

## Metal Organic Frameworks Bifunctional PGM-Free Electrocatalysts for Alkaline Electrolyzers- Trends in the Activity of Different Metal Centers

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# Authors contributed equally

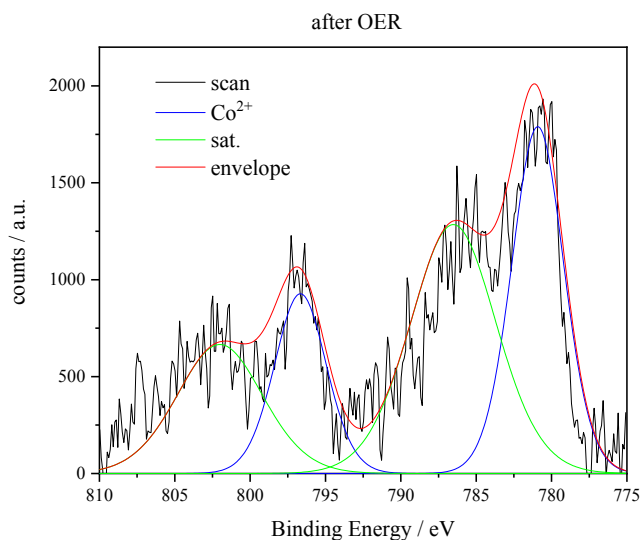
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## Supporting Information:

### Experimental Details:

#### Bulk Conductivity:

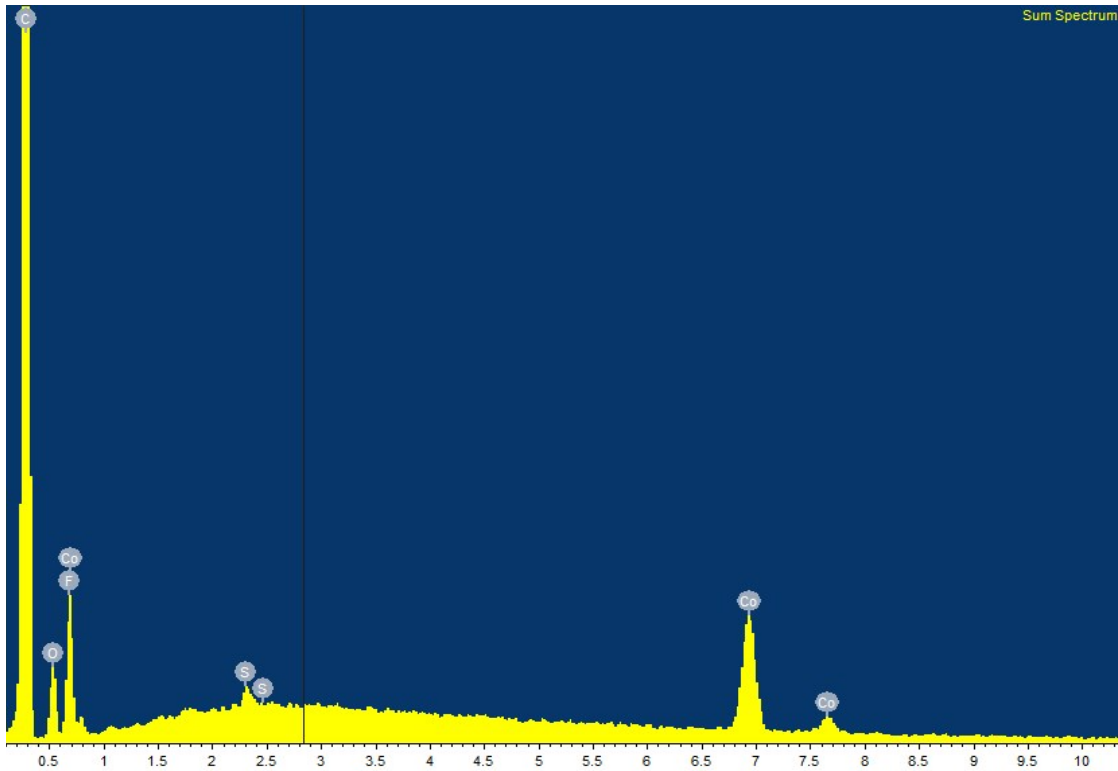
Electrical conductivity was measured using two probes as describe elsewhere.(1):(2) Pristine CoBTC MOF is not conductive as the other M-BTCs, while the CoBTC@AC composite presents conductivity of: 1.06 S/cm, which is in the same order of magnitude as the one of the activated carbon.



**Figure S1:** XPS high resolution spectrum of Co2p after OER.

**Table S1:** Metal wt% in the different MOF@AC composites by atomic absorption (AA).

MnBTC@AC	AA
CoBTC@AC	1.0% Co
CuBTC@AC	2.7% Cu
FeBTC@AC	1.9% Fe
MnBTC@AC	2.2% Mn



**Figure S2:** EDS graph of CoBTC@AC

### **Calculation of TOF**

The TOFs were calculated assuming every metal atom as an active site. Since that is not the case, because not all metal atoms are located at the surface, this TOF is an underestimate of the real numbers. The TOFs were calculated using the following equation: (3)

$$TOF = \frac{I}{z F n}$$

I is the measured current. It was chosen to use the current measured at  $\eta_{10}$  for all materials. z is the number of transferred electrons ( $z = 4$  for OER,  $z = 2$  for HER), F is the Faraday constant and n is the amount of active sites. 15  $\mu$ l of the slurry, containing 10 mg of material in 1 ml was used in every experiment. Only the metal was considered as active site, the amount of metal in the catalyst was measured with AA (see above).

### Computational Details:

For these calculations, we only considered Co based MOF structure. Initially, the bulk MOF cell parameters were relaxed, and take that structure to prepare the surfaces. We have examined 100, 010, 001 facets and found 010 facet is comparatively suitable for reactions since this surface provide Co sites to perform OER and HER. All slabs were separated from their periodic image by a minimum of 14 Å vacuum layers which converged the total energy up to 0.1 meV/atom.

OER mechanism:

$$\Delta G_A = E_A - E_{slab} - E_{H_2O} + (\Delta ZPE - T\Delta S)_A \quad 1$$

$$\Delta G_B = E_B - E_{slab} - 0.5(2E_{H_2O} + E_{H_2}) + (\Delta ZPE - T\Delta S)_B \quad 2$$

$$\Delta G_C = E_C - E_{slab} - E_{H_2O} + E_{H_2} + (\Delta ZPE - T\Delta S)_C \quad 3$$

$$\Delta G_D = E_D - E_{slab} - 2E_{H_2O} + 1.5E_{H_2} + (\Delta ZPE - T\Delta S)_D \quad 4$$

Here,  $\Delta G_A$ ,  $\Delta G_B$ ,  $\Delta G_C$ ,  $\Delta G_D$  are the adsorption free energies of  $H_2O$ , OH, O and OOH, respectively.  $E_A$ ,  $E_B$ ,  $E_C$ ,  $E_D$  are the energies of the cell with  $H_2O$ , OH, O, and OOH respectively.  $E_{slab}$  is the energy of bare slab.  $E_{H_2}$  and  $E_{H_2O}$  is the molecular energies of  $H_2$  and  $H_2O$  molecules, respectively.  $\Delta ZPE$  is the zero point energy corrections, T is the temperature and  $\Delta S$  is the correction in the entropy.  $(\Delta ZPE + T\Delta S)_A$ ,  $(\Delta ZPE + T\Delta S)_B$ ,  $(\Delta ZPE + T\Delta S)_C$ , and  $(\Delta ZPE + T\Delta S)_D$  are the total ZPE and entropy correction of cells with adsorbate  $H_2O$ , OH, O, and OOH, respectively.

**Table S2:** Adsorption free energies of Co-BTC of the intermediates of OER. A, B, C, and D belongs to  $H_2O$ , OH, O and OOH respectively.

	$\Delta ZPE + T\Delta S$	$\Delta G$ (in eV)	$\Delta G_{n+1} - \Delta G_n$ (in eV)	$\Delta G - \Delta G_A$ (in eV)
<b>Int A</b>	1.45	-0.05	1.64	0.00
<b>Int B</b>	0.81	1.59	1.62	1.64
<b>Int C</b>	0.29	3.21	0.81	3.26
<b>Int D</b>	0.86	4.03	0.41 (-4.49 eV from water)	4.08
				Overpotential = 0.52V

$$\text{Overpotential} = \text{Max} (\Delta G_{n+1} - \Delta G_n)_m - \text{Sum} \{(\Delta G_{n+1} - \Delta G_n)_m\} (2)/4 = 0.52V.$$

**Table S3:** Onsite Bader charge and magnetic moment of Co atoms in Co-BTC during OER. Co3 and Co4 are surface Co atoms, Co3 is active site.

	Co atoms	Bader charge	Magnetic moment	state
Bare	Co1	1.37	2.73	$Co^{+2}$
	Co2	1.37	2.74	$Co^{+2}$
	Co3	0.92	-3.72	$Co^{+1}$

	Co4	0.94	-2.82	Co <sup>+1</sup>
	Co5	1.38	2.63	Co <sup>+2</sup>
	Co6	1.36	2.71	Co <sup>+2</sup>
* (Int A)	Co1	1.39	2.664	Co <sup>+2</sup>
	Co2	1.47	4.451	Co <sup>+2</sup>
	Co3	1.12	1.902	Co <sup>+1</sup>
	Co4	1.00	-0.272	Co <sup>+1</sup>
	Co5	1.38	2.701	Co <sup>+2</sup>
	Co6	1.36	2.732	Co <sup>+2</sup>
OH* (Int B)	Co1	1.38	2.701	Co <sup>+2</sup>
	Co2	1.40	4.567	Co <sup>+2</sup>
	Co3	1.25	2.760	Co <sup>+2</sup>
	Co4	0.91	4.614	Co <sup>+1</sup>
	Co5	1.26	0.153	Co <sup>+2</sup>
	Co6	1.37	2.725	Co <sup>+2</sup>
O* (Int C)	Co1	1.38	2.898	Co <sup>+2</sup>
	Co2	1.33	4.544	Co <sup>+2</sup>
	Co3	1.28	-0.723	Co <sup>+2</sup>
	Co4	0.99	-0.357	Co <sup>+1</sup>
	Co5	1.37	2.727	Co <sup>+2</sup>
	Co6	1.36	2.734	Co <sup>+2</sup>
OOH* (Int D)	Co1	1.44	3.805	Co <sup>+2</sup>
	Co2	1.38	3.103	Co <sup>+2</sup>
	Co3	1.28	0.651	Co <sup>+2</sup>
	Co4	0.93	3.957	Co <sup>+1</sup>
	Co5	1.38	2.609	Co <sup>+2</sup>
	Co6	1.36	2.722	Co <sup>+2</sup>

## Cell Structures:

### Co-BTC (010) surface (Energy = -906.30 eV)

```

1.0000000000000000
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 0.0000000000000000  0.0000000000000000  27.8591003418000014

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Co C H O
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```

### Direct

```

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**Co-BTC (010) surface with adsorbate H<sub>2</sub>O (Energy = -922.03eV)**

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0.1133874060000000	16.0208981193000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8591003418000014

Co C H O  
6 36 62 49

**Direct**

0.9770600800000011	0.2598071990000008	0.2249760629999997
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0.4999212920000033 0.5000652669999965 0.0831126790000027  
0.0614085719999977 0.1568190010000023 0.3174063559999993  
0.9383441210000001 0.8432248829999978 0.3173042539999997  
0.5638307930000011 0.6556401249999979 0.0819045450000004  
0.4364179669999970 0.3443428579999974 0.0814566689999978  
0.9999768730000014 0.9999820589999970 0.0019998909999970  
0.4999208449999983 0.5000080470000015 0.2354428319999968  
0.9998882410000007 0.4999900760000031 0.1652990580000022  
0.4998027090000008 0.9999552969999996 0.4006827469999976  
0.9375131729999993 0.3670686480000001 0.0310961320000018  
0.0623712169999990 0.6330053809999967 0.0311354850000001  
0.4387206729999988 0.8684366940000032 0.2670844499999987  
0.5611772540000004 0.1318718489999995 0.2670611140000005  
0.0596904229999993 0.1321598290000026 0.4135732350000012  
0.9401937129999993 0.8677660230000015 0.4135861399999996  
0.5607756969999969 0.6319403649999984 0.1774236259999995  
0.4391508400000035 0.3680913749999988 0.1773986219999983  
0.9999580380000026 0.9999887350000023 0.2792407869999991  
0.4998762009999993 0.5001091959999968 0.0439108090000033  
0.8306207660000027 0.2181035580000028 0.1462713479999991  
0.1688741589999978 0.7818776370000009 0.1462032499999992  
0.3225767309999981 0.7155903580000000 0.3818738459999977  
0.6756923789999973 0.2839438319999985 0.3821518419999990  
0.7190305589999966 0.1486184899999969 0.1831301750000023  
0.2807203529999995 0.8514436480000001 0.1832464339999973  
0.2092459050000031 0.6446549300000015 0.4185250399999987  
0.7897146939999971 0.3554728029999978 0.4184935990000014  
0.3003934620000024 0.2564959230000028 0.1608191879999978  
0.6994223000000019 0.7435188290000028 0.1608156109999967  
0.8111053709999965 0.7558192609999992 0.3967204089999967  
0.1919220389999978 0.2438950840000018 0.3969373999999988  
0.3420973119999999 0.1879904420000003 0.2015535090000000  
0.6578039529999984 0.8120184539999968 0.2015855909999971  
0.8497351409999965 0.6839071509999997 0.4361634549999991



0.1522765759999984 0.3154894409999969 0.4365067179999969  
0.2132858630000030 0.3724642399999993 0.2695069910000001  
0.7864367959999967 0.6274604800000034 0.2694590090000020  
0.7075064180000012 0.8720538020000035 0.0346826760000027  
0.2926138340000008 0.1279311629999995 0.0346307229999994  
0.1228007079999998 0.3023084100000020 0.3048444690000025  
0.8773033020000014 0.6977565290000030 0.3048954610000010  
0.6099507209999970 0.8019502759999995 0.0664286760000010  
0.3900920150000005 0.1979961540000019 0.0664183570000034  
0.6124685999999997 0.3299386799999979 0.2536048589999993  
0.3871181609999965 0.6700429919999991 0.2535442710000027  
0.1109487940000022 0.8273982999999987 0.0183528889999991  
0.8897073859999978 0.1722955549999980 0.0184648990000014  
0.6657326819999980 0.2552209500000018 0.2891115549999981  
0.3340645130000013 0.7448794840000019 0.2891073230000032  
0.1693520099999972 0.7547253970000014 0.0520235369999966  
0.8308844570000034 0.2452244010000015 0.0521983359999965  
0.7526734469999994 0.9214147929999967 0.1527197059999992  
0.2471546379999978 0.0786011960000010 0.1527179779999983  
0.2546537220000005 0.4232364590000017 0.3886646030000023  
0.7451591490000027 0.5767476560000020 0.3886666599999984  
0.9792857770000012 0.8802869319999971 0.1556172219999965  
0.0204937760000021 0.1197364550000017 0.1556281299999966  
0.4949063059999972 0.8124108909999990 0.5403239729999996  
0.5278788210000016 0.7148041129999996 0.5403681399999982  
0.4776472149999975 0.3829000590000007 0.3907968400000001  
0.5215066080000028 0.6169919969999995 0.3906690780000019  
0.3856331409999996 0.9115512970000026 0.0695575100000028  
0.6142201420000006 0.0884339360000013 0.0695424970000005  
0.8827823999999964 0.4131442309999969 0.3049691319999965  
0.1171389820000002 0.5868664380000013 0.3049682079999982  
0.3680267330000007 0.9441835880000014 0.1221680049999989  
0.6318276519999984 0.0558234270000000 0.1221532080000003  
0.8756780619999986 0.4438043829999998 0.3581535519999974  
0.1244201140000030 0.5563067790000034 0.3581739959999979  
0.9531703589999978 0.3550057109999969 0.1770790670000011  
0.0465711650000031 0.6449035409999979 0.1770291779999980  
0.4466918999999976 0.8606428499999978 0.4113968010000022  
0.5521355870000022 0.1401916590000027 0.4114472269999965  
0.8626551030000016 0.2828180790000019 0.1113877450000018  
0.1372368339999994 0.7172822949999969 0.1113647889999996  
0.3648393750000025 0.7828034160000001 0.3467543129999981  
0.6345686909999984 0.2174481300000011 0.3472223280000009  
0.9949592950000010 0.5701668259999977 0.4210502509999969  
0.0044327499999994 0.4296206240000018 0.4210132959999981  
0.4958828689999990 0.0704118680000008 0.1855136309999992  
0.5040114520000003 0.9297710660000007 0.1855996700000020  
0.0167858949999982 0.1591325999999995 0.2731250229999986  
0.9830439090000027 0.8410292860000013 0.2730771009999984  
0.5253231530000022 0.6563351149999974 0.0376679040000027  
0.4745395180000003 0.3436554370000025 0.0379952449999976  
0.1265969130000002 0.2198244630000019 0.3411019440000018  
0.8732515570000032 0.7799587250000002 0.3410353960000023  
0.6275551319999977 0.7192263009999991 0.1055846659999986  
0.3722845910000032 0.2808490990000010 0.1055591329999999  
0.0423665160000013 0.0686356430000004 0.0180800329999968

0.9574307800000028	0.9313307399999999	0.0180562640000019
0.5376997589999988	0.5668926840000026	0.2599453930000024
0.4621558489999984	0.4330975410000022	0.2599750760000035
0.8450932499999979	0.1765643359999984	0.1759725810000035
0.1544682529999974	0.8232175110000028	0.1761128460000023
0.3332482870000035	0.6746397020000003	0.4117911160000034
0.6670035719999987	0.3245002029999995	0.4123266340000029
0.2637071309999968	0.2380150409999970	0.1945863369999969
0.7363259790000001	0.7618308070000026	0.1945806740000009
0.7836543319999976	0.7377939819999995	0.4311978819999993
0.2202557179999971	0.2622969749999982	0.4312607940000035
0.0890539589999975	0.3448120950000018	0.2791645819999999
0.9109126930000002	0.6552783249999976	0.2790426019999970
0.5804180499999987	0.8541587590000006	0.0477455219999996
0.4196598529999989	0.1457996669999986	0.0477079489999994
0.6881129149999978	0.2774573559999993	0.2563554640000021
0.3114002350000007	0.7226588730000003	0.2562983930000016
0.1778899729999992	0.7737545370000021	0.0186120179999989
0.8225409980000009	0.2261380549999998	0.0186692249999965
0.8833336229999986	0.9166719319999999	0.1368630830000015
0.1164331729999972	0.0834058820000010	0.1368901430000022
0.3810078200000007	0.4163324530000025	0.3714350460000020
0.6188163160000002	0.5835465790000001	0.3713651300000009
0.2915495929999992	0.9429396390000022	0.0919121949999990
0.7083261009999973	0.0570785439999995	0.0919087230000031
0.7964925770000022	0.4425200219999965	0.3285388350000034
0.2033362689999976	0.5571839810000014	0.3284929690000027
0.4931999149999982	0.7625563140000011	0.5199503300000003

**Co-BTC (010) surface with absorbate OH (Energy = -916.36eV)**

1.0000000000000000		
6.7042999268000001	0.0000000000000000	0.0000000000000000
0.1133874060000000	16.0208981193000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8591003418000014

Co C H O  
6 36 61 49

**Direct**

0.9770600800000011	0.2598071990000008	0.2249760629999997
0.0233121380000014	0.7404733899999982	0.2251123639999975
0.4953129889999985	0.7601102590000011	0.4478174150000029
0.5096244810000030	0.2394794969999978	0.4500997359999985
0.9999113679999994	0.9999951719999984	0.0931714179999972
0.5001361970000033	0.5001621250000028	0.3238323030000032
0.9650503399999977	0.4252223670000035	0.1021376400000022
0.0348498190000015	0.5747611520000007	0.1021379600000003
0.4632404740000027	0.9263975619999982	0.3367962239999969
0.5361987949999971	0.0739771499999975	0.3368288579999970
0.9999047519999991	0.4999978840000026	0.1262978020000034
0.4997616409999992	0.0001655889999981	0.3616590500000001

0.9998865129999999 0.5000103710000019 0.0302671919999966  
0.5000868440000019 0.0001879080000009 0.2614217400000030  
0.9643865820000030 0.4244711400000014 0.0512283300000007  
0.0354369430000006 0.5755851269999965 0.0512421800000027  
0.4653400480000016 0.9260637759999995 0.2866882679999989  
0.5346042509999975 0.0743082540000017 0.2866962550000025  
0.9251995090000023 0.3488172590000005 0.1316355909999984  
0.0749335140000014 0.6511988640000013 0.1317096949999979  
0.4221453070000010 0.8511965269999990 0.3662489060000027  
0.5768484470000033 0.1491249500000009 0.3663682640000019  
0.9998170140000013 0.4998101890000015 0.4413822590000009  
0.5000231860000000 0.0000890499999997 0.2075950059999982  
0.0321912360000027 0.0750105309999967 0.3432074790000001  
0.9675065879999991 0.9249608519999981 0.3432113229999985  
0.5315793159999984 0.5746478439999976 0.1081528220000010  
0.4682769180000008 0.4253672660000021 0.1081587449999972  
0.0341641079999988 0.0746338289999997 0.3938539330000026  
0.9656361939999982 0.9253204460000006 0.3938462730000012  
0.5335642699999994 0.5742611889999978 0.1580700430000022  
0.4663596449999972 0.4258180260000017 0.1580419240000026  
0.9998717309999989 0.9999821780000033 0.4162516000000025  
0.4999375940000022 0.5000005360000017 0.1831721659999985  
0.9998936650000019 0.9999836089999974 0.3183936180000018  
0.4999212920000033 0.5000652669999965 0.0831126790000027  
0.0614085719999977 0.1568190010000023 0.3174063559999993  
0.9383441210000001 0.8432248829999978 0.3173042539999997  
0.5638307930000011 0.6556401249999979 0.0819045450000004  
0.4364179669999970 0.3443428579999974 0.0814566689999978  
0.9999768730000014 0.9999820589999970 0.0019998909999970  
0.4999208449999983 0.5000080470000015 0.2354428319999968  
0.9998882410000007 0.4999900760000031 0.1652990580000022  
0.4998027090000008 0.9999552969999996 0.4006827469999976  
0.9375131729999993 0.3670686480000001 0.0310961320000018  
0.0623712169999990 0.6330053809999967 0.0311354850000001  
0.4387206729999988 0.8684366940000032 0.2670844499999987  
0.5611772540000004 0.1318718489999995 0.2670611140000005  
0.0596904229999993 0.1321598290000026 0.4135732350000012  
0.9401937129999993 0.8677660230000015 0.4135861399999996  
0.5607756969999969 0.6319403649999984 0.1774236259999995  
0.4391508400000035 0.3680913749999988 0.1773986219999983  
0.9999580380000026 0.9999887350000023 0.2792407869999991  
0.4998762009999993 0.5001091959999968 0.0439108090000033  
0.8306207660000027 0.2181035580000028 0.1462713479999991  
0.1688741589999978 0.7818776370000009 0.1462032499999992  
0.3225767309999981 0.7155903580000000 0.3818738459999977  
0.6756923789999973 0.2839438319999985 0.3821518419999990  
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0.2807203529999995 0.8514436480000001 0.1832464339999973  
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0.7897146939999971 0.3554728029999978 0.4184935990000014  
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0.1919220389999978 0.2438950840000018 0.3969373999999988  
0.3420973119999999 0.1879904420000003 0.2015535090000000  
0.6578039529999984 0.8120184539999968 0.2015855909999971

0.8497351409999965 0.6839071509999997 0.4361634549999991  
0.1522765759999984 0.3154894409999969 0.4365067179999969  
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0.7864367959999967 0.6274604800000034 0.2694590090000020  
0.7075064180000012 0.8720538020000035 0.0346826760000027  
0.2926138340000008 0.1279311629999995 0.0346307229999994  
0.1228007079999998 0.3023084100000020 0.3048444690000025  
0.8773033020000014 0.6977565290000030 0.3048954610000010  
0.6099507209999970 0.8019502759999995 0.0664286760000010  
0.3900920150000005 0.1979961540000019 0.0664183570000034  
0.6124685999999997 0.3299386799999979 0.2536048589999993  
0.3871181609999965 0.6700429919999991 0.2535442710000027  
0.1109487940000022 0.8273982999999987 0.0183528889999991  
0.8897073859999978 0.1722955549999980 0.0184648990000014  
0.6657326819999980 0.2552209500000018 0.2891115549999981  
0.3340645130000013 0.7448794840000019 0.2891073230000032  
0.1693520099999972 0.7547253970000014 0.0520235369999966  
0.8308844570000034 0.2452244010000015 0.0521983359999965  
0.7526734469999994 0.9214147929999967 0.1527197059999992  
0.2471546379999978 0.0786011960000010 0.1527179779999983  
0.2546537220000005 0.4232364590000017 0.3886646030000023  
0.7451591490000027 0.5767476560000020 0.3886666599999984  
0.9792857770000012 0.8802869319999971 0.1556172219999965  
0.0204937760000021 0.1197364550000017 0.1556281299999966  
0.5030587910000008 0.7101372480000023 0.5324010249999986  
0.4776472149999975 0.3829000590000007 0.3907968400000001  
0.5215066080000028 0.6169919969999995 0.3906690780000019  
0.3856331409999996 0.9115512970000026 0.0695575100000028  
0.6142201420000006 0.0884339360000013 0.0695424970000005  
0.8827823999999964 0.4131442309999969 0.3049691319999965  
0.1171389820000002 0.5868664380000013 0.3049682079999982  
0.3680267330000007 0.9441835880000014 0.1221680049999989  
0.6318276519999984 0.0558234270000000 0.1221532080000003  
0.8756780619999986 0.4438043829999998 0.3581535519999974  
0.1244201140000030 0.5563067790000034 0.3581739959999979  
0.9531703589999978 0.3550057109999969 0.1770790670000011  
0.0465711650000031 0.6449035409999979 0.1770291779999980  
0.4466918999999976 0.8606428499999978 0.4113968010000022  
0.5521355870000022 0.1401916590000027 0.4114472269999965  
0.8626551030000016 0.2828180790000019 0.1113877450000018  
0.1372368339999994 0.7172822949999969 0.1113647889999996  
0.3648393750000025 0.7828034160000001 0.3467543129999981  
0.6345686909999984 0.2174481300000011 0.3472223280000009  
0.9949592950000010 0.5701668259999977 0.4210502509999969  
0.0044327499999994 0.4296206240000018 0.4210132959999981  
0.4958828689999990 0.0704118680000008 0.1855136309999992  
0.5040114520000003 0.9297710660000007 0.1855996700000020  
0.0167858949999982 0.1591325999999995 0.2731250229999986  
0.9830439090000027 0.8410292860000013 0.2730771009999984  
0.5253231530000022 0.6563351149999974 0.0376679040000027  
0.4745395180000003 0.3436554370000025 0.0379952449999976  
0.1265969130000002 0.2198244630000019 0.3411019440000018  
0.8732515570000032 0.7799587250000002 0.3410353960000023  
0.6275551319999977 0.7192263009999991 0.1055846659999986  
0.3722845910000032 0.2808490990000010 0.1055591329999999  
0.0423665160000013 0.0686356430000004 0.0180800329999968

0.9574307800000028	0.9313307399999999	0.0180562640000019
0.5376997589999988	0.5668926840000026	0.2599453930000024
0.4621558489999984	0.4330975410000022	0.2599750760000035
0.8450932499999979	0.1765643359999984	0.1759725810000035
0.1544682529999974	0.8232175110000028	0.1761128460000023
0.3332482870000035	0.6746397020000003	0.4117911160000034
0.6670035719999987	0.3245002029999995	0.4123266340000029
0.2637071309999968	0.2380150409999970	0.1945863369999969
0.7363259790000001	0.7618308070000026	0.1945806740000009
0.7836543319999976	0.7377939819999995	0.4311978819999993
0.2202557179999971	0.2622969749999982	0.4312607940000035
0.0890539589999975	0.3448120950000018	0.2791645819999999
0.9109126930000002	0.6552783249999976	0.2790426019999970
0.5804180499999987	0.8541587590000006	0.0477455219999996
0.4196598529999989	0.1457996669999986	0.0477079489999994
0.6881129149999978	0.2774573559999993	0.2563554640000021
0.3114002350000007	0.7226588730000003	0.2562983930000016
0.1778899729999992	0.7737545370000021	0.0186120179999989
0.8225409980000009	0.2261380549999998	0.0186692249999965
0.8833336229999986	0.9166719319999999	0.1368630830000015
0.1164331729999972	0.0834058820000010	0.1368901430000022
0.3810078200000007	0.4163324530000025	0.3714350460000020
0.6188163160000002	0.5835465790000001	0.3713651300000009
0.2915495929999992	0.9429396390000022	0.0919121949999990
0.7083261009999973	0.0570785439999995	0.0919087230000031
0.7964925770000022	0.4425200219999965	0.3285388350000034
0.2033362689999976	0.5571839810000014	0.3284929690000027
0.4933681190000030	0.7623615859999973	0.5142083759999991

**Co-BTC (010) surface with absorbate O (Energy = -914.21eV)**

1.00000000000000		
6.7042999268000001	0.0000000000000000	0.0000000000000000
0.1133874060000000	16.0208981193000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8591003418000014

Co C H O  
6 36 60 49

**Direct**

0.9770600800000011	0.2598071990000008	0.2249760629999997
0.0233121380000014	0.7404733899999982	0.2251123639999975
0.4953129889999985	0.7601102590000011	0.4478174150000029
0.5096244810000030	0.2394794969999978	0.4500997359999985
0.9999113679999994	0.9999951719999984	0.0931714179999972
0.5001361970000033	0.5001621250000028	0.3238323030000032
0.9650503399999977	0.4252223670000035	0.1021376400000022
0.0348498190000015	0.5747611520000007	0.1021379600000003
0.4632404740000027	0.9263975619999982	0.3367962239999969
0.5361987949999971	0.0739771499999975	0.3368288579999970
0.9999047519999991	0.4999978840000026	0.1262978020000034
0.4997616409999992	0.0001655889999981	0.3616590500000001

0.9998865129999999 0.5000103710000019 0.0302671919999966  
0.5000868440000019 0.0001879080000009 0.2614217400000030  
0.9643865820000030 0.4244711400000014 0.0512283300000007  
0.0354369430000006 0.5755851269999965 0.0512421800000027  
0.4653400480000016 0.9260637759999995 0.2866882679999989  
0.5346042509999975 0.0743082540000017 0.2866962550000025  
0.9251995090000023 0.3488172590000005 0.1316355909999984  
0.0749335140000014 0.6511988640000013 0.1317096949999979  
0.4221453070000010 0.8511965269999990 0.3662489060000027  
0.5768484470000033 0.1491249500000009 0.3663682640000019  
0.9998170140000013 0.4998101890000015 0.4413822590000009  
0.5000231860000000 0.0000890499999997 0.2075950059999982  
0.0321912360000027 0.0750105309999967 0.3432074790000001  
0.9675065879999991 0.9249608519999981 0.3432113229999985  
0.5315793159999984 0.5746478439999976 0.1081528220000010  
0.4682769180000008 0.4253672660000021 0.1081587449999972  
0.0341641079999988 0.0746338289999997 0.3938539330000026  
0.9656361939999982 0.9253204460000006 0.3938462730000012  
0.5335642699999994 0.5742611889999978 0.1580700430000022  
0.4663596449999972 0.4258180260000017 0.1580419240000026  
0.9998717309999989 0.9999821780000033 0.4162516000000025  
0.4999375940000022 0.5000005360000017 0.1831721659999985  
0.9998936650000019 0.9999836089999974 0.3183936180000018  
0.4999212920000033 0.5000652669999965 0.0831126790000027  
0.0614085719999977 0.1568190010000023 0.3174063559999993  
0.9383441210000001 0.8432248829999978 0.3173042539999997  
0.5638307930000011 0.6556401249999979 0.0819045450000004  
0.4364179669999970 0.3443428579999974 0.0814566689999978  
0.9999768730000014 0.9999820589999970 0.0019998909999970  
0.4999208449999983 0.5000080470000015 0.2354428319999968  
0.9998882410000007 0.4999900760000031 0.1652990580000022  
0.4998027090000008 0.9999552969999996 0.4006827469999976  
0.9375131729999993 0.3670686480000001 0.0310961320000018  
0.0623712169999990 0.6330053809999967 0.0311354850000001  
0.4387206729999988 0.8684366940000032 0.2670844499999987  
0.5611772540000004 0.1318718489999995 0.2670611140000005  
0.0596904229999993 0.1321598290000026 0.4135732350000012  
0.9401937129999993 0.8677660230000015 0.4135861399999996  
0.5607756969999969 0.6319403649999984 0.1774236259999995  
0.4391508400000035 0.3680913749999988 0.1773986219999983  
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0.4998762009999993 0.5001091959999968 0.0439108090000033  
0.8306207660000027 0.2181035580000028 0.1462713479999991  
0.1688741589999978 0.7818776370000009 0.1462032499999992  
0.3225767309999981 0.7155903580000000 0.3818738459999977  
0.6756923789999973 0.2839438319999985 0.3821518419999990  
0.7190305589999966 0.1486184899999969 0.1831301750000023  
0.2807203529999995 0.8514436480000001 0.1832464339999973  
0.2092459050000031 0.6446549300000015 0.4185250399999987  
0.7897146939999971 0.3554728029999978 0.4184935990000014  
0.3003934620000024 0.2564959230000028 0.1608191879999978  
0.6994223000000019 0.7435188290000028 0.1608156109999967  
0.8111053709999965 0.7558192609999992 0.3967204089999967  
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0.3420973119999999 0.1879904420000003 0.2015535090000000  
0.6578039529999984 0.8120184539999968 0.2015855909999971

0.8497351409999965 0.6839071509999997 0.4361634549999991  
0.1522765759999984 0.3154894409999969 0.4365067179999969  
0.2132858630000030 0.3724642399999993 0.2695069910000001  
0.7864367959999967 0.6274604800000034 0.2694590090000020  
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0.2926138340000008 0.1279311629999995 0.0346307229999994  
0.1228007079999998 0.3023084100000020 0.3048444690000025  
0.8773033020000014 0.6977565290000030 0.3048954610000010  
0.6099507209999970 0.8019502759999995 0.0664286760000010  
0.3900920150000005 0.1979961540000019 0.0664183570000034  
0.6124685999999997 0.3299386799999979 0.2536048589999993  
0.3871181609999965 0.6700429919999991 0.2535442710000027  
0.1109487940000022 0.8273982999999987 0.0183528889999991  
0.8897073859999978 0.1722955549999980 0.0184648990000014  
0.6657326819999980 0.2552209500000018 0.2891115549999981  
0.3340645130000013 0.7448794840000019 0.2891073230000032  
0.1693520099999972 0.7547253970000014 0.0520235369999966  
0.8308844570000034 0.2452244010000015 0.0521983359999965  
0.7526734469999994 0.9214147929999967 0.1527197059999992  
0.2471546379999978 0.0786011960000010 0.1527179779999983  
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0.7451591490000027 0.5767476560000020 0.3886666599999984  
0.9792857770000012 0.8802869319999971 0.1556172219999965  
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0.4776472149999975 0.3829000590000007 0.3907968400000001  
0.5215066080000028 0.6169919969999995 0.3906690780000019  
0.3856331409999996 0.9115512970000026 0.0695575100000028  
0.6142201420000006 0.0884339360000013 0.0695424970000005  
0.8827823999999964 0.4131442309999969 0.3049691319999965  
0.1171389820000002 0.5868664380000013 0.3049682079999982  
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0.6318276519999984 0.0558234270000000 0.1221532080000003  
0.8756780619999986 0.4438043829999998 0.3581535519999974  
0.1244201140000030 0.5563067790000034 0.3581739959999979  
0.9531703589999978 0.3550057109999969 0.1770790670000011  
0.0465711650000031 0.6449035409999979 0.1770291779999980  
0.4466918999999976 0.8606428499999978 0.4113968010000022  
0.5521355870000022 0.1401916590000027 0.4114472269999965  
0.8626551030000016 0.2828180790000019 0.1113877450000018  
0.1372368339999994 0.7172822949999969 0.1113647889999996  
0.3648393750000025 0.7828034160000001 0.3467543129999981  
0.6345686909999984 0.2174481300000011 0.3472223280000009  
0.9949592950000010 0.5701668259999977 0.4210502509999969  
0.0044327499999994 0.4296206240000018 0.4210132959999981  
0.4958828689999990 0.0704118680000008 0.1855136309999992  
0.5040114520000003 0.9297710660000007 0.1855996700000020  
0.0167858949999982 0.1591325999999995 0.2731250229999986  
0.9830439090000027 0.8410292860000013 0.2730771009999984  
0.5253231530000022 0.6563351149999974 0.0376679040000027  
0.4745395180000003 0.3436554370000025 0.0379952449999976  
0.1265969130000002 0.2198244630000019 0.3411019440000018  
0.8732515570000032 0.7799587250000002 0.3410353960000023  
0.6275551319999977 0.7192263009999991 0.1055846659999986  
0.3722845910000032 0.2808490990000010 0.1055591329999999  
0.0423665160000013 0.0686356430000004 0.0180800329999968  
0.9574307800000028 0.9313307399999999 0.0180562640000019

0.5376997589999988	0.5668926840000026	0.2599453930000024
0.4621558489999984	0.4330975410000022	0.2599750760000035
0.8450932499999979	0.1765643359999984	0.1759725810000035
0.1544682529999974	0.8232175110000028	0.1761128460000023
0.3332482870000035	0.6746397020000003	0.4117911160000034
0.6670035719999987	0.3245002029999995	0.4123266340000029
0.2637071309999968	0.2380150409999970	0.1945863369999969
0.7363259790000001	0.7618308070000026	0.1945806740000009
0.7836543319999976	0.7377939819999995	0.4311978819999993
0.2202557179999971	0.2622969749999982	0.4312607940000035
0.0890539589999975	0.3448120950000018	0.2791645819999999
0.9109126930000002	0.6552783249999976	0.2790426019999970
0.5804180499999987	0.8541587590000006	0.0477455219999996
0.4196598529999989	0.1457996669999986	0.0477079489999994
0.6881129149999978	0.2774573559999993	0.2563554640000021
0.3114002350000007	0.7226588730000003	0.2562983930000016
0.1778899729999992	0.7737545370000021	0.0186120179999989
0.8225409980000009	0.2261380549999998	0.0186692249999965
0.8833336229999986	0.9166719319999999	0.1368630830000015
0.1164331729999972	0.0834058820000010	0.1368901430000022
0.3810078200000007	0.4163324530000025	0.3714350460000020
0.6188163160000002	0.5835465790000001	0.3713651300000009
0.2915495929999992	0.9429396390000022	0.0919121949999990
0.7083261009999973	0.0570785439999995	0.0919087230000031
0.7964925770000022	0.4425200219999965	0.3285388350000034
0.2033362689999976	0.5571839810000014	0.3284929690000027
0.4939568039999997	0.7616800070000025	0.4941115379999985

**Co-BTC (010) surface with absorbate OOH (Energy = -921.42eV)**

1.0000000000000000		
6.7042999268000001	0.0000000000000000	0.0000000000000000
0.1133874060000000	16.0208981193000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	27.8591003418000014

Co C H O  
6 36 61 50

Direct

0.9770600800000011	0.2598071990000008	0.2249760629999997
0.0233121380000014	0.7404733899999982	0.2251123639999975
0.4953129889999985	0.7601102590000011	0.4478174150000029
0.5096244810000030	0.2394794969999978	0.4500997359999985
0.9999113679999994	0.9999951719999984	0.0931714179999972
0.5001361970000033	0.5001621250000028	0.3238323030000032
0.9650503399999977	0.4252223670000035	0.1021376400000022
0.0348498190000015	0.5747611520000007	0.1021379600000003
0.4632404740000027	0.9263975619999982	0.3367962239999969
0.5361987949999971	0.0739771499999975	0.3368288579999970
0.9999047519999991	0.4999978840000026	0.1262978020000034
0.4997616409999992	0.0001655889999981	0.3616590500000001



0.9998865129999999 0.5000103710000019 0.0302671919999966  
0.5000868440000019 0.0001879080000009 0.2614217400000030  
0.9643865820000030 0.4244711400000014 0.0512283300000007  
0.0354369430000006 0.5755851269999965 0.0512421800000027  
0.4653400480000016 0.9260637759999995 0.2866882679999989  
0.5346042509999975 0.0743082540000017 0.2866962550000025  
0.9251995090000023 0.3488172590000005 0.1316355909999984  
0.0749335140000014 0.6511988640000013 0.1317096949999979  
0.4221453070000010 0.8511965269999990 0.3662489060000027  
0.5768484470000033 0.1491249500000009 0.3663682640000019  
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0.5315793159999984 0.5746478439999976 0.1081528220000010  
0.4682769180000008 0.4253672660000021 0.1081587449999972  
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0.5335642699999994 0.5742611889999978 0.1580700430000022  
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0.4999375940000022 0.5000005360000017 0.1831721659999985  
0.9998936650000019 0.9999836089999974 0.3183936180000018  
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0.4364179669999970 0.3443428579999974 0.0814566689999978  
0.9999768730000014 0.9999820589999970 0.0019998909999970  
0.4999208449999983 0.5000080470000015 0.2354428319999968  
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0.0596904229999993 0.1321598290000026 0.4135732350000012  
0.9401937129999993 0.8677660230000015 0.4135861399999996  
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0.1109487940000022 0.8273982999999987 0.0183528889999991  
0.8897073859999978 0.1722955549999980 0.0184648990000014  
0.6657326819999980 0.2552209500000018 0.2891115549999981  
0.3340645130000013 0.7448794840000019 0.2891073230000032  
0.1693520099999972 0.7547253970000014 0.0520235369999966  
0.8308844570000034 0.2452244010000015 0.0521983359999965  
0.7526734469999994 0.9214147929999967 0.1527197059999992  
0.2471546379999978 0.0786011960000010 0.1527179779999983  
0.2546537220000005 0.4232364590000017 0.3886646030000023  
0.7451591490000027 0.5767476560000020 0.3886666599999984  
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0.8756780619999986 0.4438043829999998 0.3581535519999974  
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0.8626551030000016 0.2828180790000019 0.1113877450000018  
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0.3648393750000025 0.7828034160000001 0.3467543129999981  
0.6345686909999984 0.2174481300000011 0.3472223280000009  
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0.0044327499999994 0.4296206240000018 0.4210132959999981  
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0.5040114520000003 0.9297710660000007 0.1855996700000020  
0.0167858949999982 0.1591325999999995 0.2731250229999986  
0.9830439090000027 0.8410292860000013 0.2730771009999984  
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0.1265969130000002 0.2198244630000019 0.3411019440000018  
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0.5376997589999988 0.5668926840000026 0.2599453930000024  
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0.8450932499999979 0.1765643359999984 0.1759725810000035  
0.1544682529999974 0.8232175110000028 0.1761128460000023  
0.3332482870000035 0.6746397020000003 0.4117911160000034  
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0.2637071309999968 0.2380150409999970 0.1945863369999969  
0.7363259790000001 0.7618308070000026 0.1945806740000009  
0.7836543319999976 0.7377939819999995 0.4311978819999993  
0.2202557179999971 0.2622969749999982 0.4312607940000035  
0.0890539589999975 0.3448120950000018 0.2791645819999999  
0.9109126930000002 0.6552783249999976 0.2790426019999970  
0.5804180499999987 0.8541587590000006 0.0477455219999996  
0.4196598529999989 0.1457996669999986 0.0477079489999994  
0.6881129149999978 0.2774573559999993 0.2563554640000021  
0.3114002350000007 0.7226588730000003 0.2562983930000016  
0.1778899729999992 0.7737545370000021 0.0186120179999989  
0.8225409980000009 0.2261380549999998 0.0186692249999965  
0.8833336229999986 0.9166719319999999 0.1368630830000015  
0.1164331729999972 0.0834058820000010 0.1368901430000022  
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0.6188163160000002 0.5835465790000001 0.3713651300000009  
0.2915495929999992 0.9429396390000022 0.0919121949999990  
0.7083261009999973 0.0570785439999995 0.0919087230000031  
0.7964925770000022 0.4425200219999965 0.3285388350000034  
0.2033362689999976 0.5571839810000014 0.3284929690000027  
0.4931999149999982 0.7625563140000011 0.5199503300000003  
0.4923161569999976 0.8330591320000025 0.5423172710000017

**Co-BTC (010) surface with absorbate H (Energy = -909.58eV)**

1.0000000000000000  
6.7042999268000001 0.0000000000000000 0.0000000000000000  
0.1133874060000000 16.0208981193000000 0.0000000000000000  
0.0000000000000000 0.0000000000000000 27.8591003418000014

Co C H O  
6 36 61 48

Direct

0.9774245590088830 0.2593219836314903 0.2256105103176932  
0.0221001037537946 0.7404701644603587 0.2256169023834948  
0.5067042961227669 0.7599631423635969 0.4468812716470280  
0.4984366198652727 0.2410646399035093 0.4526629847670197  
0.9997896179994006 0.0001160511150941 0.0993049817787585  
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