HOW DOES PENTAGONAL MOLECULES SELF-ASSEMBLE ON A SIX-FOLD SYMMETRY SURFACE?
THE CASE OF PENTA-TERT-BUTYL-CORANNULENE MOLECULE ON CU(111)

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Among point group symmetries, five-fold rotational symmetry plays a special role because of its incompatibility with translational symmetry. Our focus is on tiling of penta-tert-butyl-corannulene molecules (PTBC, $C_{40}H_{50}$) on a hexagonal Cu(111) surface. Corannulene buckybowl is the smallest separable fullerene C_{60} fragment, and in the study it is functionalized with five tert-butyl legs in order to enhance the five-fold symmetrical properties.

We have investigated the deposition of PTBC submonolayer on Cu(111) surface by means of low temperature STM and adsorption simulations. In these experiments, annealing at 100°C for one hour leads to the formation of two coexisting island structures. The first ressembles a slightly disordered hexagonal phase, while the second one forms rosette structures consisting of units of seven molecules.

The adsorption simulations were performed with ASED+ approach. In the simulations for few molecules, PTBC molecules tend to form rigid dimer and trimer structures, which adapt to the hexagonal surface symmetry. The interplay between the adsorption of one molecule and the interaction between the tertbutyl legs leads to the formation of observed rosette superstructure.

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Figures:

PTBC molecules on Cu(111). Top, STM image presents the observed rosette superstructure, and, bottom, the optimized adsorption geometry of six trimers PTBC molecules adapts to the hexagonal surface symmetry.