Supporting Information

A Chiral Surface From Achiral Ingredients: Modification of Cu(110) With Phthalic Acid

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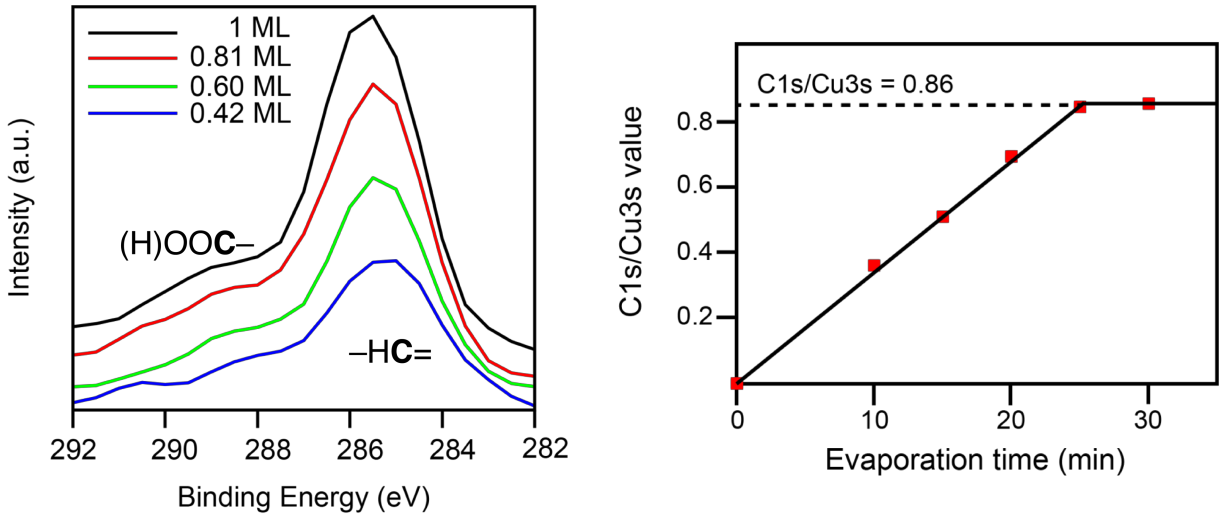

Figure S1. C1s spectra for different amounts of PHTA on the Cu(110) surface with the crystal held at RT during evaporation (left). The high energy shoulder at 288.5 eV represents the carbon in the carboxyl groups and the peak at 285 eV the carbon in the benzo group. At a C 1s/Cu 3s ratio of 0.86 the C 1s signal saturates (left). This coverage has been assigned to one monolayer.

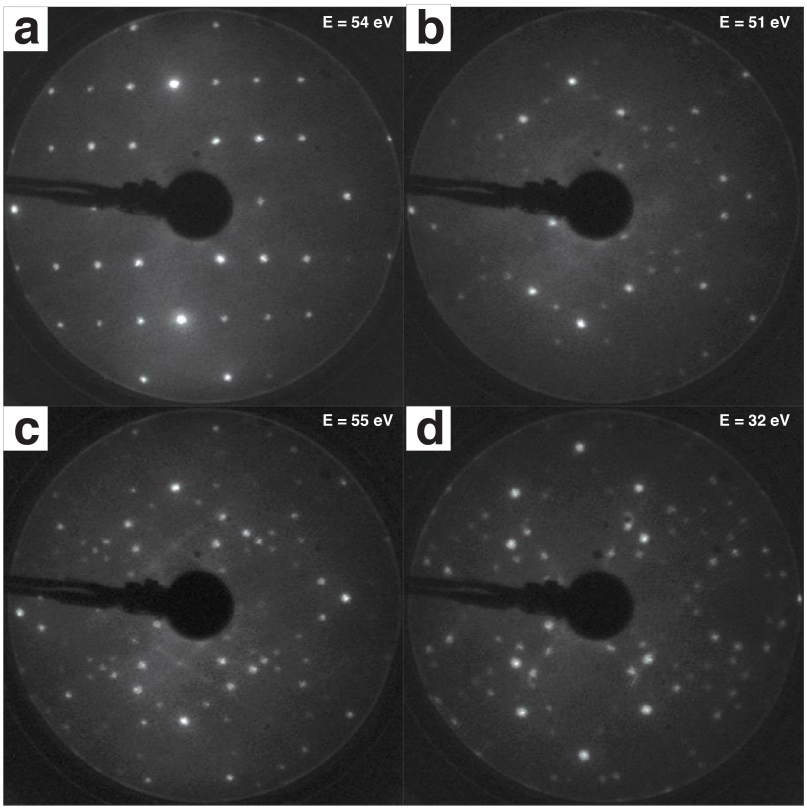

Figure S2. LEED patterns of CHDCA on Cu(110). (a) p2gg(2×4) structure (deposition onto surface at 373 K for 15 to 30 minutes). (b) (1 1, –5 2) structure, preparation as in (a) and annealing at 423 K. The faint lines in the background suggest an additional (2, ±2) periodicity. (c) p2gg(2×4) structure coexisting with a (1 1, –5 2) and a (1 2, –5 4) structure (deposition onto surface at 423 K until saturation coverage is reached). (d) As in (c), but at different primary energy. Note that these structures were also observed for other BADs: p2gg(2×4): FUA, MAL and DMSU; (1 1, –5 2): FUA and MAL; (1 2, –5 4): DMSU.

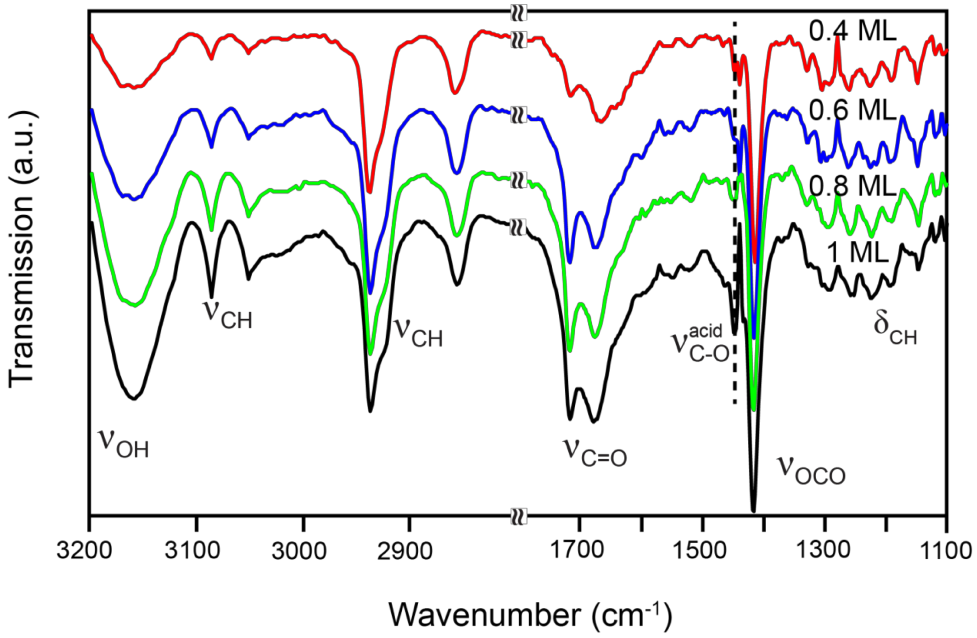

Figure S3. RAIR spectra of CHDA with the Cu(110) surface at room temperature. All spectra are dominated by ν_{CH}, νC=O and νOCO modes, indicating a monocarboxylate on the surface. ν_{CH} modes above 3000 cm^{-1} are not expected for CHDA and are assigned to spectrometer contaminations.

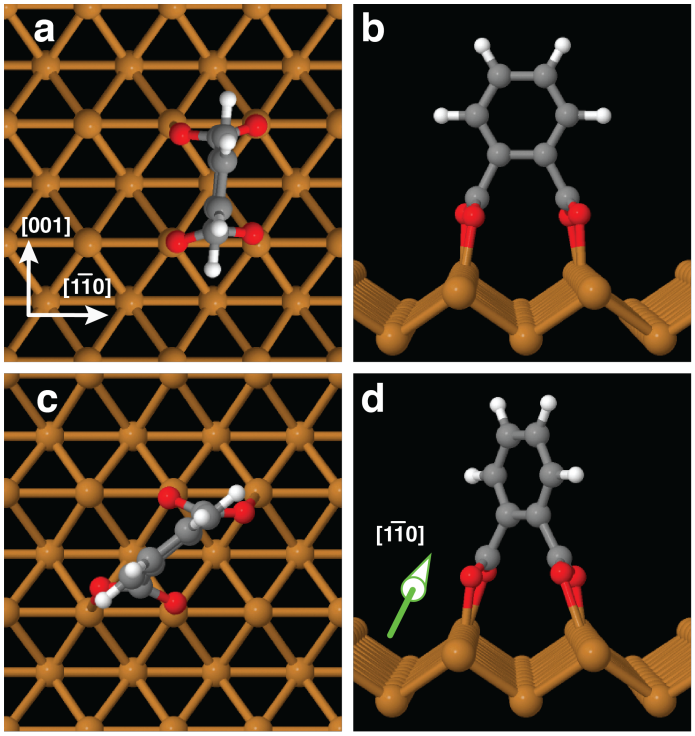

Figure S4. Molecular models derived from DFT calculations for two different adsorption modes of PHTA on Cu(110) as dicarboxylate on a two-layer Cu-slab. The Cu crystal directions are indicated. The PHTA adsorbate is in both modes chirally distorted.

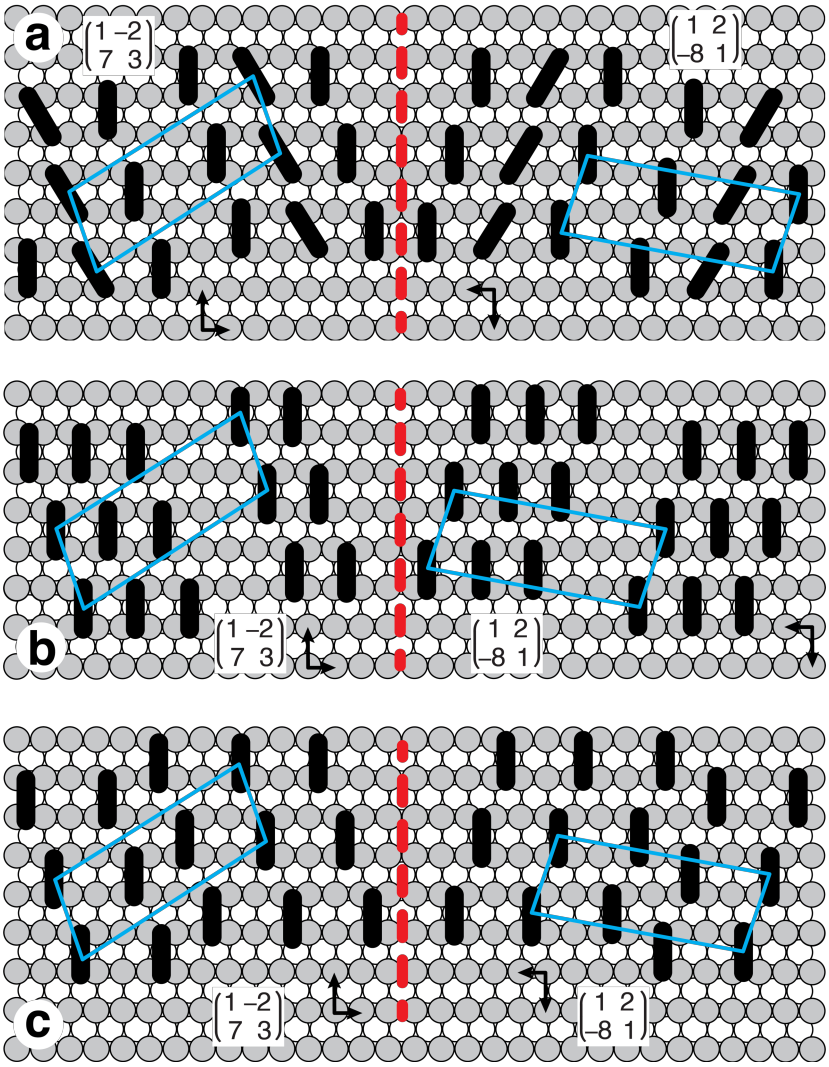

Figure S5. Different structure models for the (1 –2, 7 3) / (1 2, –8 1) enantiomorphs of phthalic acid on Cu(110). Black bars represent the rectangular or oblique diphthalate adsorbate bound to four surface copper atoms. The choices of substrate unit cell vectors are indicated by arrows.

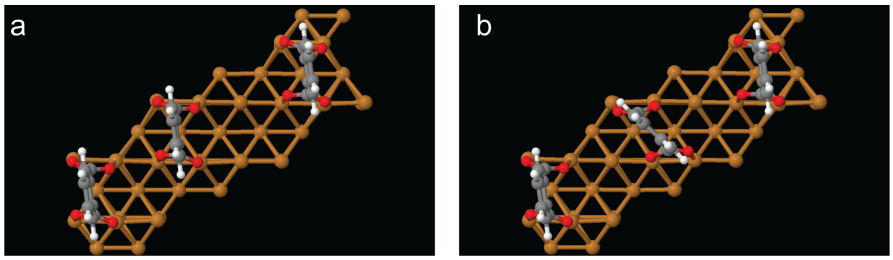

Figure S6. Configurations of the DFT calculation for the two triplet structures, namely three perpendicular footprints (a) and a combination of one oblique and two perpendicular footprints (b).

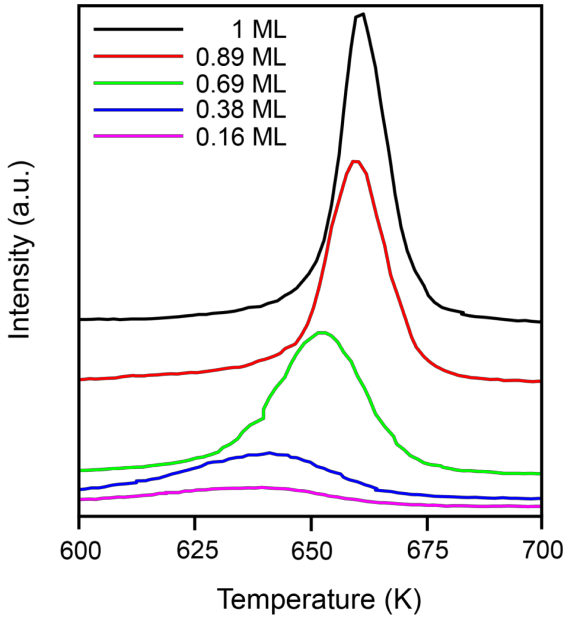

Figure S7. TPD spectra (44 amu) of CHDA showing surface explosion decomposition in a narrow peak shifting from 638 K to 661 K with increasing coverage.