Supplemental Information for:

Rhodizonic Acid on Noble Metals: Surface Reactivity and Coordination Chemistry

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Vacuum Dehydration Procedure

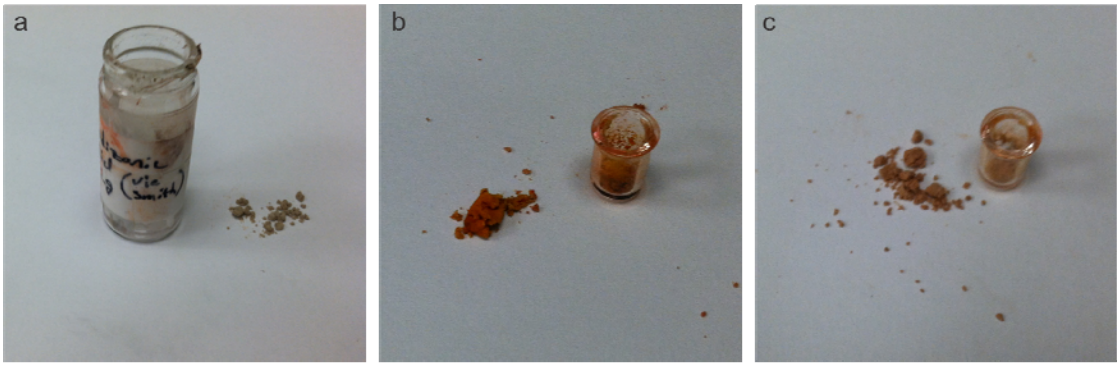


Figure S1. (a) Dihydrate rhodizonic acid, image taken before vacuum dehydration procedure. (b) Rhodizonic acid after heating the molecules shown to approximately 140°C for six hours in ultra high vacuum. (c) 90 minutes after being removed from vacuum the rhodizonic acid is transforming back into dihydrate rhodizonic acid, with concomitant color change.

We monitored the color of the rhodizonic acid powder carefully, to compare with colors reported in the literature (Figure S1). The color of the dihydrate RA, which is typically present under ambient conditions, has been described in the literature as colorless [s1]. De-hydration of the dihydrate rhodizonic acid has been reported to occur upon heating the molecules to approximately 140°C for six hours in vacuum. Characteristic for the dehydrated form of RA is a deep orange hue, as reported in [s2]. The image in figure S1b was taken promptly after being removed from the vacuum chamber. After being removed from vacuum the rhodizonic acid is transforming back into dihydrate rhodizonic acid by adsorbing water vapor from the atmosphere. Concomittantly, the orange tone fades slowly back to colorless. The picture in figure S1c has been taken 90 minutes after removal from vacuum. The rhodizonate ion, discussed in the main article, has a reported deep yellow color [s3].

[s1] Patton, E.; West, R. New Aromatic Anions. VIII. Acidity Constants of Rhodizonic Acid. *J. Phys. Chem.* **1970**, *74* (12), 2512-2518.
[s2] Braga, D.; Cojazzi, G.; Maini, L.; Greponi, F. Reversible Solid-State Interconversion of Rhodizonic Acid $H_2C_6O_6$ into $H_6C_6O_8$ and the Solid-State Structure of the Rhodizonate Dianion $C_6O_6^{-2}$ (Aromatic or Non-aromatic?), *New J. Chem.* **2001**, *25*, 1221-1223.
[s3] Preisler, P. W.; Berger, L.; Hill, E. S. Oxidation-Reduction Potentials of Thiol-Dithio Systems: Thiourea-Formamidine Disulfide, *J. Am. Chem. Soc*. **1947**, *69* (2), 326–329.

Computational Details

All of the results reported in the main text were obtained from surface models which used two-layer 2D Cu(111) or Au(111) slab models with the organic network adsorbed onto only one face, the other face is left exposed to a vacuum measuring at least 20 Å. All of the cells were hexagonal and a dipole correction was applied along the direction perpendicular to the metal surface (using the IDIPOL tag in VASP). Preliminary calculations using four-layer slabs were performed with RA monomers and are reported in this SI. All of the Cu slabs on which the MOCN networks were adsorbed were built from a bulk fcc lattice with the experimental 3.61 Å lattice constant. For the Au slabs, both the experimental lattice constant (4.08 Å) and the optimal vdW-DF2 lattice constant (4.35 Å) were used with the RA networks and their corresponding hydrated networks. Although the changes in binding energies and slight shifts in some peaks of their site-projected densities of state are to be expected, the asymmetric profile of the PDOS peaks as discussed in the main text and the computed hydration reaction energies were unaffected.

From the main text:

> (Periodic) "Density Functional Theory (DFT) calculations (geometry optimizations, electronic densities of states, charge densities) were performed using the Vienna Ab–initio Simulation Package (VASP) version 5.2.11. The projector augmented wave (PAW) method was used to treat the core states along with a plane–wave energy cutoff of 500 eV, and the C/N/O 2s/2p, H 1s and Au 6s/5d electrons were treated explicitly. The non–local correlation functional of Langreth and Lundqvist (vdW–DF2) was employed to account for the dispersion interactions."

The G-centered Monkhorst–Pack scheme was used to generate k-point grids for various RA networks. A 3x3x1 grid was used for the gas-phase optimizations/scans (reported in this SI and referenced in the main text) and 7x7x1 grids were used to produce all of the DOS/PDOS plots and charge densities. The PDOS curves were smoothed slightly by applying running averages over 0.003 eV energy windows to improve visibility. In cases where relative energies were reported, they were compared with the results from 5x5x1 grids and found to vary by less than 2 meV/atom. The surface-adsorbed RA network geometries were initially converged using a 3x3x1 k-point grid and then raised to 5x5x1 and 7x7x1 grids. In the optimized structures, the magnitude of the largest force acting on the optimized atoms was less than 0.05 eV/Å.

The molecular calculations performed on the Cu-/Au- substituted molecular fragments (RA dimers and trimers) were performed using the ADF molecular program [s4]. The revPBE functional with the Grimme DFT-D3 dispersion correction were used with the TZP basis set from the ADF basis set library; the frozen core approximation was used for the Cu and Au atoms with the Cu.3p and Au.4f entries in the library. Scalar relativistic effects (using ZORA) [s5] were included.

[s4] ADF2012, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com

[s5] van Lenthe, E.; Baerends, E. J.; Snijders. J. G. Relativistic Regular Two-component Hamiltonians. *J. Chem. Phys.* **1993**, *99*, 4597.

RA monomers

Rhodizonic acid (RA) has three possible conformers when considering the rotation of the hydroxyl groups (Figure S2). Using DFT-D3, it was determined that the relative energy of the monomers, in the gas phase, was 0, 5.5, and 20.4 kcal/mol for monomer i, monomer ii, and monomer iii.

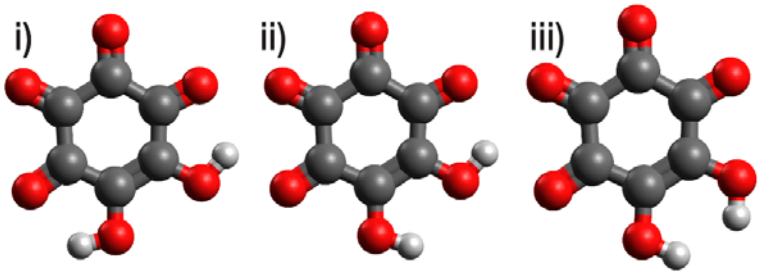


Figure S2: Conformers of rhodizonic acid.

Frontier Orbitals of Various RA Species

The calculated spatial distribution of the frontier orbitals of the RA molecules in three different conformations (Monomers i-iii) and a deprotonated RA molecule (Monomer iv). The MOs of monomer iv no longer has a "crescent shaped" topology, like that of monomers i and ii.

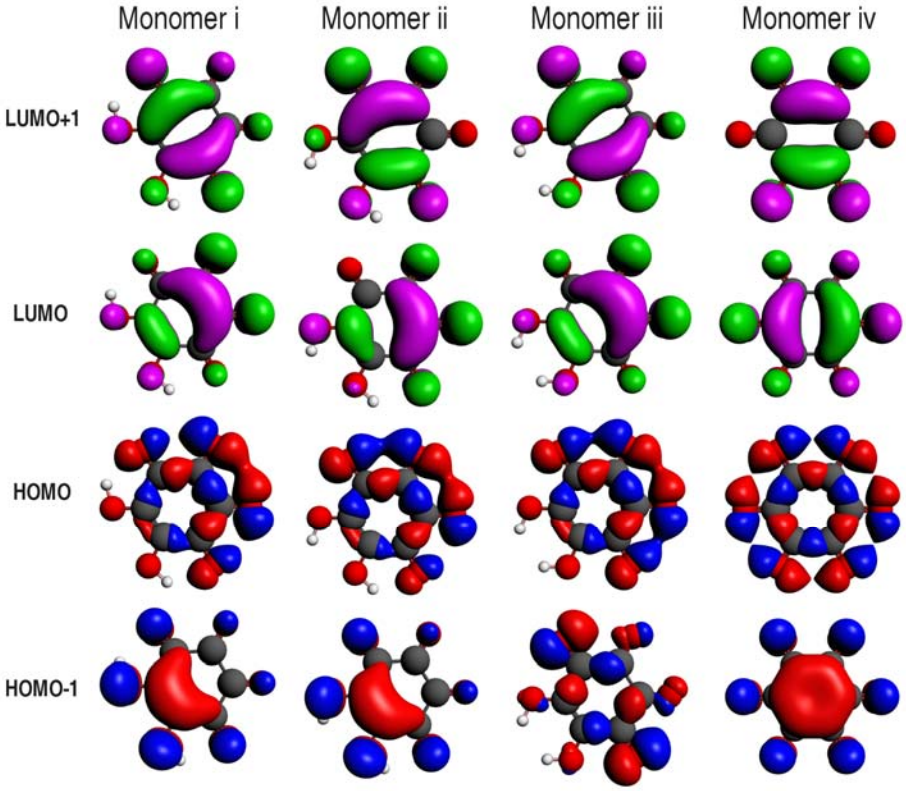


Figure S3: The frontier orbitals of the difference RA monomers and the dehydrogenated RA molecule (Monomer iv in the figure). Isovalue = +/-0.03 au.

Alternative RA network on Au (111)

An alternative RA network to that shown in figure 1 of the main text is shown in Figure S4(a). The network is constructed from a different monomer, monomer i from Figure S2 instead of monomer ii, and the dipole moments of each molecule are aligned. This network is 0.030 eV/molecule higher in energy than the figure 1 model when placed on the two layer Au(111) slab built with 13.40 Å lattice vectors (4.35 Å bulk lattice constant).

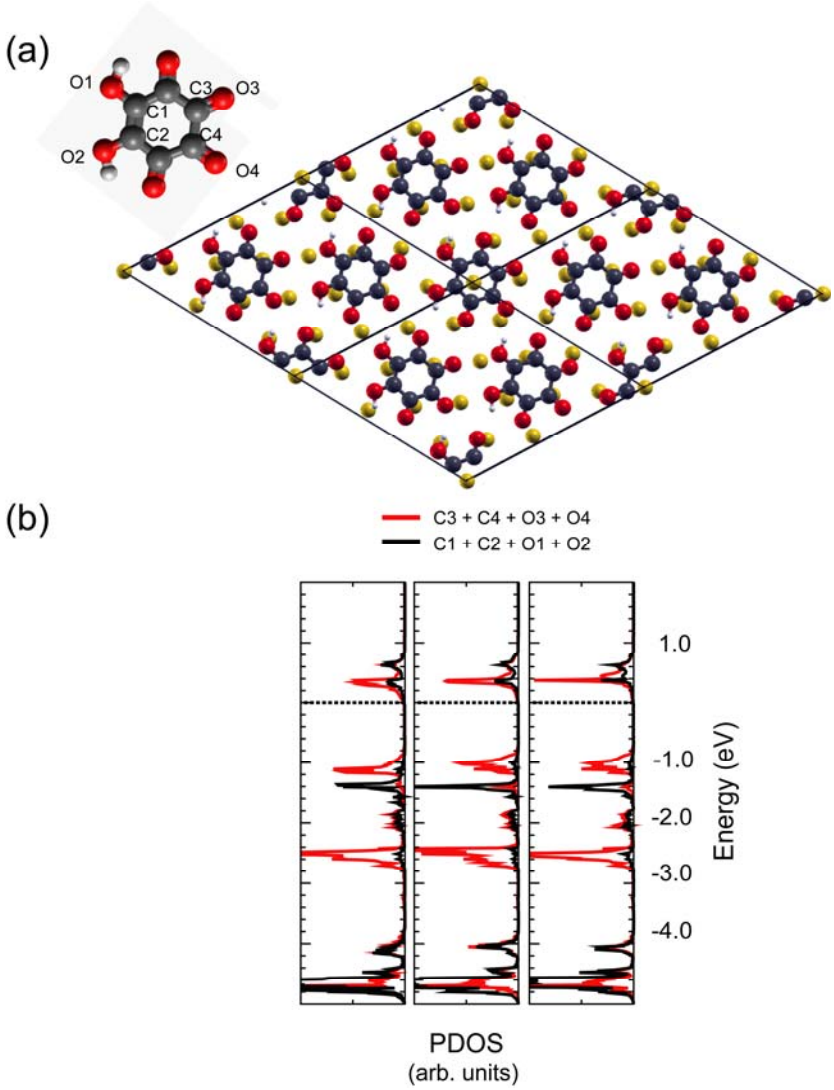


Figure S4: (a) An alternative RA network to the one shown in figure 1 of the main text. In addition, the top layer of Au is shown as well. (b) The summed site-projected densities are similar to what is shown in figure 1 of the main text. All three molecules in the simulation cell are shown. Unlike the model from the main text, all three molecules are symmetrically equivalent with respect to the organic network and this symmetry is broken slightly by the Au surface (eg. "T" site or "H" site).

Gas Phase Reactions : Hydrates

Bulk rhodizonic acid is hydroscopic. The dihydrated form of RA has been crystallized in bulk, as cited in the main text. In this section we investigate the relative stabilities of the dihydrate RA (1) with respect to the mono-hydrate RA (2) and unadulterated RA (3) via various density functionals (Figure S5).

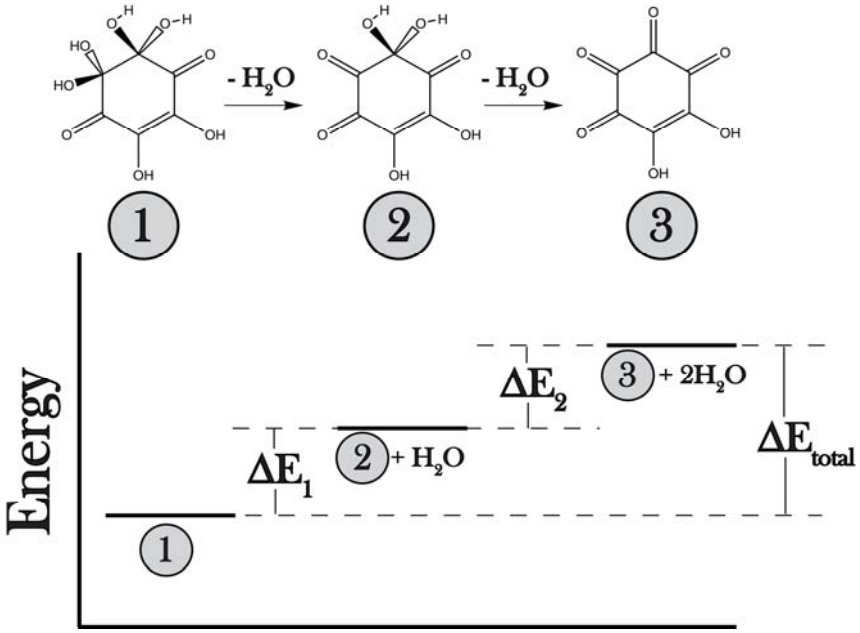


Figure S5: A partial sketch of the potential energy landscape of the dehydration of the dihydrated RA (1) to mono-hydrate RA (2) to RA (3).

Functional	ΔE_1	ΔE_2	ΔE_{total}
DFT-D3	0.49	1.40	1.90
revPBE	0.24	0.60	0.84
PBE	0.52	1.14	1.67
B3LYP	0.46	1.05	1.51

Table S1: The change in energy to go from the dihydrate RA to the mono-hydrate RA (DE_1) and the energy to go from the mono-hydrate RA to RA (DE_2), along with the energy to go from the di-hydrate RA to RA (DE_{total}), as calculated by revPBE-D3, revPBE, PBE and B3LYP functionals (in ADF). The reaction energies are given in eV.

For the hydration of the network shown in figure 1 of the main text (the hydrated networks are shown further down in Figures S7 and S9 of this SI) the DE_1 / DE_2 reaction energies were calculated (with VASP) as 0.67/0.75 eV/molecule and 0.26/0.43 eV/molecule using the DFT-D2 and vdW-DF2 functionals, respectively. When optimized over the Au(111) surface and the vdW-DF2 functional, the ratio becomes 0.07/0.44. The reduction of DE_1 is the result of the "RA sheets" lying further from the surface in the dihydrated species, due to the presence of the extra hydroxyl group between them.

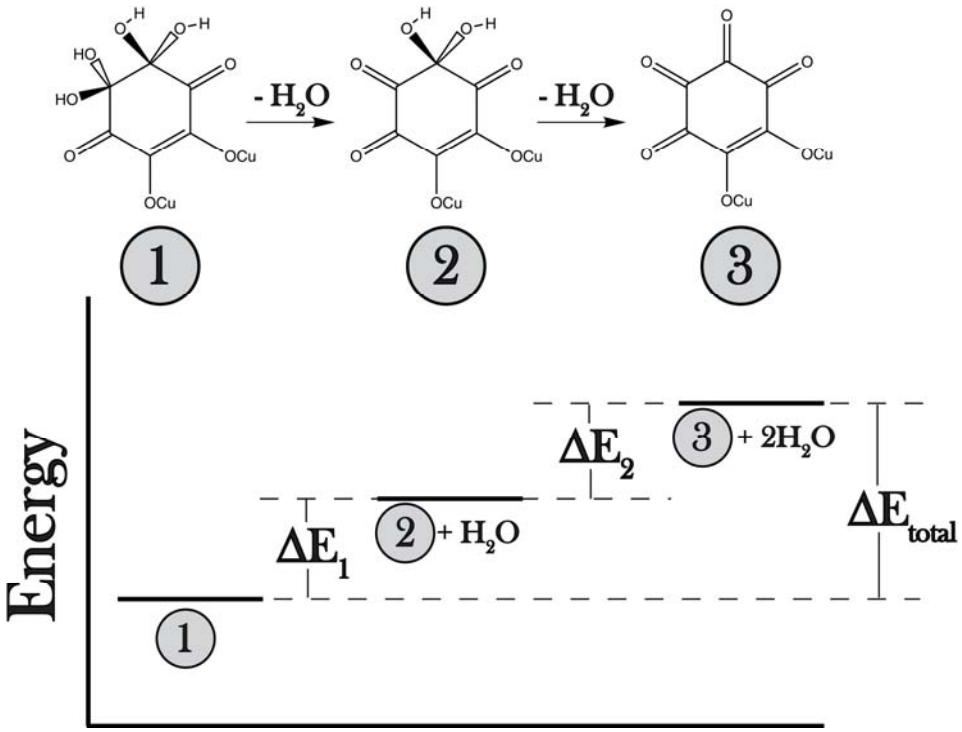


Figure S6 : A partial sketch of the potential energy landscape of the dehydration of the dihydrated RA-2Cu (1) to mono-hydrate RA-2Cu (2) to RA-2Cu (3).

Functional	ΔE_1	ΔE_2	ΔE_{total}
DFT-D3	0.16	0.27	0.43
PBE	0.18	0.55	0.73
B3LYP	0.15	0.46	0.60

Table S2: The change in energy to go from the dihydrate RA-2Cu to the mono-hydrate RA-2Cu (DE_1) and the energy to go from the mono-hydrate RA-2Cu to RA-2Cu (DE_2), along with the energy to go from the di-hydrate RA to RA (DE_{total}), as calculated by revPBE-D3, revPBE, PBE and B3LYP functionals (in ADF). The reaction energies are given eV.

Hydrated RA Sheet - Structure Model

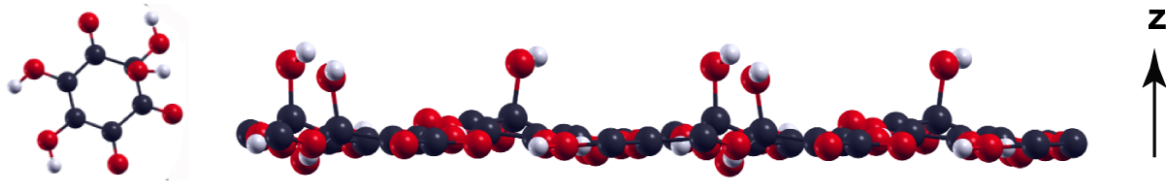


Figure S7: The mono-hydrated RA molecule and the extended structure of a sheet of hydrated RA molecules.

Figure S7 shows a planar hydrated network of RA constructed from the RA network in figure 1a of the main text; the hydration of a carbonyl yields two hydroxyl groups, one participates in a hydrogen bond within a layer and the other would connect molecules between layers in the 3D solid. In the gas-phase, periodic computations suggest that this network is energetically favored by 0.400, 0.630, and 0.750 eV/molecule with respect to decomposition into the RA network illustrated in figure 1a and molecular H_2O using the vdW-DF2, PBE, and DFT-D2 functionals, respectively. The vdW-DF2 value is only slightly larger than the 0.360 eV/molecule reaction energy computed for the hydration of a single RA molecule. When modeled over a two-layer Au(111) slab with 13.4 Å lattice vectors (4.35 Å bulk lattice constant), the hydrated network is favored by 0.440 eV/molecule.

Frontier Orbitals of Hydrate RA

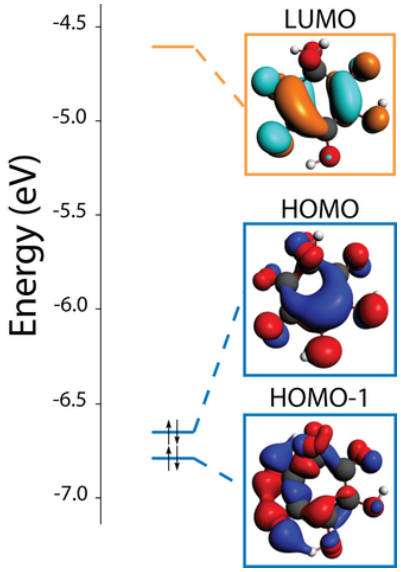


Figure S8: Frontier Orbitals of mono-hydrated RA.

The frontier orbitals of the hydrated RA molecule were calculated using ADF, the revPBE functional, and the Grimme3 empirical dispersion correction.

Hydrated RA networks on a Au(111) surface

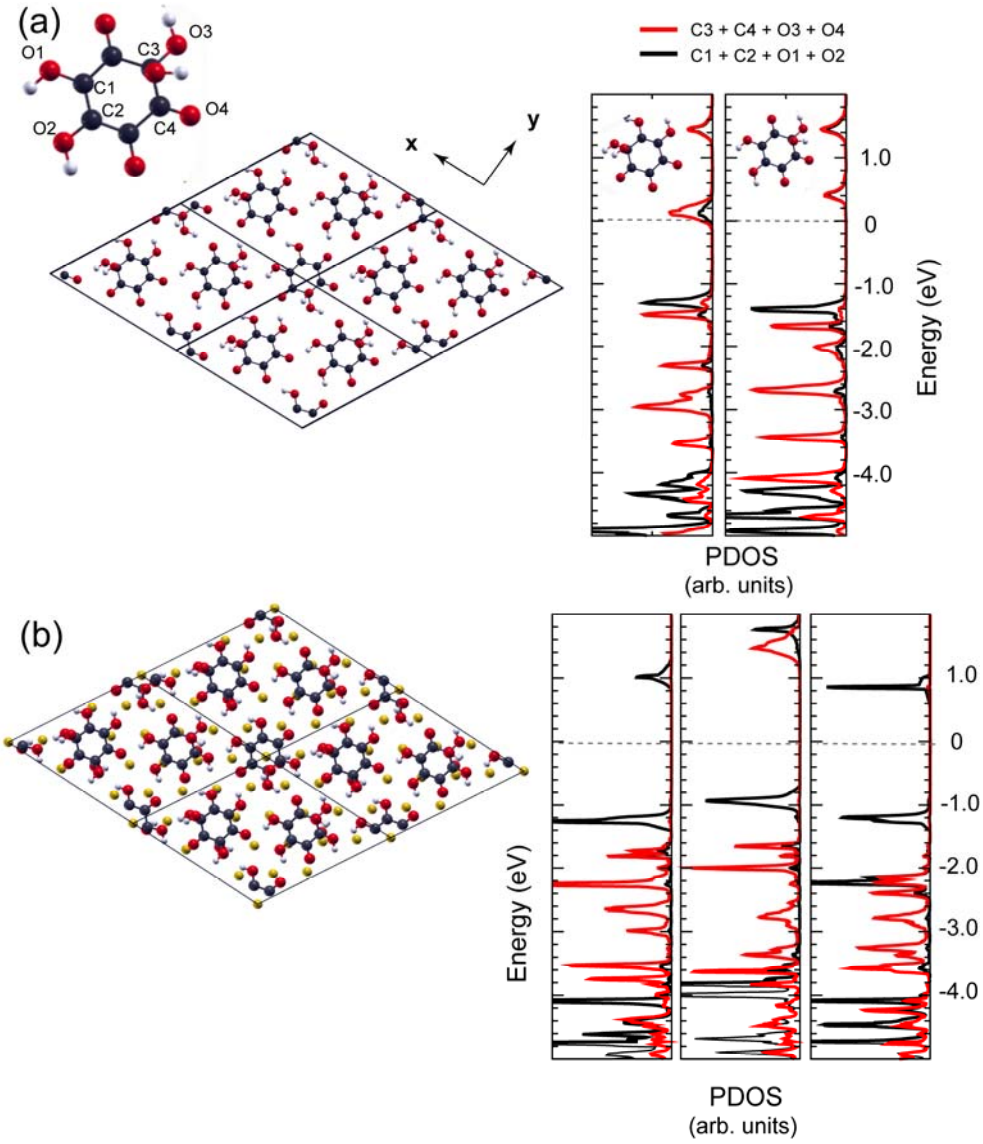
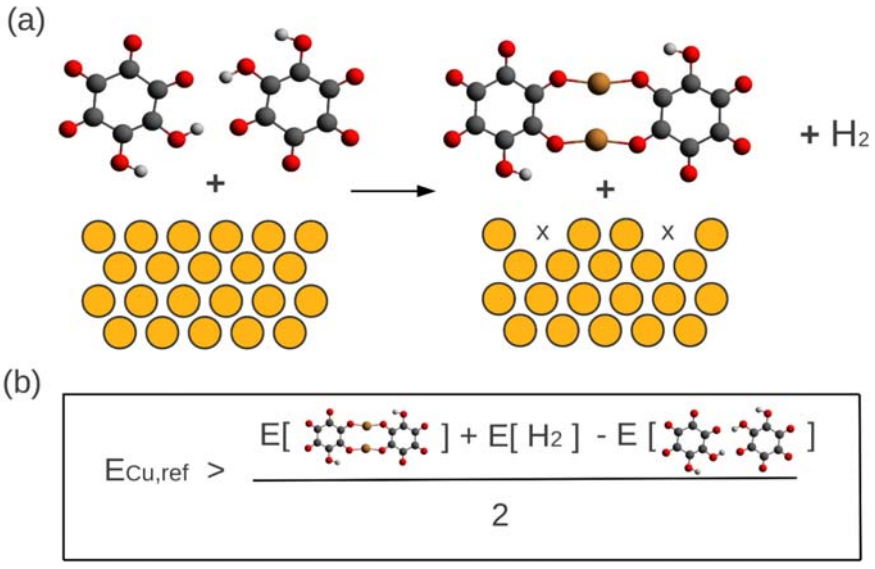


Figure S9 : (a) The overhead view of the hydrated RA network (one H_2O added per molecule) shown in figure S7. The summed site-projected densities are shown to the right, wherein the assymetric profiles of the peaks can still be seen and, in addition, there are considerable differences between molecules due to the presence of different configurational isomers. Note that only two of the three molecules are shown, the third indeed represents a different isomer but behaves similarly to the right plot. (b) The overhead view of a further hydrated RA network (two H_2O's per molecule). The top layer of Au atoms are also shown. The summed site-projected densities are shown to the right, Note that the underlying "RA sheet" is further off the surface because there is now a second set of hydroxyl groups attached to the molecules which lie between them and the surface.

Gas Phase Substitution Reactions

RA dimer and trimer models were used to preliminarily assess trends in substituting hydrogen bonding bridges with Cu bridges. This was done to help explore why MOCN's are thought to form on the Cu (111) surface but not the Au(111) surface. A number of Cu-containing monomer and dimer geometries were initially considered, encompassing different interactions between the Cu atom and the RA monomers/dimers, and it was found that it was preferable for the Cu atom to bridge a pair of nearby carbonyl groups.

Figure S10(a) shows the reaction discussed in the main text, wherein the condition for the reaction being exothermic (where E is the internal electronic energy) or spontaneous (where E is the Gibb's Free energy) is outlined in part (b). The values of the right hand side (R.H.S.) of the inequality for both the electronic energy and the computed Gibb's Free energy at zero pressure are also given in part (b). The trend shows that the reaction is stable for a wider range of values for the Cu reference state than Ag or Au, suggesting the reaction itself is more likely.

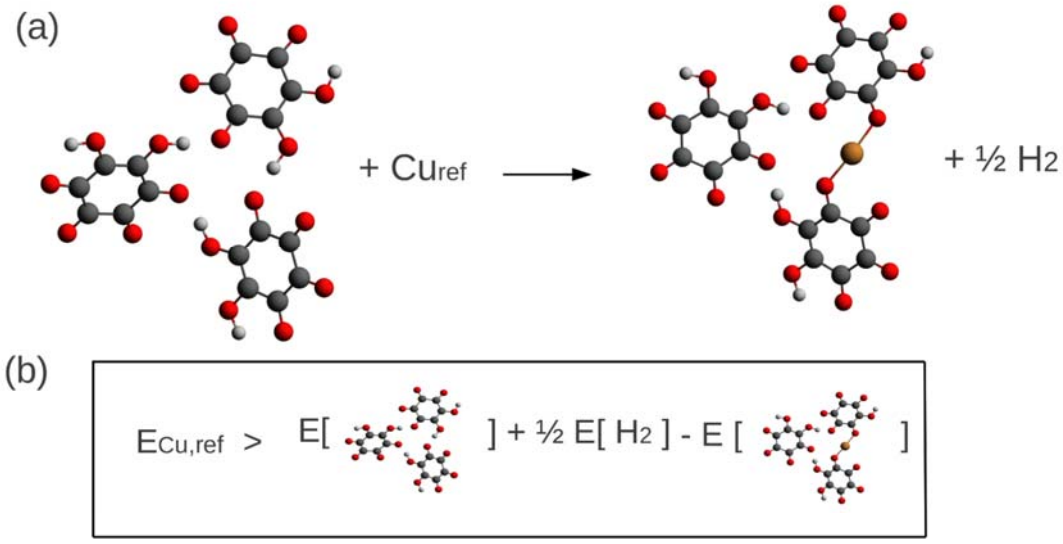


Metal atom	Internal Energy R. H. S. (eV)	Gibb's Free Energy R. H. S. (eV @ 300 K)
Cu	-2.10	-2.82
Ag	-0.86	-1.63
Au	-0.86	-1.64

Figure S10. (a) Schematic illustration of a simple substitution reaction of hydrogen with Cu within an RA dimer. For the purposes of this study, the reference state of the Cu is treated as arbitrary, but the picture shows one model of removing the Cu atoms from the surface. (b) The condition for spontaneity of the reaction shown in part (a). The table shows the computed values for the right hand side (R.H.S.) of the inequality.

The metal atom is in an unspecified reference state, M_{ref} (specifically, the default reference state which the ADF program uses). It would be reasonable to define a reference state which could, for example, be related to the atom's binding energy to the surface or to the surface's vacancy formation energy, but here we only comment on the trend in going from Cu to Au. In order for the right hand side of the above reaction to be favored, M_{ref} must be > -2.10/-0.86/-0.88 eV for Cu/Ag/Au. The trend suggests that Cu favors the substituted dimer in contrast to what is found for Ag and Au. Similar energies were seen for substituted trimers (see Figure S11).

Figure S11 (a) shows a related reaction with an RA trimer. The trends agree with those shown in Figure S10, again suggesting the reaction is more likely with Cu than with Ag or Au.



Metal atom	Internal Energy R. H. S. (eV)
Cu	-2.13
Ag	-1.19
Au	-0.77

Figure S11. (a) Schematic illustration of a simple substitution reaction of hydrogen with Cu within an RA trimer. For the purposes of this study, the reference state of the Cu (Cu_{ref}) is treated as arbitrary. (b) The condition for spontaneity of the reaction shown in part (a). The table shows the values of the right hand side (R.H.S.) of the inequality.

Molecular Orbital Level Diagram of $C_6O_6^{2-}$

The frontier molecular orbitals of rhodizonate were calculated using revPBE+D3. It is noted that the molecule retains D_{6h} symmetry, similar to benzene. The LUMO and LUMO+1 are degenerate in energy.

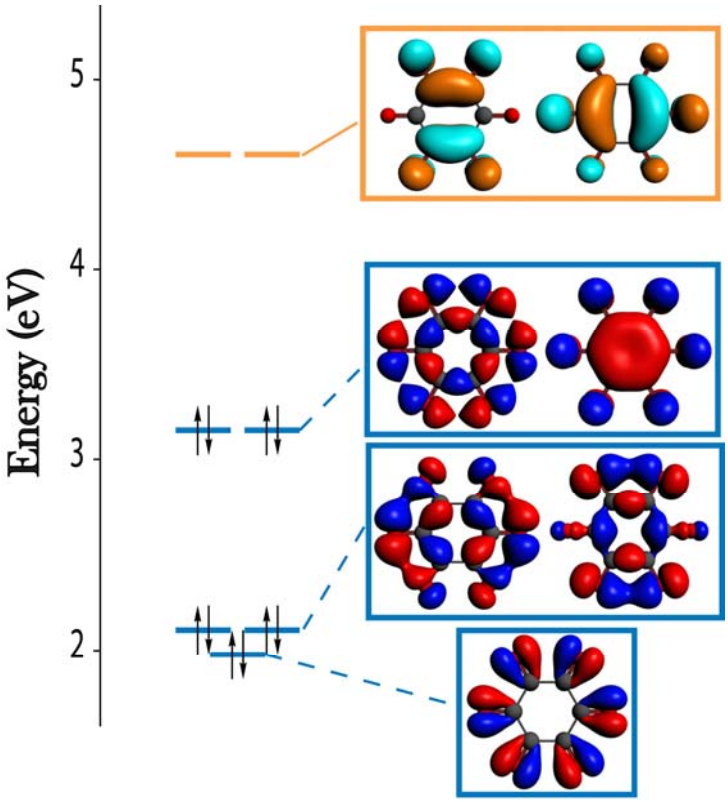


Figure S12: Schematic level diagram of the rhodizonate anion. An isovalue of +/- 0.03 au was used to generate the isosurfaces.

Gas Phase MOCN Networks

A number of plausible MOCN structures were modeled in the gas phase, constructed by effectively substituting each H atom for a Cu atom. The specifics of all these structures is outside the scope of this study, but the two structures shown in figure S13 (a) were the focus.

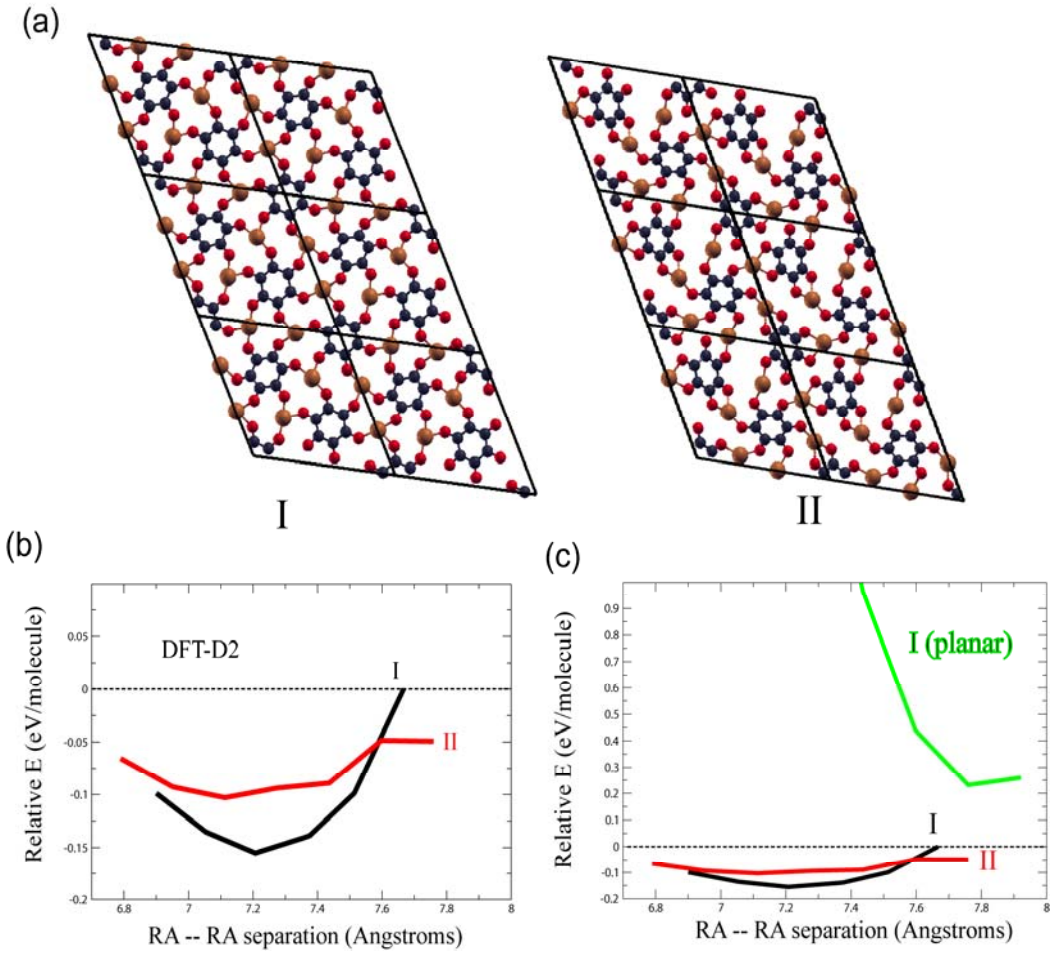


Figure S13: (a) Two model gas-phase MOCN networks; network I is what was initially placed on the model Cu (111) slab and optimized to what is shown in Figure 3 of the main text. The relative energies of the two are shown in (b), where zero is referenced to the absolute electronic energy of I when it crosses the dashed line in the plot. (c) The same as (b) except the energies of network I when constrained to be planar are added as well.

Note that these energies are taken from a rough scan of the cells' lattice constant as it is incrementally decreased. When intermolecular RA-RA spacings of ~7 Å or less are reached, the sheets can buckle somewhat to lower the energy further and create a myriad of structures which are subtly different but comparable in energy. However, our focus here was not on the precise atomic structure but more on the influence the surrounding Cu atoms can have on the molecules' electronic structure.

Figure S14 shows the summed site-projected densities of states over each molecule in structures I and II from figure S13. The qualitative behavior of the peak near the Fermi energy (outlined by a think yellow line) is similar to what is discussed in the main text concerning the surface-adsorbed networks.

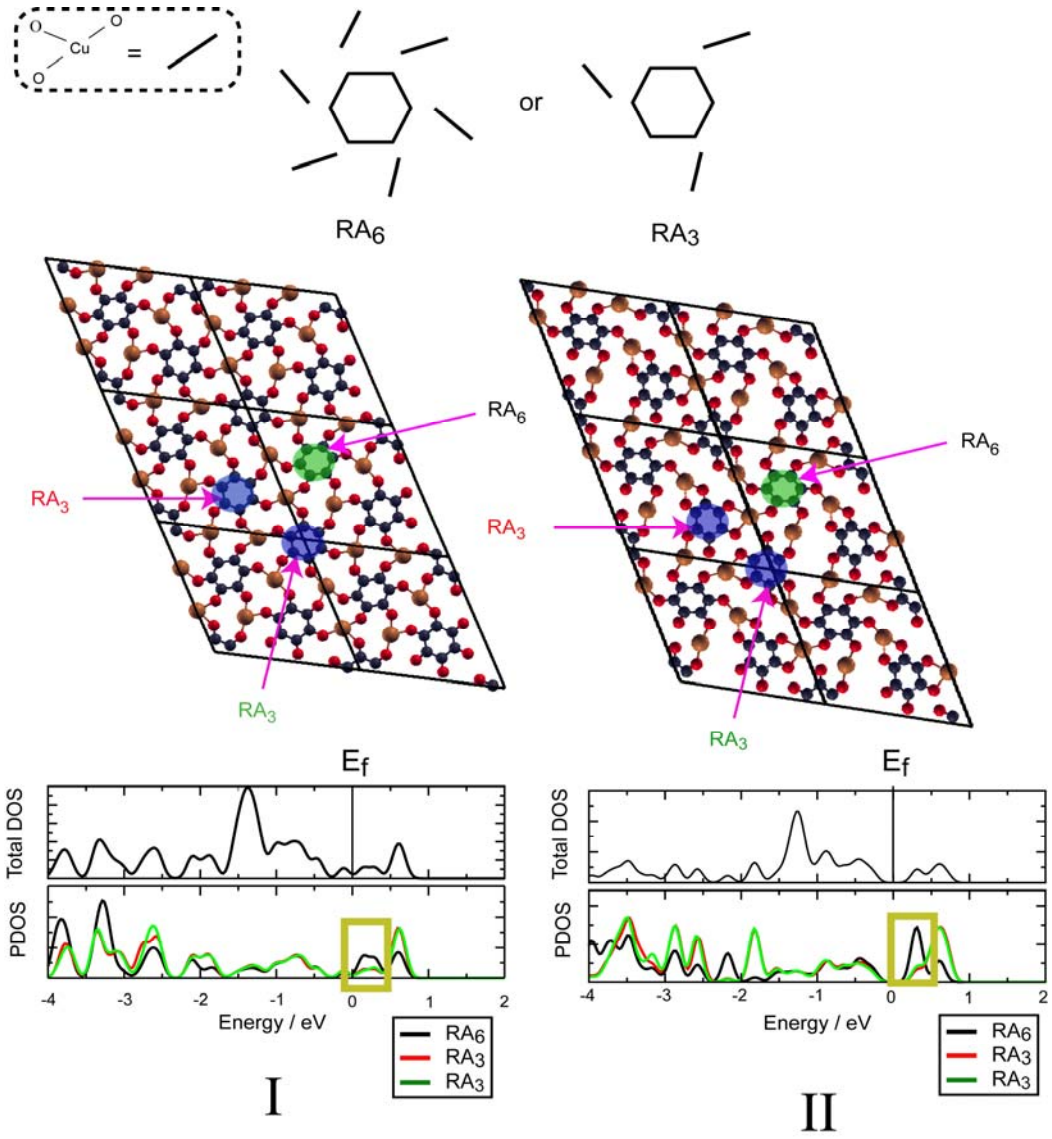


Figure S14: (top) Extended representations of structures I and II from Figure S13; the molecules are labeled according to how they are coordinated to the Cu motifs around them, similar to what is described for figure 3 of the main text. (bottom) The summed site-projected densities of states over molecules in the two structures; the enhanced RA_6 character near the Fermi energy is highlighted.

MOCN adsorbed on Cu(111): "T" vs. "H" site

Figure S15 expands upon figure 3 from the main text. In addition to figure 3, it shows the summed site-projected densities of states over all three molecules in the simulation cell when the RA_6 molecule is placed over an "H" site instead of a "T" site.

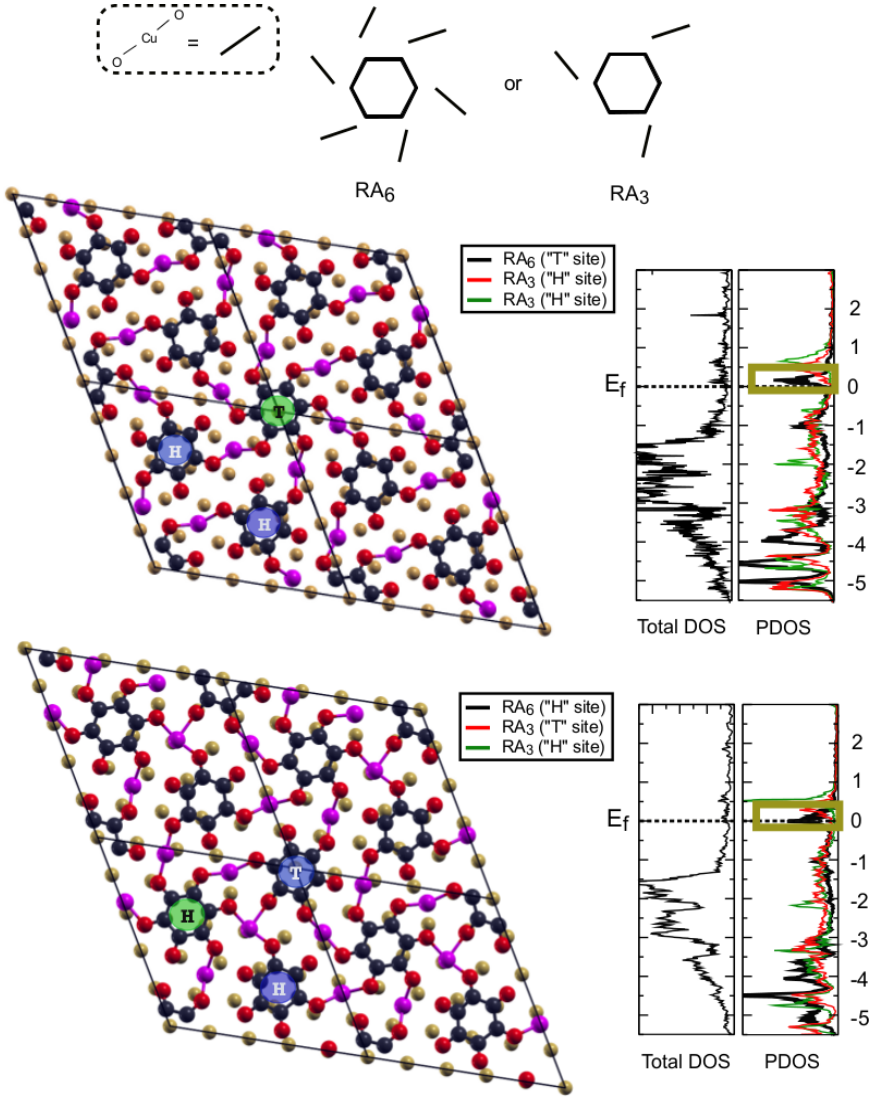


Figure S15: The total and summed site-projected densities densities of states over RA molecules in an MOCN network adsorbed on a two-layer Cu(111) slab (12.77 Å lattice vectors). The top and bottom plots represent model where the RA6 molecule is placed over (top) the "T" site or (bottom) the "H"site.

The similarities between the two sites reflects how the organic layer itself in these models is lifted slightly off the surface compared to how it would sit in the absence of Cu adatoms; the Cu adatoms lie mostly underneath them. The top plot was also computed using the vdW-DF2 functional and found to behave quite similarly.

Simulated STM image of Benzene on Pd(111)

To complement the MOCN image in Figure 3c of the main text, we computed a similar image of benzene on a Pd(111) surface to compare with the previous literature.

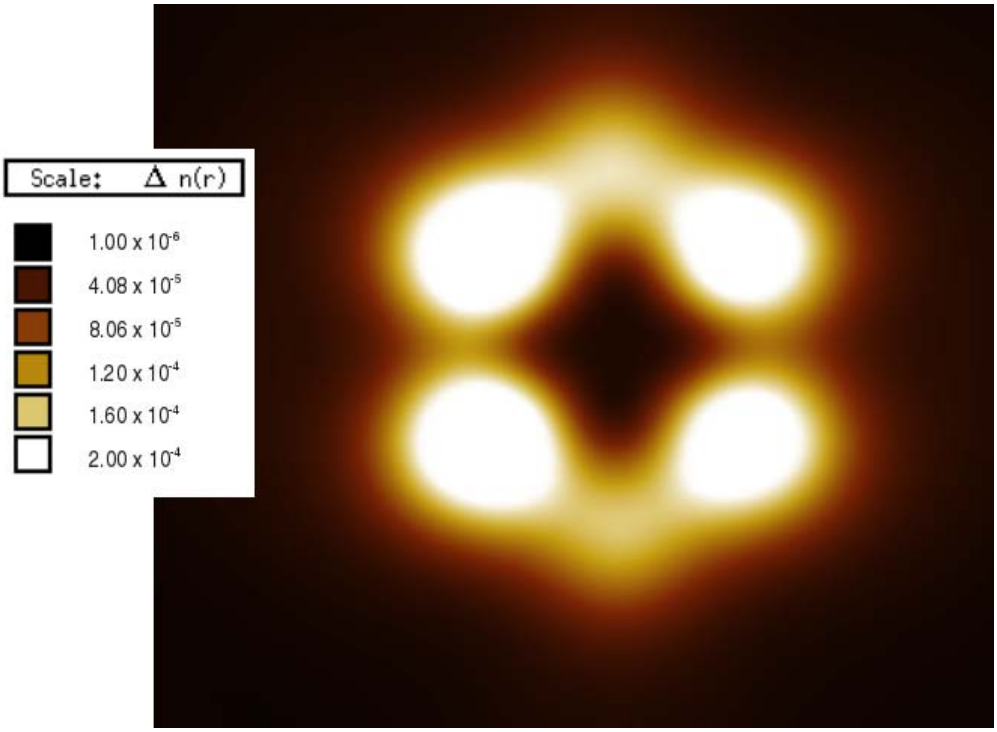


Figure S16: Simulated STM image of Benzene adsorbed on the Pd(111) surface in the B30 binding configuration. The legend shows the density in e/Å^3.

Using VASP, the adsorbtion of benzene was simulated on a four layer Pd(111) slab comprised of 100 atoms. The Grimme2 semi-empirical dispersion correction was used to account for van der Waals forces. The bottoms two layers of the slab were fixed at the experimental lattice constant, while the top two layers were permitted to relax.

The STM image was simulated using the Tersoff-Hamann approximation, representing a plane of the charge density generated from bands within 0.08 eV of the Fermi energy. The plane is approximately 4 Å from the metal surface. This is in good agreement with previously observed/calculated STM images.[s6,s7,s8]

[s6] Futaba, D. N.; Chiang, S. Calculations of Scanning Tunneling Microscopic Images of Benzene on Pt(111) and Pd(111), and Thophene on Pd(111). *Jpn. J. Appl. Phys.* **1999**, *38*, 3809-3812.

[s7] Weiss, P. S.; Eigler, D. M. Site dependence of the apparent shape of a molecule in scanning tunneling microscope images: Benzene on Pt(111). *Phys. Rev. Lett.*, **1993**, *71*, 3139-3142.

[s8] Javier, A.; Li, D.; Balbuena, P. B.; Soriaga, M. P. Simulation of scanning tunneling microscope image of benzene chemisorbed on Pd(111) electrode surface by density functional theory. *Reports in Electrochemistry*, **2013**, *3*, 1-5.

Monomers on Cu(111) and Au(111)

The adsorption of four different monomers on Cu(111) and Au(111) was modelled using VASP. The DFT-D2 dispersion correction parameter set does not include the required parameters for Au, so vdW-DF2 was used to account for dispersion in Au-containing systems. The relative energies of the adsorbed monomers i and ii, as computed by DFT-D2, are reversed from what they are the gas phase and monomer iii was unstable upon geometry optimization. In contrast, the vdW-DF2 numbers retain the same approximate energy ranking as the gas phase calculations. This is similar to what we found for CA monomers [*Phys. Rev. B*, 87 (2013) 041402] and is likely related to how DFT-D2 is known to overbind adsorbates at the surface-adsorbate interface and vdW-DF2 tends to underbind.

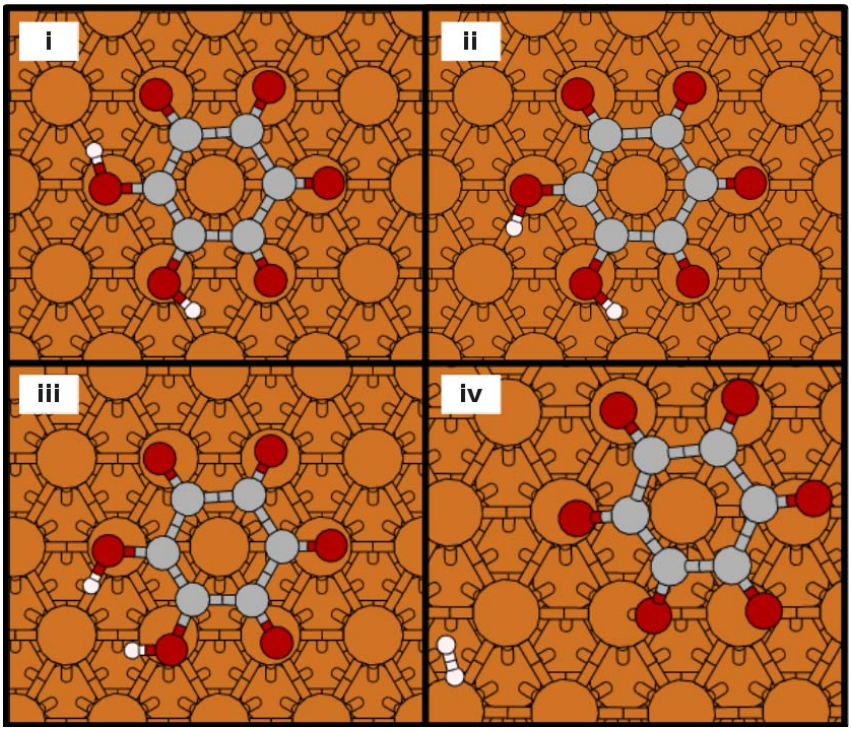


Figure S17: Structures of monomers on Cu(111) as obtained using first-principles calculations. Note that in monomer iv the H atoms are removed from RA to form an H_2 molecule in the simulation cell; its energy was always found to be higher than the other monomers.

Monomer	E_{rel} Gas (revPBE)	E_{rel} Gas (DFT-D3)	E_{rel} Cu (vdW-DF2)	E_{rel} Cu (DFT-D2)	E_{rel} Au (vdW-DF2)
I	0.0	0.0	0.0	3.9	0.0
ii	5.5	5.2	3.8	0.0	3.9
iii	20.4	19.9	16.5	-[A]	26.0

Table S3: Relative energies (E_{rel}) of RA monomers in the gas phase, on Cu(111), and on Au(111). The values are reported in kcal/mol.

[A] Monomer iii optimized to monomer ii on the Cu(111) and Au(111) surface

Coordinates

Slab model from Figure 1b of the main text – RA on Au(111)

POSCAR format

```
C O H Au
  1.00000000000000
    13.4076000000000004    0.0000000000000000    0.0000000000000000
    -6.7038000000000002   11.6113219999999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.0000000000000000
    18   18    6   38
Direct
0.4443763214459153 0.8151543373968977 0.2443112775694729
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0.4757034387567742 0.7298158230403189 0.2449780128864703
0.3240376808561223 0.7910289976966070 0.2415416797007808
0.2284951124136683 0.6657696237770594 0.2339176633861442
0.0946939451236517 0.1529771550734225 0.2446242650243846
0.9786706256081743 0.1237235846349520 0.2458675977598190
0.8834447408731663 0.0043600811316438 0.2435074799398151
0.9107812114449416 0.9088493871893775 0.2314282395656733
0.0378052838838272 0.9397067361345179 0.2298534285159590
0.1312025009940001 0.0662785505771026 0.2382645641065935
0.5531852570261222 0.3214688937928045 0.2435496169858524
0.5764899002144617 0.2259427047885154 0.2424408833076086
0.7014498867658929 0.2540832020261163 0.2450527317638347
0.7969181280051316 0.3796285161832316 0.2544595769859583
0.7649373648587598 0.4748485570445169 0.2516834484304340
0.6402760293527052 0.4376820339928926 0.2466427648457312
0.1851153262388863 0.4704808069358535 0.2463715374608100
0.4144664010780232 0.5289962623886595 0.2447553015172517
0.5851771105762253 0.7533247593821457 0.2466430618700812
0.3036470092381691 0.8709249421244181 0.2440375134500812
0.1308188110855895 0.6408781708062534 0.2210353325928409
0.1822165339071873 0.2612333712658241 0.2471300739953222
0.9566699520955382 0.2107892683274031 0.2488567905643961
0.7819421985564361 0.9823334540810578 0.2485504140285499
0.8325529255384438 0.8113506587759645 0.2214245597800613
0.0640063937093061 0.8663475731000432 0.2202680937764256
0.2340945947300526 0.0936489728678609 0.2364807528720050
0.5291435830271425 0.9250080777520751 0.2447743450565270
0.4446994371519395 0.3014647131658847 0.2404190112542040
0.4962729400164676 0.1241142864115758 0.2392390754908575
0.7250262769410583 0.1765937500980002 0.2409022192195067
0.8946896417475401 0.4011325668795394 0.2648792898155605
0.8392987652479249 0.5766804894276376 0.2547857754109515
0.6191519918121671 0.5244581509364110 0.2461324671699217
0.1612567509558644 0.3226187993907104 0.2489203108729328
0.6446486426365681 0.8368494368022183 0.2459625966658336
0.3839805338144444 0.2185804073059145 0.2388220560020002
0.5367328467313328 0.5039500173549669 0.2442836084423803
0.5005901188789892 0.9812135938343545 0.2430360937765101
0.8728941707007962 0.1855492166632402 0.2480247335447601
0.0000000000000000 0.0000000000000000 0.1004590000000007
0.2105260000000015 0.5263160000000013 0.1004590000000007
0.5263160000000013 0.3157890000000023 0.1004590000000007
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0.2456140000000033 0.2807019999999980 0.0000000000000000
0.8421049999999966 0.1052630000000008 0.1004590000000007
0.5614040000000031 0.0701749999999990 0.0000000000000000
0.7368420000000029 0.8421049999999966 0.1004590000000007
0.4561399999999978 0.8070179999999993 0.0000000000000000
0.7719299999999976 0.5964910000000003 0.0000000000000000
0.0526320000000027 0.6315790000000021 0.1004590000000007
0.3684209999999979 0.4210530000000006 0.1004590000000007
0.0877189999999999 0.3859649999999988 0.0000000000000000
0.6842109999999977 0.2105260000000015 0.1004590000000007
0.4035089999999997 0.1754389999999972 0.0000000000000000
0.5789469999999994 0.9473679999999973 0.1004590000000007
0.2982459999999989 0.9122810000000001 0.0000000000000000
0.8947369999999992 0.7368420000000029 0.1004590000000007
0.6140350000000012 0.7017540000000011 0.0000000000000000
0.9298250000000010 0.4912279999999996 0.0000000000000000
0.2631579999999971 0.1578950000000034 0.1004590000000007
0.1578950000000034 0.8947369999999992 0.1004590000000007
0.4736839999999987 0.6842109999999977 0.1004590000000007
0.1929820000000007 0.6491230000000030 0.0000000000000000
0.7894739999999985 0.4736839999999987 0.1004590000000007
0.5087720000000004 0.4385970000000015 0.0000000000000000
0.8245610000000028 0.2280700000000024 0.0000000000000000
0.7192980000000020 0.9649119999999982 0.0000000000000000
0.1052630000000008 0.2631579999999971 0.1004590000000007
0.4210530000000006 0.0526320000000027 0.1004590000000007
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0.3157890000000023 0.7894739999999985 0.1004590000000007
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0.3508769999999970 0.5438600000000022 0.0000000000000000
0.9473679999999973 0.3684209999999979 0.1004590000000007
0.6666669999999968 0.3333330000000032 0.0000000000000000
0.9824559999999991 0.1228070000000017 0.0000000000000000
0.8771929999999983 0.8596489999999974 0.0000000000000000

Slab model from Figure 1c of the main text – hydrated RA on Au(111)

POSCAR format

```
C O H Au
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    13.4076000000000004    0.0000000000000000    0.0000000000000000
    -6.7038000000000002   11.6113219999999995    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.0000000000000000
    18    21    12    38
Direct
0.4355115899217026 0.8119835145411542 0.2438451017695940
0.2552554589487883 0.5680484340888299 0.2435932932921006
0.3828870883093032 0.6043077168689308 0.2430112044899815
0.4666227064016297 0.7273014887808955 0.2421989840111181
0.3133340186318634 0.7871728335994135 0.2536298975028402
0.2207952233623587 0.6617071165472836 0.2405593633242162
0.1024505115514529 0.1475323431627089 0.2421337002801422
0.9862662118702588 0.1153174105754502 0.2417304450143405
0.8917848951924370 0.9948828944049026 0.2431694857230227
0.9200554320172500 0.8983882533976342 0.2556341839296792
0.0472767063778505 0.9335941502541090 0.2434990253038265
0.1396859709007003 0.0616627934661906 0.2414804384730544
0.5571741994859707 0.3261399724346958 0.2426656540475207
0.5830849256217121 0.2322989198354719 0.2427875147815470
0.7096775243641318 0.2624679458109753 0.2433425655650936
0.8028048379369963 0.3880889804918368 0.2558728079212145
0.7662634979130942 0.4793019126701665 0.2444581979347831
0.6426060619121259 0.4422263143664225 0.2424803905263744
0.1790866229249701 0.4661591478244347 0.2458976992952486
0.4099076602392273 0.5278018462206546 0.2412141721955194
0.5778078743532120 0.7526405452103049 0.2381935366825161
0.2999545494111757 0.8694003069426870 0.2247070110538161
0.1211770250010673 0.6376181941104662 0.2314649119718197
0.1889772825487768 0.2571843733157095 0.2400108331462789
0.9605096396003958 0.2003613357933318 0.2388611462330914
0.7909062741216104 0.9740505974472597 0.2385126881503510
0.8401268931191836 0.7995117762612267 0.2285607081982022
0.0734964103793416 0.8589279442016959 0.2369856455483514
0.2424091629888565 0.0877163343830958 0.2383849939549734
0.5202579766842277 0.9213017494196905 0.2383434569185852
0.4474763016072174 0.3033935351868280 0.2404173591337866
0.5041840385344898 0.1297342221153457 0.2411959828161372
0.7336795657466055 0.1857450337165716 0.2380430245294320
0.9036517641946347 0.4109855597885783 0.2293284690796042
0.8424372441153096 0.5810376220450948 0.2389284042179156
0.6206493537538478 0.5291517432306136 0.2390084727843629
0.3046531373395069 0.7976088779016308 0.3117331316334102
0.8154513761220059 0.3924313835670219 0.3142288198656331
0.9136290951331674 0.8839314092388761 0.3136939881801766
0.1656831448544764 0.3167593045367454 0.2405400527651551
0.6346096816444984 0.8359635666975507 0.2368415916186848
0.3888409409237354 0.2199453741526156 0.2391940965550248
0.9633868808039452 0.4929036917548046 0.2325734514187801
0.5378217929557252 0.5075947213258161 0.2386070951445873
0.4958011682437800 0.9804444285956677 0.2390960369634243
0.8763865872096233 0.1713181471879537 0.2365050848737695
```

0.8535708089903693 0.7342713271432757 0.2347643104243460
0.2210200542443559 0.8571318247324129 0.2274185522742300
0.8327318109377515 0.8522670140054842 0.3236663882743613
0.2314491060558623 0.7946745337439651 0.3189532540924418
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0.8421049999999966 0.1052630000000008 0.1004590000000007
0.5614040000000031 0.0701749999999990 0.0000000000000000
0.7368420000000029 0.8421049999999966 0.1004590000000007
0.4561399999999978 0.8070179999999993 0.0000000000000000
0.7719299999999976 0.5964910000000003 0.0000000000000000
0.0526320000000027 0.6315790000000021 0.1004590000000007
0.3684209999999979 0.4210530000000006 0.1004590000000007
0.0877189999999999 0.3859649999999988 0.0000000000000000
0.6842109999999977 0.2105260000000015 0.1004590000000007
0.4035089999999997 0.1754389999999972 0.0000000000000000
0.5789469999999994 0.9473679999999973 0.1004590000000007
0.2982459999999989 0.9122810000000001 0.0000000000000000
0.8947369999999992 0.7368420000000029 0.1004590000000007
0.6140350000000012 0.7017540000000011 0.0000000000000000
0.9298250000000010 0.4912279999999996 0.0000000000000000
0.2631579999999971 0.1578950000000034 0.1004590000000007
0.1578950000000034 0.8947369999999992 0.1004590000000007
0.4736839999999987 0.6842109999999977 0.1004590000000007
0.1929820000000007 0.6491230000000030 0.0000000000000000
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0.5087720000000004 0.4385970000000015 0.0000000000000000
0.8245610000000028 0.2280700000000024 0.0000000000000000
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0.0350880000000018 0.7543859999999967 0.0000000000000000
0.6315790000000021 0.5789469999999994 0.1004590000000007
0.3508769999999970 0.5438600000000022 0.0000000000000000
0.9473679999999973 0.3684209999999979 0.1004590000000007
0.6666669999999968 0.3333330000000032 0.0000000000000000
0.9824559999999991 0.1228070000000017 0.0000000000000000
0.8771929999999983 0.8596489999999974 0.0000000000000000

Slab model from Figure 3b of the main text – MOCN on Cu(111)

POSCAR format

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C O Cu
   1.00000000000000
     12.7799999999999994    0.0000000000000000    0.0000000000000000
      6.3899999999999997   11.0678049999999999    0.0000000000000000
      0.0000000000000000    0.0000000000000000   30.0000000000000000
     18    18    56
Direct
0.8645040977635361 0.0906895981111546 0.1678958163900290
0.9517588444560587 0.1300266578172042 0.1705875400201009
0.0780488862107234 0.0426353631917706 0.1715610359236805
0.1161000345570571 0.9153028787280633 0.1705787651144064
0.0272158265438378 0.8772754866039136 0.1678305692592303
0.9015916325238038 0.9645488153041555 0.1669612043020834
0.2129600374809115 0.4687221730873077 0.1893558573079019
0.3377612772562344 0.4486719001937729 0.1816139401827499
0.4420725118167752 0.3232506687452386 0.1867983055042330
0.4181312985410344 0.2286415749257031 0.1693454584756680
0.2962831339659004 0.2590225475968779 0.1573677437418155
0.1925700297462498 0.3706675007807689 0.1724074105517275
0.5522621201321627 0.8063044177120844 0.1727338734616097
0.5360653829578368 0.7073181955404024 0.1575029525864480
0.6335309582532247 0.5821178538223748 0.1622874117657531
0.7544018517109521 0.5656674065893270 0.1590995817942584
0.7767692111781983 0.6600123812206817 0.1747790524299546
0.6733843261496233 0.7796639918873183 0.1897033012833873
0.3568750970532051 0.5334759375250542 0.1730116667517052
0.5418608111566030 0.3024806215256888 0.2001763417482181
0.5035200794550860 0.1238095199228511 0.1595048815054838
0.2805985430927151 0.1833798015693375 0.1337111909282882
0.0855899619685019 0.3910356471110248 0.1678232888596582
0.1338668450703224 0.5625356046351797 0.2064952047978110
0.4679370277660198 0.9148735118160829 0.1696236428463038
0.4408974705017030 0.7289538362732628 0.1361303642121356
0.6104157732083593 0.4971685951992555 0.1564968623609744
0.8340774285302146 0.4763452714721126 0.1360490696168952
0.8814178233061938 0.6457502712574126 0.1712895693873193
0.6894002822605714 0.8557306481457303 0.2086079186206149
0.9144339512608255 0.2438204793099956 0.1653301934614078
0.1551624795180686 0.0788986451520302 0.1672366731578094
0.2272993173560636 0.8370705736779982 0.1655798746619155
0.0643534108595674 0.7652234556051312 0.1588838274778297
0.8239220832652023 0.9305867355336872 0.1578291587498768
0.7528862416781408 0.1679998739824171 0.1592237983122473
0.0236293899062900 0.2951613509685060 0.1411320287433853
0.6634793979744416 0.0612886783244520 0.1376598628780812
0.2594508105929236 0.6769241241351907 0.1363713200774299
0.9376131054486407 0.7304878653432425 0.1353269393097492
0.7107463784879613 0.3306112213286525 0.1397250079823493
0.3131851111017241 0.9787625131373900 0.1405347260769574
0.0000000000000000 0.0000000000000000 0.0695649999999972
0.0000000000000000 0.2000000000000028 0.0695649999999972
0.0000000000000000 0.3999999999999986 0.0695649999999972
0.0000000000000000 0.6000000000000014 0.0695649999999972
0.0000000000000000 0.7999999999999972 0.0695649999999972
0.2000000000000028 0.0000000000000000 0.0695649999999972
0.2000000000000028 0.2000000000000028 0.0695649999999972
```

0.2000000000000028 0.3999999999999986 0.0695649999999972
0.2000000000000028 0.6000000000000014 0.0695649999999972
0.2000000000000028 0.7999999999999972 0.0695649999999972
0.3999999999999986 0.0000000000000000 0.0695649999999972
0.3999999999999986 0.2000000000000028 0.0695649999999972
0.3999999999999986 0.3999999999999986 0.0695649999999972
0.3999999999999986 0.6000000000000014 0.0695649999999972
0.3999999999999986 0.7999999999999972 0.0695649999999972
0.6000000000000014 0.0000000000000000 0.0695649999999972
0.6000000000000014 0.2000000000000028 0.0695649999999972
0.6000000000000014 0.3999999999999986 0.0695649999999972
0.6000000000000014 0.6000000000000014 0.0695649999999972
0.6000000000000014 0.7999999999999972 0.0695649999999972
0.7999999999999972 0.0000000000000000 0.0695649999999972
0.7999999999999972 0.2000000000000028 0.0695649999999972
0.7999999999999972 0.3999999999999986 0.0695649999999972
0.7999999999999972 0.6000000000000014 0.0695649999999972
0.7999999999999972 0.7999999999999972 0.0695649999999972
0.0666662000000002 0.0666662000000002 0.0000000000000000
0.0666662000000002 0.2666662000000031 0.0000000000000000
0.0666662000000002 0.4666661999999988 0.0000000000000000
0.0666662000000002 0.6666662000000017 0.0000000000000000
0.0666662000000002 0.8666661999999974 0.0000000000000000
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0.2666662000000031 0.2666662000000031 0.0000000000000000
0.2666662000000031 0.4666661999999988 0.0000000000000000
0.2666662000000031 0.6666662000000017 0.0000000000000000
0.2666662000000031 0.8666661999999974 0.0000000000000000
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0.4666661999999988 0.2666662000000031 0.0000000000000000
0.4666661999999988 0.4666661999999988 0.0000000000000000
0.4666661999999988 0.6666662000000017 0.0000000000000000
0.4666661999999988 0.8666661999999974 0.0000000000000000
0.6666662000000017 0.0666662000000002 0.0000000000000000
0.6666662000000017 0.2666662000000031 0.0000000000000000
0.6666662000000017 0.4666661999999988 0.0000000000000000
0.6666662000000017 0.6666662000000017 0.0000000000000000
0.6666662000000017 0.8666661999999974 0.0000000000000000
0.8666661999999974 0.0666662000000002 0.0000000000000000
0.8666661999999974 0.2666662000000031 0.0000000000000000
0.8666661999999974 0.4666661999999988 0.0000000000000000
0.8666661999999974 0.6666662000000017 0.0000000000000000
0.8666661999999974 0.8666661999999974 0.0000000000000000

Slab model from Figure 3c of the main text – MOCN on Cu(111)

POSCAR format

```
C  O  Cu
  1.00000000000000
    13.5250000000000004    0.0000000000000000    0.0000000000000000
    -6.7625000000000002   11.7129940000000001    0.0000000000000000
     0.0000000000000000    0.0000000000000000   25.0000000000000000
    18    18    62
Direct
0.9774708089573707 0.0917255168635833 0.1946744294559508
0.0908575510065290 0.1064618692162043 0.1945615012172226
0.1055562527996443 0.0078089184614569 0.1947730459067429
0.0068132854591667 0.8944281261376688 0.1950458507251227
0.8934139141778203 0.8797178348071597 0.1952335673544923
0.8787465844194671 0.9784037065344506 0.1949595094247627
0.6875130053582978 0.4473780831915306 0.1959539035682383
0.7780344939696278 0.4171840654522683 0.1957448808374593
0.7506089962598850 0.2978825319954197 0.1957170280257614
0.6299124964057796 0.2073008580200124 0.1952056755559326
0.5380056436889404 0.2346758175164609 0.1953497938270203
0.5682558073932640 0.3554257824375071 0.1953283994647776
0.3539994440945122 0.7789334382884618 0.1960312399325801
0.2332972937481088 0.6883150885752158 0.1961419480369386
0.2061894250414937 0.5690720117737911 0.1956367359693090
0.2967925181556552 0.5390028408047414 0.1960122737223031
0.4160171258768628 0.6309826589953857 0.1960115527828705
0.4460022179237271 0.7516616250202404 0.1963447777801974
0.8825526006136215 0.4965927011386384 0.1922719197158500
0.8260882216444045 0.2694826728558155 0.1926373782911526
0.6051271754184455 0.1028572876100355 0.1914489965058337
0.4340787155891448 0.1592831453921804 0.1923222006860144
0.4888209706485398 0.3804982470980178 0.1914712427696230
0.7158907070046965 0.5512559580543410 0.1933471989755660
0.3791536538777933 0.8834372090075533 0.1921043396754456
0.1577022396284917 0.7164849290509068 0.1931357262615307
0.1018045190531254 0.4894537456581887 0.1914384258999604
0.2684404739346533 0.4351610860700532 0.1925788488260025
0.4955790498943742 0.6061309023409223 0.1922260609224367
0.5497824625639893 0.8272401540150227 0.1930524663241613
0.1759615815948052 0.2093574380257763 0.1920049486017774
0.2084295095779751 0.0255409590613240 0.1926014936925284
0.0244360746306000 0.8092407300354694 0.1931565421736323
0.8082262112513163 0.7768742466501806 0.1934163563805811
0.7759581325543365 0.9608881891034216 0.1928069979409130
0.9597267682531694 0.1768644840361802 0.1922425671091545
0.3328088481558638 0.2721571227168980 0.1696025236999787
0.7144050850534214 0.0561458316413308 0.1707658906222846
0.9301432142348389 0.6524836823661744 0.1725798499016662
0.6514783401220114 0.7145027389985188 0.1723817317294731
0.0545615206707595 0.3335270700084649 0.1697846864183319
0.2719750032806445 0.9322916431757662 0.1713517904762654
0.0000000000000000 0.0000000000000000 0.0834779999999995
0.0000000000000000 0.5000000000000000 0.0834779999999995
0.5000000000000000 0.0000000000000000 0.0834779999999995
0.5000000000000000 0.5000000000000000 0.0834779999999995
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0.1428569999999993 0.9285704999999993 0.0834779999999995
0.6428569999999993 0.4285704999999993 0.0834779999999995
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0.6428569999999993 0.9285704999999993 0.0834779999999995
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0.9285704999999993 0.2857135000000000 0.0834779999999995
0.9285704999999993 0.7857135000000000 0.0834779999999995
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0.2857135000000000 0.8571420000000032 0.0834779999999995
0.7857135000000000 0.3571420000000032 0.0834779999999995
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0.2142849999999967 0.6428569999999993 0.0834779999999995
0.7142849999999967 0.1428569999999993 0.0834779999999995
0.7142849999999967 0.6428569999999993 0.0834779999999995
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0.9047610000000006 0.3809515000000019 0.0000000000000000
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0.2619040000000012 0.4523799999999980 0.0000000000000000
0.2619040000000012 0.9523799999999980 0.0000000000000000
0.7619040000000012 0.4523799999999980 0.0000000000000000
0.7619040000000012 0.9523799999999980 0.0000000000000000

Gas-Phase Models for Substitution Reaction – RA dimer

XYZ format

28

C	14.296116	6.867626	5.902752
C	15.833100	6.786423	5.864487
C	16.496817	5.377459	5.858945
C	15.586892	4.125020	5.962393
C	14.122495	4.360131	6.001770
C	13.536176	5.624961	5.957698
O	16.504089	7.800272	5.843289
O	17.702460	5.261409	5.780055
O	16.060219	2.997761	6.004492
O	13.357969	3.261145	6.078547
O	12.193030	5.652163	5.990658
O	13.724963	7.969417	5.891568
O	10.525981	7.801408	5.855315
C	9.959958	8.905775	5.871275
C	8.427451	8.997551	5.756034
C	7.761982	10.401793	5.859046
C	8.674120	11.651597	5.954238
C	10.135687	11.409865	6.033952
C	10.719818	10.143938	5.992817
O	7.760201	7.995742	5.586274
O	6.553417	10.514997	5.864002
O	8.205477	12.781911	5.962576
O	10.900870	12.504348	6.150228
O	12.061314	10.114331	6.067802
H	12.418613	9.186477	6.000659
H	11.837787	12.209808	6.191019
H	11.836411	6.581788	5.945322
H	12.418997	3.551759	6.085630

Gas-Phase Models for Substitution Reaction – Cu-substituted RA dimer

XYZ format

28

C	14.819896885	6.640232308	5.970618933
C	16.336309472	6.439944304	5.979353104
C	16.911780448	5.023607792	5.729636460
C	15.939995369	3.835187679	5.792871063
C	14.503039021	4.178770873	5.848546276
C	13.938551849	5.485942244	5.895909859
O	17.078068496	7.389578522	6.168269804
O	18.096621755	4.866411126	5.505234797
O	16.331647405	2.672405577	5.784999259
O	13.650517291	3.156535997	5.819460878
O	12.627646405	5.509071259	5.905446171
O	14.441287433	7.847801080	6.036554054
O	9.753227414	7.881168273	6.005554313
C	9.382906247	9.093397801	5.976988058
C	7.868812788	9.305234585	5.963627212
C	7.315936271	10.717326508	5.647694309
C	8.280744257	11.905411366	5.782378426
C	9.710114434	11.557409176	5.919176670
C	10.268068987	10.247427115	5.968194533
O	7.112782439	8.372766087	6.180133849
O	6.154827775	10.870782834	5.320838985
O	7.889539139	13.068577926	5.766177191
O	10.567245014	12.576137548	5.946203163
O	11.576876733	10.222236997	6.044779911
Cu	12.879183392	8.873122542	6.030154117
H	11.459101685	12.144401075	6.002590761
Cu	11.318915134	6.856394466	5.953750284
H	12.754319868	3.582875477	5.839322463

Gas-Phase Models for Substitution Reaction – Au-substituted RA dimer

XYZ format

28
TIME: 1.02000

C	14.907415373	6.521717971	6.163186581
C	16.394607260	6.237028417	6.417769223
C	17.027233740	4.983435461	5.770198459
C	16.081574718	3.819055916	5.464788821
C	14.637537363	4.139717598	5.525433211
C	14.038372414	5.406584599	5.811153272
O	17.066508736	7.008539119	7.078213221
O	18.220285301	4.936684816	5.542568865
O	16.489524621	2.691346911	5.206170155
O	13.814148094	3.146567163	5.202142396
O	12.725221737	5.368057010	5.737039966
O	14.611268318	7.744659743	6.332156326
O	9.579105834	7.978396242	6.250098590
C	9.287793137	9.205174558	6.097633815
C	7.787977466	9.479811315	6.287945003
C	7.189770487	10.784108943	5.710859110
C	8.153470802	11.958742435	5.524417121
C	9.591472857	11.616525472	5.587277536
C	10.170473725	10.326960600	5.804378221
O	7.078595596	8.664435011	6.849301224
O	6.005426362	10.862613537	5.449493042
O	7.763028513	13.107802863	5.346433721
O	10.432497025	12.617918791	5.345402574
O	11.484233629	10.355487443	5.738425020
Au	12.961816076	8.948316955	6.035987698
H	11.333144009	12.200416885	5.388731110
Au	11.237508436	6.774127249	6.005896509
H	12.907112937	3.547825747	5.259147954

Optimized Monomers Adsorbed to Cu(111)/Au(111) surfaces

POSCAR format

Monomer i on Cu(111) -DFT-D2
Cu O C H
1.00000000000000
12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
100 6 6 2
Direct
0.8008127847410684 0.8007077725762377 0.1546228984433817
0.4045666159519344 0.7976326915392286 0.1544762208006889
0.7973799723540553 0.4045821558629951 0.1544230971291763
0.6020915084153259 0.8002604836883862 0.1544257485582362
0.8003115223348179 0.6019893713815018 0.1544256332759013
0.6006662538540152 0.6007182466181862 0.1544246305922634
0.9995693080983339 0.8003264414483904 0.1543709890565424
0.4003296382012997 0.4003406275316412 0.1543828063178355
0.2053040223032948 0.7926868997342539 0.1564940140031432
0.4025090269376389 0.5980890841930930 0.1542851382505721
0.2005122564841558 0.5985284129774017 0.1544830536830882
0.8005095220097118 0.9992276527222188 0.1543143756213308
0.5982031541142615 0.4023503608607882 0.1542766060498474
0.7927516172006557 0.2047380168245203 0.1565836878185426
0.5984562989318619 0.2004305486871319 0.1544899323535846
0.0002923158528443 0.4055296738131860 0.1539011991170525
0.0006547757543540 0.6019021202757824 0.1545306918088530
0.4056302685713933 0.0003262980865450 0.1538849254407836
0.2008672435378165 0.4012316068953615 0.1543581693706739
0.4011797453286332 0.2008881215030870 0.1543472245726673
0.2024953227864608 0.2027245568027246 0.1540493575352928
0.6019694654342177 0.0005635559943436 0.1545055119024007
0.0009103963246676 0.9999378857441802 0.1551495224350336
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0.2093361544497089 0.9999752882837000 0.1546698363924854
0.8673546784807982 0.8672517981697820 0.1030601019616434
0.6670059948147543 0.6670065383327785 0.1031218819380892
0.6672517360287801 0.8669210308938423 0.1031634759370913
0.4667917596059412 0.8668066763773794 0.1031858330032387
0.8669569907786469 0.6671964958489798 0.1031735078498815
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0.2664307632031015 0.6679438117180130 0.1035114906255699
0.2659153240819067 0.8672969131503251 0.1041071408188445
0.0683845685020696 0.8676845052466692 0.1041523260330083
0.6680552047386300 0.2663390685590374 0.1035432682319370
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0.8671917082046964 0.2658852290713530 0.1041028178566963
0.8678522335278906 0.0682866358438672 0.1041717608132692
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0.0672304690075874 0.6675117105177116 0.1031487237273749
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0.3333299999999966 0.1333300000000008 0.0521799999999999
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0.7999900000000011 0.2000000000000028 0.0000000000000000
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0.0000000000000000 0.3999900000000025 0.0000000000000000
0.0000000000000000 0.5999899999999982 0.0000000000000000
0.3999900000000025 0.0000000000000000 0.0000000000000000
0.2000000000000028 0.3999900000000025 0.0000000000000000
0.3999900000000025 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.2000000000000028 0.0000000000000000
0.5999899999999982 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.0000000000000000 0.0000000000000000
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0.0154920472345369 0.7783209870801067 0.2442487630989822
0.7897403987055981 0.9978740915583203 0.2442448611156453
0.7800828168030581 0.1901872000399290 0.2148838323337886
0.9844895900976428 0.2095983856176135 0.2031930775649921
0.1082102485148889 0.9946837606850839 0.2107368415407849
0.1099219673295296 0.8820167382964292 0.2201578241511519
0.0031760519756163 0.8851893850636391 0.2347206815461252
0.8942561681614132 0.9911264049101697 0.2347057536507149

0.8851828633487048 0.1006675396674131 0.2201385921385703
0.9946531291380675 0.1049897613928324 0.2106544288956974
0.1006189074523850 0.7180893136547155 0.2391844582112729
0.7265521167369192 0.0817580734917384 0.2392266701005140

Monomer ii on Cu(111) -DFT-D2
Cu O C H
1.00000000000000
12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
100 6 6 2
Direct
0.8007501556083627 0.8005229239044892 0.1548752568395629
0.3989477612536516 0.8002571656778702 0.1547870351684750
0.8006277738646583 0.3987699220195552 0.1549009759775590
0.6001144345306827 0.8007109330210309 0.1544454718167534
0.8008114160816224 0.5995501818103227 0.1543429609193348
0.6000534281057052 0.5992067261483622 0.1543192866842444
0.0000903272226685 0.8014939018222419 0.1550170554401940
0.3999511898323623 0.4000872244490184 0.1545273693851305
0.1973440683572498 0.8004857117871280 0.1549825319264171
0.3998097509137572 0.5987892168111028 0.1545877096472600
0.1991993887873321 0.6002100490219949 0.1550578043089465
0.8022531673188020 -0.0009245941615469 0.1548693753529942
0.5998277275234952 0.3992008368566493 0.1544051706533827
0.8010776871755119 0.1975374376385657 0.1554761890673246
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0.0006541387188236 0.5996116936196929 0.1547557380451649
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0.0000000000000000 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.0000000000000000 0.0000000000000000
0.9951184069922653 0.2127902061434796 0.2095290810968127
0.7881157768013355 0.1976098780027169 0.2094771448178180
0.7814537915453725 0.9947694963704421 0.2338623637845311
0.0085102922388988 0.7841595077462827 0.2371924837116901
0.2206796124012179 0.7824269499756238 0.2202504360279655
0.2224293889115088 0.0017391918800241 0.2038292062451185
0.0061922691108413 0.1114320492947199 0.2127677998140792
0.8872481689364773 0.1044122545772618 0.2168041960105484
0.8893617921614284 0.9953332880505618 0.2291016763068130
0.0040225107184211 0.8928264918962723 0.2310280764578105
0.1273117581333502 0.8834143067175555 0.2211250782501520

0.1255167328557818 -0.0005799490620670 0.2122822196236620
0.8117156500985336 0.9089393578315039 0.2411380211785014
0.0954572268567551 0.7330077580760661 0.2374029425866215

Monomer iii on Cu(111) -DFT-D2
Cu O C H
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12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
100 6 6 2
Direct
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0.4049164258899600 0.7979098968002148 0.1547550972736923
0.7972858232835178 0.4042807810941827 0.1546195928558374
0.6021988242387564 0.7997916115577129 0.1543134324862501
0.8005331195314606 0.6012682222686092 0.1543376141897681
0.6010580274695023 0.6004731915365157 0.1544188036128594
0.9986858589433448 0.7993029631831162 0.1532988155409630
0.4002434185632656 0.3999207503173178 0.1540922994612696
0.2068600647927966 0.7906898974506051 0.1567576108908218
0.4036438112717831 0.5971645837083966 0.1541235185758552
0.2003206105828493 0.5974858870026585 0.1544561168827394
0.7991048945825012 0.9969149668447761 0.1523078488854257
0.5976486430232772 0.4026785980464427 0.1540736891254013
0.7896155402958716 0.2050334433863265 0.1564711783360867
0.5964435613342794 0.1994655441088695 0.1541314428784402
0.0001888083254667 0.4048246033693010 0.1540903434205206
0.0004555557539904 0.6009218370268771 0.1543226524326550
0.4051524014534399 -0.0000859607684773 0.1540821601340906
0.2007911949885189 0.4003861833248559 0.1541915870970539
0.4001695791697460 0.2003737891718138 0.1542455961632551
0.2016750657253793 0.2025966411574210 0.1542216422657027
0.6009771571428508 -0.0001397044051220 0.1541913697921444
0.0009633349384990 0.9997026604079881 0.1547993766274472
-0.0012378114808350 0.2099220242218360 0.1551982616776440
0.2093887978370410 0.0006609674091555 0.1550962882704684
0.8678507711185742 0.8663634358808451 0.1025793000046927
0.6671160321964776 0.6667458790322721 0.1032750409766239
0.6672408487099774 0.8665820077418349 0.1032073987900850
0.4666635040883372 0.8667033678079378 0.1033910569030995
0.8670902734246584 0.6666010923268009 0.1032519856164968
0.8668875567834281 0.4661452049477636 0.1033733506119504
0.2662408615086399 0.6681862546681235 0.1037808609529994
0.2656453238177073 0.8673696939917462 0.1046225412700773
0.0691923003386573 0.8675033726302178 0.1043154260954829
0.6679775887556690 0.2660676046626576 0.1036637448240498
0.4663942948835328 0.6674123010197986 0.1033660948219301
0.6672529632853933 0.4663600986116344 0.1033092832819128
0.4667419056500106 0.4668606193400054 0.1029768194370221
0.8668060020693239 0.2653204336421084 0.1045593185060506
0.8681191108246230 0.0685298328406238 0.1040241586707835
0.2667608293957023 0.2666670894449109 0.1031525089143675
0.0680027657059599 0.6664255592905460 0.1031613146957818
0.2671780419017003 0.4671294736279035 0.1031096877946917
0.0672383753881859 0.4667249715773606 0.1031626880065988
0.4669499969677341 0.2671333878535772 0.1030049933453115
0.6664941542372917 0.0675715971807016 0.1028143706688300
0.4669826215323981 0.0669717148842030 0.1031047166933506
0.0663738070955835 0.2663049673475689 0.1034883606103872
0.2668083614960577 0.0665137700286626 0.1034250119971073
0.0680548369912570 0.0678716271327094 0.1045694362045110

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0.0000000000000000 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.0000000000000000 0.0000000000000000
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0.7995704718726805 0.9611758152883947 0.2286234126202213
0.7755377648634574 0.1750719653536653 0.2076460404098461
0.9784423530859868 0.2059711784965603 0.2033151252994145
0.1088801973576464 0.9901303251540418 0.2086075920244762
0.1185857378151242 0.8702895972105491 0.2141890463826600
0.0119426513035978 0.8667347569737519 0.2248252490153576
0.8996745743999041 0.9704884694403968 0.2231656316663062
0.8843483843791810 0.0859918747540688 0.2126792671169015
0.9908823789265039 0.0984167513931262 0.2079396399116810

0.9453797730519857 0.7673202029492406 0.2366241684979844
0.7294013081207172 0.0382313115620109 0.2213715611698112

Monomer iv on Cu(111) -DFT-D2
Cu O C H
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12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
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Direct
0.7989227363789594 0.7980411685606988 0.1546575956946580
0.4053733736787644 0.7985238733183048 0.1547950344420266
0.7979781583136257 0.4050376722085496 0.1547815231009662
0.6013581395922197 0.7995211250637505 0.1543273694736084
0.7998597268536881 0.6007830674423755 0.1543446316805874
0.6006020308432691 0.6005597082451993 0.1542736781106601
0.0018311445539581 0.7912084046092666 0.1556116924133161
0.4000834206423570 0.3998936975865606 0.1540841721960888
0.2107112268925198 0.7916754001995092 0.1553906545555152
0.4036775765459201 0.5969106330605481 0.1539891568572670
0.2029185554449664 0.5963496278949199 0.1543774654570007
0.7916914168239676 0.0004602189944297 0.1555321570298767
0.5967015526639871 0.4035694934223155 0.1539241520137208
0.7908710803040042 0.2099022274401612 0.1550728011816765
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0.0004308645134290 0.4042598121048784 0.1539521204087861
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0.4004680211002406 0.2008299326803967 0.1541155207736220
0.2027928133842382 0.2034109999203324 0.1545741591755459
0.5976313861130171 1.0000276244469644 0.1540076011331172
0.0007620789598856 0.0009633693167317 0.1547099256162950
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0.2098769214161051 0.0020069140755390 0.1552271100786127
0.8682603717411678 0.8676980819068884 0.1044380409889836
0.6669016265826655 0.6667277682718643 0.1032208741708781
0.6677231332714542 0.8666735070713574 0.1033020542591102
0.4663771572408231 0.8668767471879238 0.1033381937748546
0.8669062539998075 0.6673295419982086 0.1033005128525227
0.8668693506450853 0.4660923288695599 0.1033535898339728
0.2658996944854379 0.6681844037027788 0.1034599649985363
0.2649919437211961 0.8684028068174651 0.1043523330617531
0.0673978659199371 0.8664134189848650 0.1048611043875013
0.6675606106185344 0.2660017537811666 0.1033451776942352
0.4660242617091997 0.6676966621811888 0.1033404651023520
0.6674947381948412 0.4660676441098308 0.1033275830489059
0.4665451781564920 0.4668241866448427 0.1029193364030764
0.8678931390475324 0.2649935171374178 0.1042129097308363
0.8664431016636328 0.0671090932679103 0.1048022963395191
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0.0667211197162190 0.6679268817755116 0.1034791429980029
0.2665687312677646 0.4675441508669553 0.1030032621836601
0.0671640544770819 0.4668581226466131 0.1029456600402950
0.4674146643733572 0.2665371840765031 0.1030164930522892
0.6681115014173303 0.0664640818990299 0.1034713164175562
0.4669455113629476 0.0670686069919366 0.1029594997966120
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0.7922155819720432 0.0038422422656104 0.2057332139657719
0.7875185653493433 0.2218984577992100 0.2055302705074545
0.0005938232523135 0.2267328974720387 0.2057508295809390
0.1198663303243803 0.0112388440778039 0.2099701422186282
0.1221530663225382 0.8945142176389359 0.2097868398747333
0.0078580204150340 0.8921559135031563 0.2095846928318691
0.8912954349112541 0.0061435568295852 0.2095508749474669
0.8885967996388007 0.1229945129988759 0.2096002987559918
0.0028016489103905 0.1257399582831277 0.2098107147000429
0.8061558013273350 0.7089831505850457 0.2615095833436326

0.7944512134471161 0.7683035857147840 0.2544259306433823

Monomer i on Cu(111) -vdW-DF2
Cu O C H
1.00000000000000
12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
100 6 6 2
Direct
0.7989227363789594 0.7980411685606988 0.1546575956946580
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0.7979781583136257 0.4050376722085496 0.1547815231009662
0.6013581395922197 0.7995211250637505 0.1543273694736084
0.7998597268536881 0.6007830674423755 0.1543446316805874
0.6006020308432691 0.6005597082451993 0.1542736781106601
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0.4000834206423570 0.3998936975865606 0.1540841721960888
0.2107112268925198 0.7916754001995092 0.1553906545555152
0.4036775765459201 0.5969106330605481 0.1539891568572670
0.2029185554449664 0.5963496278949199 0.1543774654570007
0.7916914168239676 0.0004602189944297 0.1555321570298767
0.5967015526639871 0.4035694934223155 0.1539241520137208
0.7908710803040042 0.2099022274401612 0.1550728011816765
0.5962642477329901 0.2021887411646239 0.1543673063583841
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0.3999900000000025 0.3999900000000025 0.0000000000000000
0.2000000000000028 0.7999900000000011 0.0000000000000000
0.3999900000000025 0.5999899999999982 0.0000000000000000
0.2000000000000028 0.5999899999999982 0.0000000000000000
0.7999900000000011 0.0000000000000000 0.0000000000000000
0.5999899999999982 0.3999900000000025 0.0000000000000000
0.7999900000000011 0.2000000000000028 0.0000000000000000
0.5999899999999982 0.2000000000000028 0.0000000000000000
0.0000000000000000 0.3999900000000025 0.0000000000000000
0.0000000000000000 0.5999899999999982 0.0000000000000000
0.3999900000000025 0.0000000000000000 0.0000000000000000
0.2000000000000028 0.3999900000000025 0.0000000000000000
0.3999900000000025 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.2000000000000028 0.0000000000000000
0.5999899999999982 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.0000000000000000 0.0000000000000000
0.2187520352165749 0.0133380207767751 0.2060365668275000
0.2232446767826674 0.7956184001448341 0.2057602656582518
0.0099837405871183 0.7908819231969311 0.2057206214627311
0.7922155819720432 0.0038422422656104 0.2057332139657719
0.7875185653493433 0.2218984577992100 0.2055302705074545
0.0005938232523135 0.2267328974720387 0.2057508295809390
0.1198663303243803 0.0112388440778039 0.2099701422186282
0.1221530663225382 0.8945142176389359 0.2097868398747333
0.0078580204150340 0.8921559135031563 0.2095846928318691
0.8912954349112541 0.0061435568295852 0.2095508749474669
0.8885967996388007 0.1229945129988759 0.2096002987559918
0.0028016489103905 0.1257399582831277 0.2098107147000429
0.8061558013273350 0.7089831505850457 0.2615095833436326
0.7944512134471161 0.7683035857147840 0.2544259306433823

Monomer ii on Cu(111) -vdW-DF2
Cu O C H
1.00000000000000
12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
100 6 6 2
Direct
0.7999647818459525 0.7999345595242519 0.1635314152795916
0.4001351657207248 0.7999518576844356 0.1636671763076643
0.7999794240681548 0.4001074679584999 0.1636703003441196
0.6000673605573995 0.8001160608548856 0.1635906514515084
0.8001543615527161 0.6000311209789541 0.1635803290941763
0.5999706213818622 0.5999836417473533 0.1635523440578293
0.9999077066758031 0.7997821436201422 0.1631812638372241
0.3999491425215670 0.4000993828840284 0.1636374170926839
0.2000697458580785 0.7997596132281939 0.1634452692348061
0.4001065400503976 0.5998298340797261 0.1636623788232590
0.1999825036977062 0.5999116715432894 0.1635982314645259
0.7999533254309120 0.9997276282821647 0.1632414960276132
0.5997758682141863 0.4002168246587476 0.1636406624327218
0.7998416749773218 0.1999787413613848 0.1635130403051376
0.5998667160964359 0.2000061149082456 0.1636952647289368
0.0000061745365825 0.4001283175094317 0.1636726933296846
-0.0000129013244835 0.5998169728290867 0.1636052401289923
0.4000913521269617 0.9999759018608255 0.1637021558422160
0.1998618912540031 0.4001815389425733 0.1636449284416695
0.4000857934166543 0.1998785560401888 0.1636184286446280
0.2000802940237754 0.2000861796274003 0.1637650467333583
0.5998587755400215 0.9998517195308392 0.1635906155349574
0.0001586380006840 0.9998708995158748 0.1632245870475592
-0.0000278255014667 0.1999399186018300 0.1635747984534510
0.1999581289683882 0.9999309058518313 0.1636040105873773
0.8666291274312695 0.8666227756850038 0.1075252087907925
0.6666673151556144 0.6666620039627702 0.1076843446306657
0.6666117426772564 0.8666243571493113 0.1075970871625528
0.4666812561929444 0.8666352594171253 0.1076842265387636
0.8666568162186001 0.6665972043146609 0.1076081408243378
0.8666379630833155 0.4666834678404572 0.1076809735997496
0.2666144829120279 0.6665531770196278 0.1076849823437960
0.2667147042380466 0.8666486819507329 0.1076865457945825
0.0667823691020370 0.8664439236754652 0.1075072634449928
0.6665603859378364 0.2665983439011879 0.1077529198341130
0.4666808212072881 0.6666632412361033 0.1076907428271152
0.6666604236423721 0.4666993677947274 0.1076885599107983
0.4666229067871764 0.4666478308974555 0.1076720087057274
0.8666444143196731 0.2666995964375748 0.1077045564209537
0.8664630837044163 0.0667620732813419 0.1075723053970323
0.2666140221049242 0.2666399153606613 0.1077010328762022
0.0668708409037364 0.6664585367640153 0.1075825769720760
0.2666590965125513 0.4666630259858462 0.1076439093256235
0.0667124598922214 0.4666242489342375 0.1076524707834979
0.4666790023558964 0.2666560942576989 0.1077009036101022
0.6664557325291642 0.0668835820541170 0.1076516995599078
0.4666159494291481 0.0667064299174867 0.1076687222411407
0.0668379445015878 0.2665873471212653 0.1077781885889958
0.2665956711634409 0.0668291618006408 0.1077858411518065
0.0667783527591844 0.0667597924981162 0.1076130889092784
0.9333200000000019 0.9333200000000019 0.0521799999999999
0.5333299999999994 0.9333200000000019 0.0521799999999999
0.9333200000000019 0.5333299999999994 0.0521799999999999

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0.5333299999999994 0.5333299999999994 0.0521799999999999
0.3333299999999966 0.9333200000000019 0.0521799999999999
0.5333299999999994 0.7333199999999991 0.0521799999999999
0.3333299999999966 0.7333199999999991 0.0521799999999999
0.9333200000000019 0.1333300000000008 0.0521799999999999
0.7333199999999991 0.5333299999999994 0.0521799999999999
0.9333200000000019 0.3333299999999966 0.0521799999999999
0.7333199999999991 0.3333299999999966 0.0521799999999999
0.1333300000000008 0.5333299999999994 0.0521799999999999
0.1333300000000008 0.7333199999999991 0.0521799999999999
0.5333299999999994 0.1333300000000008 0.0521799999999999
0.3333299999999966 0.5333299999999994 0.0521799999999999
0.5333299999999994 0.3333299999999966 0.0521799999999999
0.3333299999999966 0.3333299999999966 0.0521799999999999
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0.3333299999999966 0.1333300000000008 0.0521799999999999
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0.5999899999999982 0.5999899999999982 0.0000000000000000
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0.2000000000000028 0.7999900000000011 0.0000000000000000
0.3999900000000025 0.5999899999999982 0.0000000000000000
0.2000000000000028 0.5999899999999982 0.0000000000000000
0.7999900000000011 0.0000000000000000 0.0000000000000000
0.5999899999999982 0.3999900000000025 0.0000000000000000
0.7999900000000011 0.2000000000000028 0.0000000000000000
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0.0000000000000000 0.3999900000000025 0.0000000000000000
0.0000000000000000 0.5999899999999982 0.0000000000000000
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0.2000000000000028 0.3999900000000025 0.0000000000000000
0.3999900000000025 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.2000000000000028 0.0000000000000000
0.5999899999999982 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 0.2000000000000028 0.0000000000000000
0.2000000000000028 0.0000000000000000 0.0000000000000000
0.9934792819496966 0.2184611359401609 0.2491779516586259
0.7823092966419674 0.2042477248569879 0.2489263756208565
0.7907727871212222 0.9868111449236271 0.2500266530215509
0.0114593877044682 0.7775969189674585 0.2503085447212658
0.2174301798415704 0.7824141438024055 0.2492758744803151
0.2186696560364060 0.0040583605094323 0.2490903229354767
0.9998004436489617 0.1197146935774704 0.2497944508515393
0.8820777048808860 0.1119784823197689 0.2500813335506680
0.8952956409586574 0.9901889118811245 0.2508090469469355
0.0068046674971256 0.8863769962251266 0.2508990162716505
0.1234606024344480 0.8827413238393260 0.2501699291197318
0.1236908603686577 0.0019429961233783 0.2497440440146526
0.8088879322258926 0.9027413717858452 0.2498352585056217
0.0980905668600823 0.7153630818973832 0.2498514908524087

Monomer iii on Cu(111) -vdW-DF2
Cu O C H
1.00000000000000
12.7810000000000006 0.0000000000000000 0.0000000000000000
6.3905000000000003 11.0686699999999991 0.0000000000000000
0.0000000000000000 0.0000000000000000 40.0000000000000000
100 6 6 2
Direct
0.8000764778646540 0.7999286241806879 0.1638161971263025
0.4001661674759750 0.7999751093750395 0.1636726044584075
0.7999791180331695 0.4001340810759249 0.1636709457754643
0.6001713185824736 0.8001163937075609 0.1636271061829444
0.8001426449367505 0.6001396421856470 0.1636391524837008
0.6000185754712908 0.6000008418729000 0.1635366236355734
0.9996930623782142 0.7998850331535085 0.1631661401863516
0.4000138878335274 0.4000291996711017 0.1635945582389547
0.2000303968006672 0.7998398869011953 0.1634271982504698
0.4001962876125217 0.5998091491248738 0.1636450978200583
0.1999110408146675 0.5999362953063943 0.1636764924889853
0.7999698843234155 0.9995917698260209 0.1632221086931995
0.5998318758502502 0.4001823133988639 0.1636348915211474
0.7998371565255649 0.1999470010645638 0.1635290556302514
0.5999252425973793 0.1999194042793602 0.1636808500826356
0.9999521917874765 0.4001558019682865 0.1636875222535202
0.9997298082547839 0.5999758441183354 0.1636469613005801
0.4001409658453121 0.9999539068320642 0.1636900301109335
0.1997972687541212 0.4001636781238478 0.1635959137427055
0.4001254439054837 0.1998243668695365 0.1635904892257452
0.2000645587871476 0.2000880553141037 0.1637587637504881
0.5999541789357079 0.9997337616183150 0.1636128237415525
0.0000677388800911 0.9999215511620989 0.1631664224273255
0.9999299689523788 0.1999635117978001 0.1636306726438863
0.1999355053922156 -0.0000104894434209 0.1635954318584560
0.8665751724012311 0.8665822105549029 0.1074745722911669
0.6666992126420613 0.6666829604135995 0.1076923551690874
0.6666883696224815 0.8665751419434071 0.1076084696510438
0.4667390349113106 0.8666140944507160 0.1076862139900455
0.8665922476799718 0.6666596996472702 0.1075885843005931
0.8666122875538925 0.4667368918262361 0.1076848032590748
0.2665851771318699 0.6665554623529044 0.1077507351783951
0.2667308662088155 0.8666535685745144 0.1076893366502041
0.0667488845314547 0.8664254714291499 0.1075061780608836
0.6665803645215940 0.2665771645054636 0.1077615732465405
0.4667047718498708 0.6666710336923631 0.1076845675737330
0.6666748427889092 0.4667049064750723 0.1076786989641318
0.4666484736956616 0.4666433730373998 0.1076663924475519
0.8666396636174664 0.2667155633802382 0.1077102638826829
0.8664270537625377 0.0667521267914799 0.1075491426932881
0.2666092524071526 0.2666236692301203 0.1076801956524447
0.0668580476318466 0.6664421868508954 0.1076143788909248
0.2666308345838275 0.4666840236808309 0.1076818724508963
0.0666459038881266 0.4666771140690840 0.1076708310147767
0.4666939861113765 0.2666311429867314 0.1076818181524119
0.6664715774755514 0.0668472467773120 0.1076457732127361
0.4666677714489232 0.0666560417140709 0.1076670915912475
0.0668063626537014 0.2666014162953193 0.1077904088802593
0.2665997159845251 0.0668278874964076 0.1077848131140633
0.0667559766410533 0.0667792503619626 0.1076077325594198
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0.9333200000000019 0.5333299999999994 0.0521799999999999
0.7333199999999991 0.9333200000000019 0.0521799999999999

0.9333200000000019	0.7333199999999991	0.0521799999999999
0.7333199999999991	0.7333199999999991	0.0521799999999999
0.1333300000000008	0.9333200000000019	0.0521799999999999
0.5333299999999994	0.5333299999999994	0.0521799999999999
0.3333299999999966	0.9333200000000019	0.0521799999999999
0.5333299999999994	0.7333199999999991	0.0521799999999999
0.3333299999999966	0.7333199999999991	0.0521799999999999
0.9333200000000019	0.1333300000000008	0.0521799999999999
0.7333199999999991	0.5333299999999994	0.0521799999999999
0.9333200000000019	0.3333299999999966	0.0521799999999999
0.7333199999999991	0.3333299999999966	0.0521799999999999
0.1333300000000008	0.5333299999999994	0.0521799999999999
0.1333300000000008	0.7333199999999991	0.0521799999999999
0.5333299999999994	0.1333300000000008	0.0521799999999999
0.3333299999999966	0.5333299999999994	0.0521799999999999
0.5333299999999994	0.3333299999999966	0.0521799999999999
0.3333299999999966	0.3333299999999966	0.0521799999999999
0.7333199999999991	0.1333300000000008	0.0521799999999999
0.1333300000000008	0.1333300000000008	0.0521799999999999
0.1333300000000008	0.3333299999999966	0.0521799999999999
0.3333299999999966	0.1333300000000008	0.0521799999999999
0.7999900000000011	0.7999900000000011	0.0000000000000000
0.3999900000000025	0.7999900000000011	0.0000000000000000
0.7999900000000011	0.3999900000000025	0.0000000000000000
0.5999899999999982	0.7999900000000011	0.0000000000000000
0.7999900000000011	0.5999899999999982	0.0000000000000000
0.5999899999999982	0.5999899999999982	0.0000000000000000
0.0000000000000000	0.7999900000000011	0.0000000000000000
0.3999900000000025	0.3999900000000025	0.0000000000000000
0.2000000000000028	0.7999900000000011	0.0000000000000000
0.3999900000000025	0.5999899999999982	0.0000000000000000
0.2000000000000028	0.5999899999999982	0.0000000000000000
0.7999900000000011	0.0000000000000000	0.0000000000000000
0.5999899999999982	0.3999900000000025	0.0000000000000000
0.7999900000000011	0.2000000000000028	0.0000000000000000
0.5999899999999982	0.2000000000000028	0.0000000000000000
0.0000000000000000	0.3999900000000025	0.0000000000000000
0.0000000000000000	0.5999899999999982	0.0000000000000000
0.3999900000000025	0.0000000000000000	0.0000000000000000
0.2000000000000028	0.3999900000000025	0.0000000000000000
0.3999900000000025	0.2000000000000028	0.0000000000000000
0.2000000000000028	0.2000000000000028	0.0000000000000000
0.5999899999999982	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	0.2000000000000028	0.0000000000000000
0.2000000000000028	0.0000000000000000	0.0000000000000000
0.2164658463333731	0.0027626688727221	0.2489526662580838
0.2203323174711699	0.7826517227127827	0.2487945309543622
0.0219339181606854	0.7665777711607215	0.2504339959358485
0.7864569431102062	0.9909401356220296	0.2503757393296715
0.7825099759949105	0.1997667694534256	0.2487997820307468
0.9914947680552859	0.2170720402044608	0.2489722583893291
0.1217270326277131	0.0005467944794954	0.2497206615394252
0.1238539739169684	0.8786432847914840	0.2500521479561882
0.0065274515097226	0.8805888269048747	0.2509254504399661
0.8960420659712611	0.9858583574354630	0.2509103071500124
0.8828374648054718	0.1082568522057832	0.2500485397977198
0.9985989946251919	0.1178075451857335	0.2497265535440399
0.9463824407047551	0.7652639138663688	0.2492401143972317
0.7925386583650615	0.9118592948213715	0.2491994076169751

Monomer iv on Cu(111) -vdW-DF2

```
Cu O C H
   1.00000000000000
    12.7810000000000006    0.0000000000000000    0.0000000000000000
     6.3905000000000003   11.0686699999999991    0.0000000000000000
     0.0000000000000000    0.0000000000000000   40.0000000000000000
   100     6     6     2
Direct
  0.7977608097424104  0.7968327618880485  0.1624802285259039
  0.4007064893092180  0.7991424581614044  0.1638004862734654
  0.7998817539107794  0.4001935221176079  0.1636947190036759
  0.5991055201885214  0.7989393311315015  0.1636305796861179
  0.7995292905248149  0.5984643853201468  0.1636569771153520
  0.6000261361644194  0.5993676385408307  0.1635141126951738
  0.9997116917497587  0.7952898119714522  0.1641866342171021
  0.4006616642415491  0.3983759138215748  0.1634774119699896
  0.2040168681381880  0.7967646814268194  0.1620670143333928
  0.4014237147682139  0.5981888448153523  0.1635440769589360
  0.2035024297865035  0.5946534161432021  0.1623361986224598
  0.7968316430174023  0.0005366881616362  0.1653812403042731
  0.5993745311695349  0.4003542817846744  0.1636252719921522
  0.7978304204385783  0.2031937902542897  0.1626501031705498
  0.5980046141679675  0.2010183148905111  0.1632074542189147
  0.0003092726091551  0.3985687177915239  0.1636560738821486
  0.9997254306036455  0.5959260384155289  0.1623634022635529
  0.3995200951549238  0.9994072298119886  0.1636525213492509
  0.2004368603085376  0.3981857442930899  0.1632766527932601
  0.3998174043905132  0.1991763451586351  0.1632999857238404
  0.2004928783267269  0.1994101969588549  0.1635690323628177
  0.5973539323223095  0.9989789270789110  0.1625855194216038
  0.0022765114337220  0.0029677417925884  0.1595407323899379
  0.0004561728793369  0.2007948675845384  0.1626643413377548
  0.2011796004705204  0.9999403221871057  0.1624104792845218
  0.8674279507392303  0.8665309583520158  0.1091993772582194
  0.6666803019414176  0.6662466401454723  0.1075883804026738
  0.6668436574271585  0.8662228027865581  0.1072605609798875
  0.4667234110596167  0.8662313858860989  0.1076322365756448
  0.8666537067432826  0.6662533282149006  0.1072134268936836
  0.8667395734720280  0.4662779215854948  0.1076324913183720
  0.2669693331577584  0.6656708188463084  0.1073909991057373
  0.2668013521902019  0.8660201336189197  0.1074795553236281
  0.0665803346648376  0.8651916570511909  0.1075410712342349
  0.6663179408090170  0.2664159616030327  0.1075098326743307
  0.4668481309634488  0.6662133107977301  0.1076393459637485
  0.6667289952768368  0.4663163245734415  0.1076690206220415
  0.4668552572915274  0.4660672916830164  0.1075105426019679
  0.8665373432795346  0.2664305424562193  0.1074396919334770
  0.8654274402737261  0.0661313471744077  0.1077257497310075
  0.2670443279667902  0.2660853618609623  0.1074337594397872
  0.0661101969058885  0.6670213605514592  0.1080775788710197
  0.2668480972678082  0.4658103297054909  0.1071993527774097
  0.0670104016072054  0.4658955661373072  0.1071776642853285
  0.4671069914420845  0.2657667021360070  0.1073678508617432
  0.6682571766360554  0.0651851039318849  0.1085246659843655
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