Supporting Information

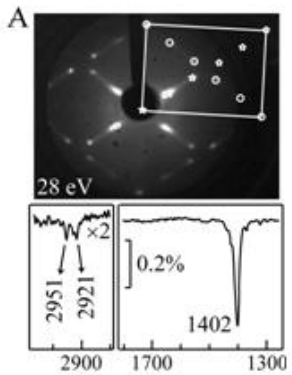
Methods:

Experimental Details: All STM measurements were carried out with a SPECS STM Aarhus 150, which is housed in an ultra-high vacuum chamber with base pressure 2×10^{-10} mbar. All measurements were taken in constant current mode, using a tungsten tip and at a base pressure of 1.5×10^{-10}mbar. Bias voltages are measured at the sample ($V = V_{sample}$). The Cu(110) single crystal was cleaned by repeated Ar^+ sputtering and consecutive annealing to 850 K. After the sample was cooled down to RT, Succinic Acid (99% Sigma Aldrich) was thermally sublimed from a Knudsen cell onto the clean surface held at room temperature. The (5 0, ±1 1) phase is created by heating to about 420K and the recooling to room temperature. LEED data was obtained via a CCD video camera interfaced to a computer. The succinic acid coverage on the Cu(110) surface is quoted in terms of fractional monolayers (ML) quoted with respect to the number density of Cu atoms.

Computational Details: The periodic DFT calculations in this study were performed using version 4.6 of the VASP code [x1], with the standard ultra-soft pseudopotentials and the PW91 version of generalised gradient approximation for the exchange-correlation functional [x2], with a plane-wave cutoff energy of 396 eV The calculations of the bisuccinate in the (5 0, ±11) periodic structure were based on a unit cell that was evaluated directly from LEED and STM data and carried out on a 6×2×1 *k*-point grid. The copper surface was modelled using a five layer slab, with the bottom three layers fixed in their calculated bulk positions and the top two layers allowed to relax. The vacuum separation between the copper slabs was 17 Å, leaving about 10Å between the molecule and the back of the next slab. Adsorption geometries were calculated by placing a bisuccinate molecule above the surface and allowing all molecular atoms and the top two layers of the copper slab to relax until all the forces on the atoms were less than 0.02 eV $Å^{-1}$. For the calculations of the chiral flipping defect structures, a 4x2 supercell of the (5 0, 11) unit cell was used with a defect in the centre. To make the calculations tractable, the slab thickness was reduced to 3 layers with the bottom two layers fixed, and a 3x2x1 k-point grid was used. STM images were calculated using the Tersoff-Hamann approximation in the implementation by Lorente and Persson [x3].

[x1] G. Kresse and J. Furthmuller, Phys. Rev. B, 54 (1996) 11169; G. Kresse and J. Hafner, Phys. Rev. B, 47 (1993) 558.
[x2] 33) Perdew, J. P.; Chevary, J. A.; Vosko, S. H.; Jackson, K. A.; Pederson, M. R.; Singh, D. J.; Fiolhais, C. Phys. Rev. B 1992, 46, 6671.
[x3] Tersoff, J.; Hamann, D. R. Phys. Rev. Lett. 1983, 50, 1998. Lorente, N.; Persson, M. Faraday Discuss. 2000, 117, 277.

LEED and RAIRS data:



Top: LEED Diffraction spots from both the (5 0, -11) and the mirror (1 1,-5 0) enantiomorphs are observed. The unit cell of the clean surface is marked.
Bottom: Reflection Absorption IR Spectroscopy (RAIRS) data show bands that are consistent with the presence of the bisuccinate form only.