

On-Surface Design of Highly-Ordered Two-Dimensional Networks Stabilized by Nonmetal Atoms

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In this work we show the adatom-mediated synthesis of highly ordered two-dimensional nanostructures, stabilized by either hydrogen bonds or by nonmetal adatoms on Ag(111). The phase transition from triangular packing (see Figure 1a and b) to inverted packing (see Figure 1d and e) is mediated by an unconventional interaction between the pre-adsorbed Cl adatoms and the hydrogens of the TPyPPB arms. Our DFT calculations (see Figures 1c and f) shows that the halogens are mandatory to stabilize the inverted phase.

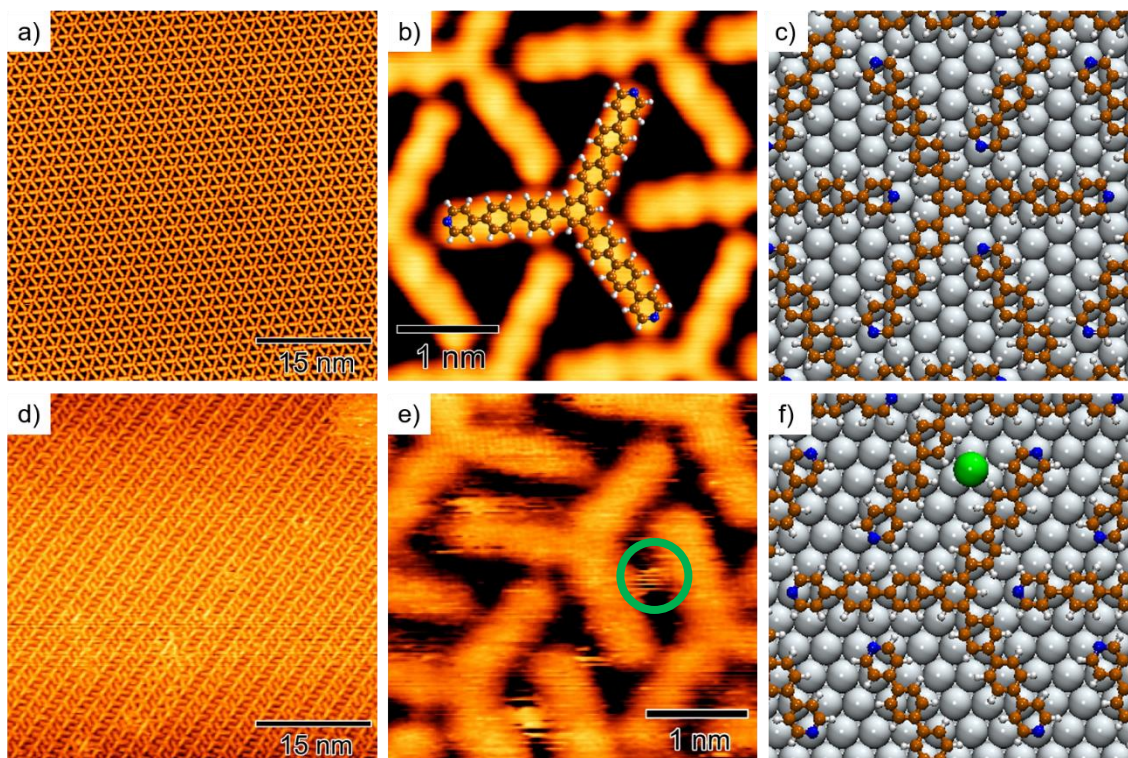


Figure 1: a) STM images of the triangular packing forming extended domains on Ag(111); b) High-resolution STM image with superimposed TPyPPB molecular structure showing the intermolecular interactions; c) Top-view of the DFT adsorption configuration of the triangular packing (Ag in gray, C in brown, and N in blue); d) STM overview image of the extended domains of inverted packing; e) High-resolution STM image with the bright protrusion assigned to Cl adatoms highlighted in green; f) Top-view of the DFT adsorption configuration of the inverted packing with one Cl adatom (Ag in gray, C in brown, N in blue, and Cl in green)