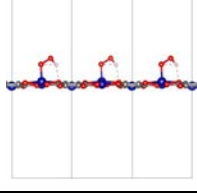
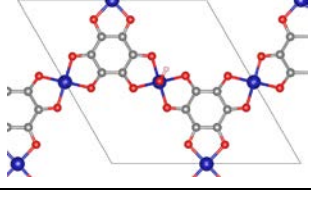
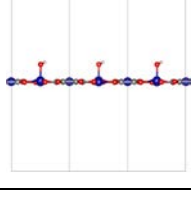
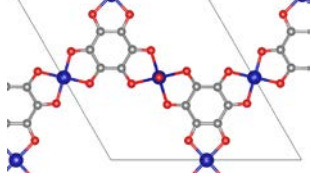
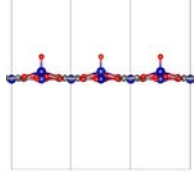
Materials	Adsorbate/ Site	Top view	Side view
Co-O-MOF	-		
Co-O-MOF	H/ Co		
Co-O-MOF	H/ O		
Co-O-MOF	H/C		
Co-O-MOF	OOH/Co		
Co-O-MOF	OH/Co		
Co-O-MOF	O/Co		

Figure S2. The optimized top and side views of H, OOH, O, and OH on Co-O MOF monolayer.

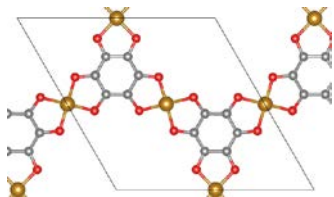

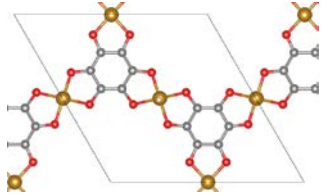
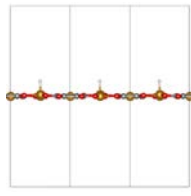
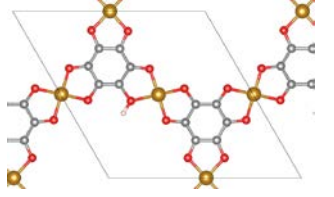

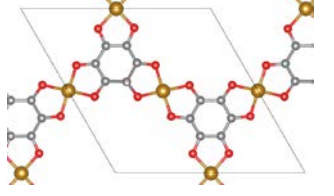

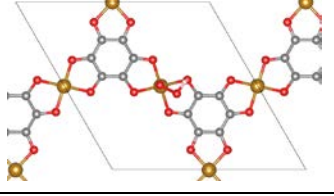

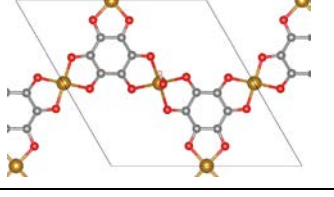
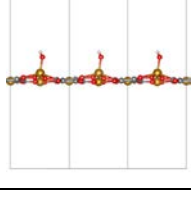
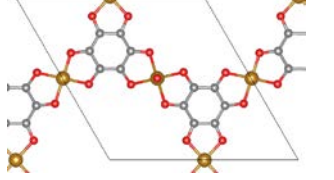
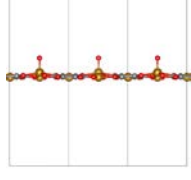
Materials	Adsorbate/ site	Top view	Side view
Fe-O-MOF	-		
Fe-O-MOF	H/ Fe		
Fe-O-MOF	H/ O		
Fe-O-MOF	H/C		
Fe-O-MOF	OOH/Fe		
Fe-O-MOF	OH/Fe		
Fe-O-MOF	O/Fe		

Figure S3. The optimized top and side views of H, OOH, O, and OH on Fe-O MOF monolayer.

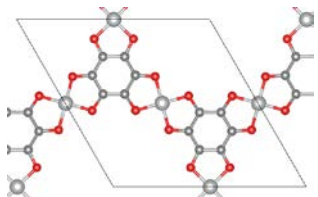
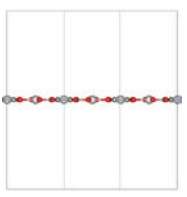
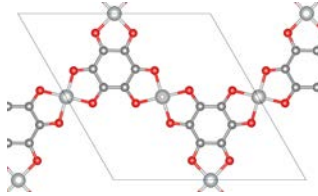
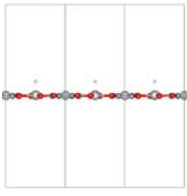
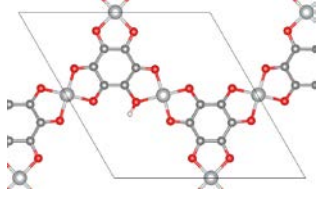

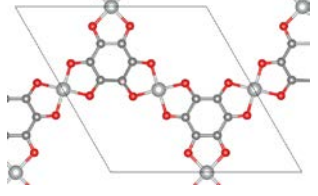
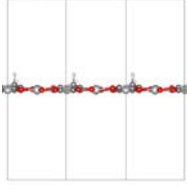
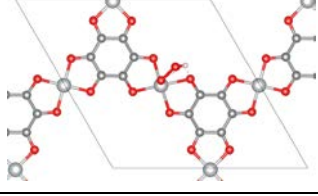
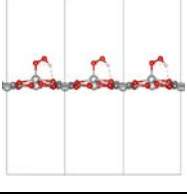
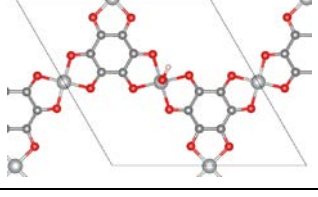
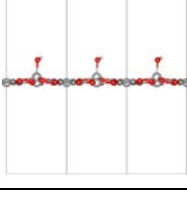
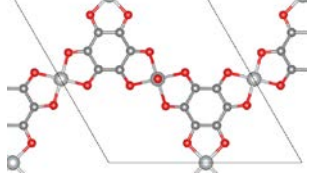
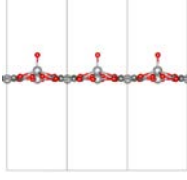
Materials	Adsorbate/ site	Top view	Side view
Ni-O-MOF	-		
Ni-O-MOF	H/ Ni		
Ni-O-MOF	H/ O		
Ni-O-MOF	H/C		
Ni-O-MOF	OOH/Ni		
Ni-O-MOF	OH/Ni		
Ni-O-MOF	O/Ni		

Figure S4. The optimized top and side views of H, OOH, O, and OH on Ni-O MOF monolayer.