Supporting Information

Molecules coining patterns into a metal: the hard core of soft matter

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Estimate of step formation energy

A reliable estimate of the change in cohesion energy accompanying the creation of a pair of steps was estimated by employing effective medium theory. The cohesion energy E per atom can be described by the number of nearest and next nearest neighbours, N_1 and N_2, respectively, which yields for a *fcc* lattice

$$E(N_1, N_2) \approx V_2(12 - N_1) + \tfrac{1}{2} V_3(12 - N_1)^2 + V_2'(6 - N_2),$$

where V_2 and V_2' denote the effective nearest and next-nearest neighbor pair potentials and V_3 is the effective nearest neighbor three-body interaction potential (S1). Using previously published parameters for the pair potentials of copper (S1) and considering the change in coordination accompanied with the creation of a pair of steps thus yields a reconstruction energy per (1×5) unit cell of the underlying copper surface of

$$\Delta E_{rec} = E_{(110)} - E_{(110)\text{-}(1x5)} = -4\,V_3 + 2\,V_2' = 0.04 \text{ eV}.$$

Considering that this energy has to be expended 5 times to form a (5×5) unit cell of the HT phase which on the other hand contains 2 molecules and thus yields a reconstruction energy of about 0.1eV per adsorbed perylene molecule.

(S1) O.B. Christensen and K.W. Jacobsen, *Phys. Rev. B* **1992**, ***45***, 6393.