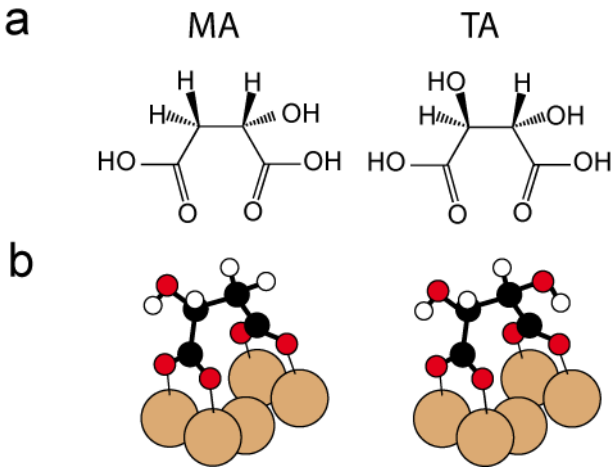
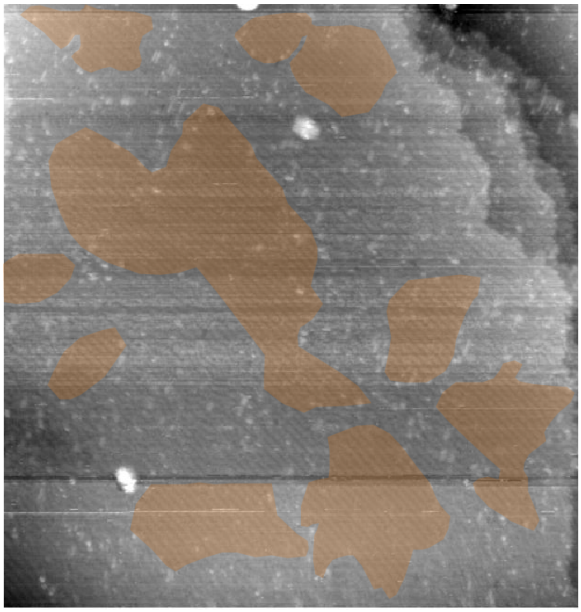
Supplementary Information

# Pasteur's quasiracemates in 2D: chiral conflict between structurally different enantiomers induces single-handed enantiomorphism

Christian Roth, Daniele Passerone and Karl-Heinz Ernst*

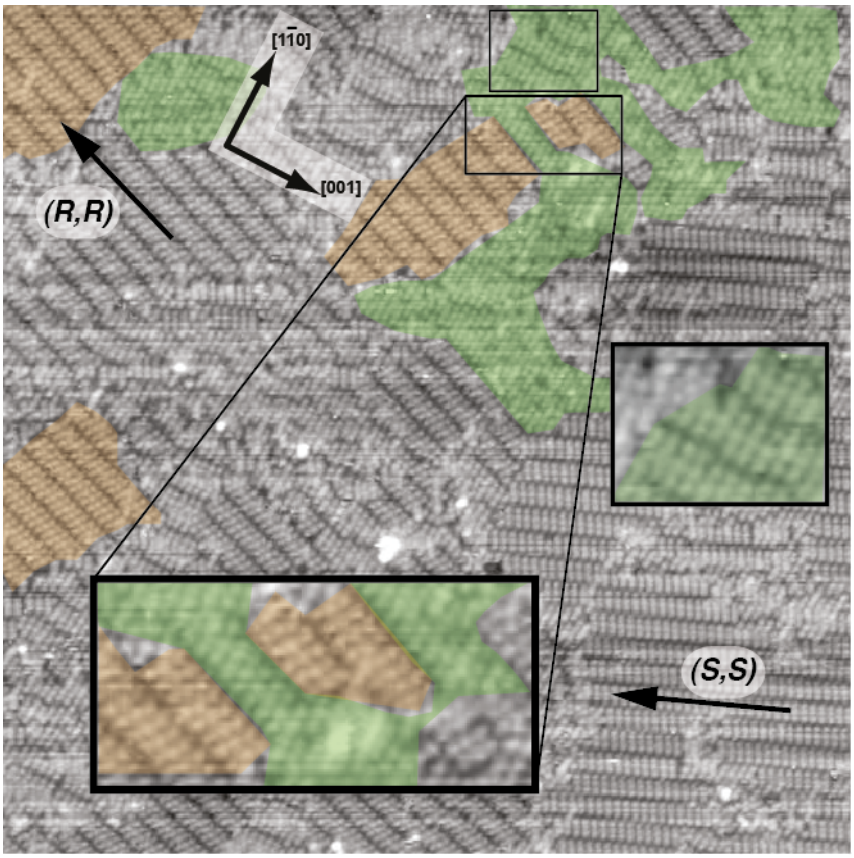



**Supplementary Information Figure 1**. Adsorption modes of tartaric acid and malic acid on Cu(110). (a) Structural formulas for (*S*)-malic acid (MA) and (*S,S*)-tartaric acid (TA). (b) Sketches for bimalate (left) and bitartrate (right) in the adsorbed state.



**Supplementary Information Figure 2**. Long-range STM scan (180 nm × 190 nm, U = –1930 mV, I = 65pA). About 33% of the surface is covered with (1 2, –9 0) domains (orange).

* e-mail: karl-heinz.ernst@empa.ch




**Supplementary Information Figure 3**. STM image (70 nm × 70 nm, U = - 2V, I= 50 pA) showing the coexistence of all phases at a ratio of 90% *rac.*-TA to 10% *(R)*-MA. The *(S,S)*-TA domains are still of substantial size. Some of the *(R,R)*-TA areas are coloured in orange. Triplets in the enantiopure (1 2, –9 0) domains are aligned along the [1 $\bar{1}$ 1] direction, i.e. the trimer rows run parallel to the [1 $\bar{1}$ 4] direction. The green areas show examples where the molecules are aligned along the [1 $\bar{1}$ 0] direction. The insets show the presence of triplets in the green areas, one row going through a (1 2, –9 0) island.

## DFT calculations

For DFT modelling we used a Gaussian plane wave (GPW) approach as implemented in the code cp2k in the local density approximation (LDA). The electron-ion interaction was described by the norm-conserving pseudo-potentials of Goedecker-Teter-Hutter (GTH) and we used a TZV2P basis set for all elements of the molecule, and DZVP basis sets for the copper atoms; all bases are optimized for molecular and condensed phase systems. Our Cu(110) was modelled with 4 layers of 24 atoms each. Only the top line was allowed to relax during our geometry optimizations. A vacuum region of 20 Å was included in the direction orthogonal to the surface, and full periodic boundary conditions were adopted