

Supporting information to

On the critical role of the substrate: the adsorption behavior of tetrabenzoporphyrins on different metal surfaces

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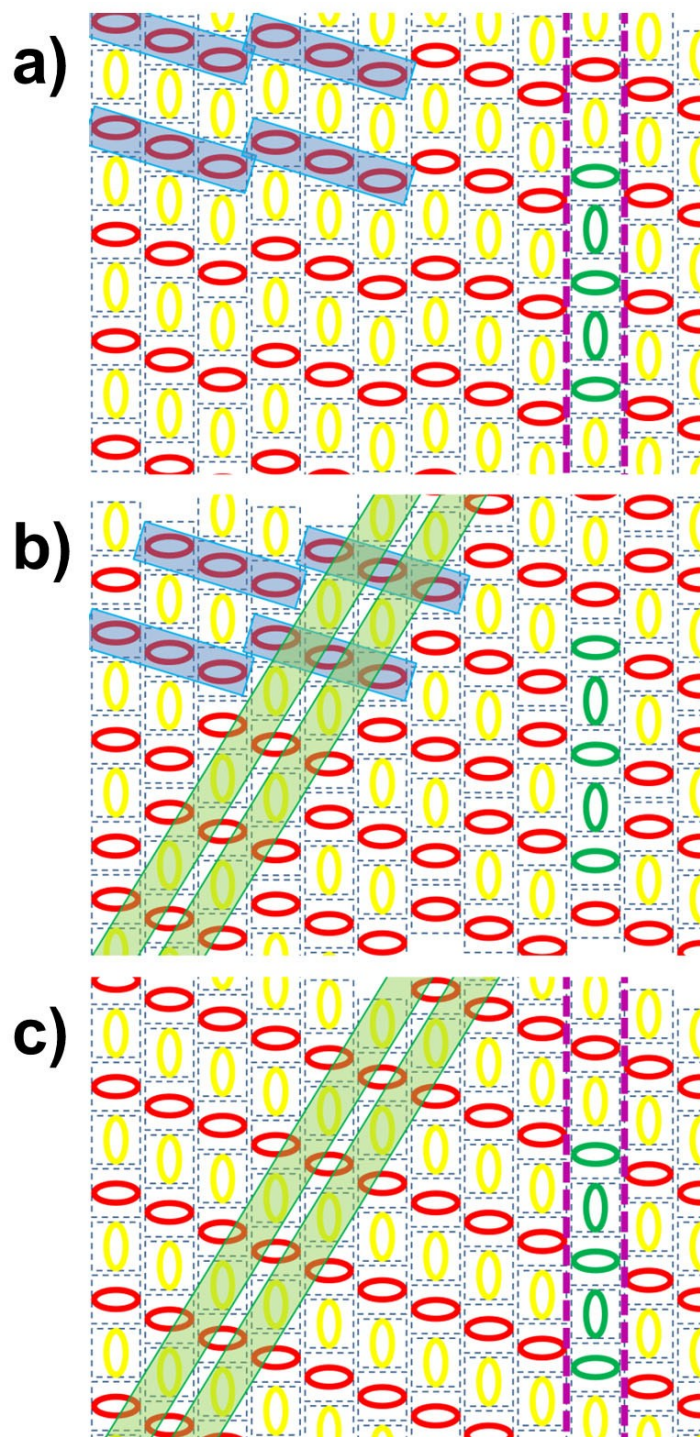


Figure S1. Proposed structural models for 2HTPTBP on Cu(111) with different coverages: (a) relatively low coverage; (b) medium coverage; (c) monolayer coverage. The red and yellow ovals indicate the individual molecules with different orientations. The blue, green, and purple bars highlight the similarities between the structures with different coverages.

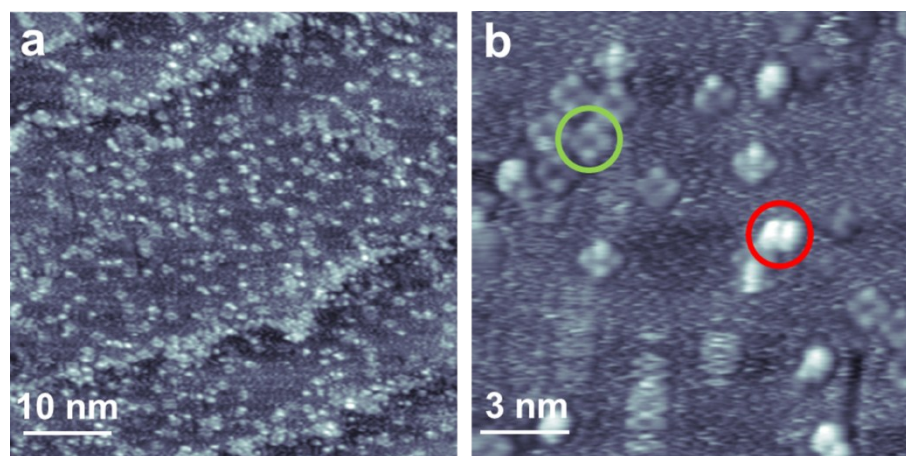


Figure S2. STM images of 2HTPTBP on Cu(110) after annealing to 450 K for 10 min. The intramolecular conformation changes from saddle shape to four-protrusion structure. The red and green circles highlight the intact and the deformed molecules, respectively. The deformed molecules show a four-protrusion conformation, which most probably results from the self-metalation and/or dehydrogenation of 2HTPTBP on Cu(110).

Molecular geometry of 2HTPBP optimized using DFT in the gas phase

Atomic Cartesian coordinates optimized at the BP-D3/SV(P) level of theory; see the main text for further information.

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Energy = -2526.744377580

C	5.4358407	-5.5558644	-0.0484157
C	5.4995854	-4.5314310	0.9132188
C	4.5273341	-3.5194655	0.9280631
C	3.4746985	-3.5231223	-0.0123181
C	3.4164558	-4.5567749	-0.9709163
C	4.3930117	-5.5646679	-0.9919135
C	2.4321675	-2.4524254	0.0080278
C	2.8508847	-1.1516309	-0.3465004
C	4.1305994	-0.7167505	-0.8975519
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C	2.8508847	1.1516309	-0.3465004
N	2.1217143	0.0000000	-0.1250052
C	2.4321675	2.4524254	0.0080278
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C	1.1062450	2.8213285	0.3713255
C	0.7124959	4.1213825	0.9542217
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C	-1.1062450	2.8213285	0.3713255
N	0.0000000	2.0517784	0.1251252
C	-2.4321675	2.4524254	0.0080278
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N	0.0000000	-2.0517784	0.1251252
C	5.2244300	-1.4273153	-1.4466598
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C	1.4243646	5.1972146	1.5261114
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C	-5.2244300	1.4273153	-1.4466598
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C	-1.4243646	-5.1972146	1.5261114
C	1.4243646	-5.1972146	1.5261114
H	-4.5745013	-2.7107073	1.6752642
H	-2.5908594	-4.5620460	-1.7006262
H	-6.3137408	-4.5213481	1.6568043
H	-4.3387733	-6.3650334	-1.7484363
H	-6.2007060	-6.3500261	-0.0622140
H	-4.5745013	2.7107073	1.6752642
H	-2.5908594	4.5620460	-1.7006262
H	-6.3137408	4.5213481	1.6568043
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H	6.3137408	-4.5213481	1.6568043
H	4.3387733	-6.3650334	-1.7484363
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H	-1.1389691	0.0000000	0.1803058
H	1.1389691	0.0000000	0.1803058
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C	6.3004825	0.7079192	-1.9736917
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C	0.7055501	6.2639233	2.0858039
C	-0.7055501	6.2639233	2.0858039
C	0.7055501	-6.2639233	2.0858039
C	-0.7055501	-6.2639233	2.0858039
H	-2.5217426	-5.2064052	1.5602068
H	-1.2530548	-7.1054724	2.5419590
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H	2.5217426	-5.2064052	1.5602068
H	5.2285967	-2.5241987	-1.4841191
H	7.1536570	-1.2532636	-2.4097700
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H	5.2285967	2.5241987	-1.4841191

H	2.5217426	5.2064052	1.5602068
H	1.2530548	7.1054724	2.5419590
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H	-2.5217426	5.2064052	1.5602068
H	-7.1536570	1.2532636	-2.4097700
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