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Hydrogen-bonded Molecular Network of Anthraquinone on Au(111)

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Supramolecular structures of anthraquinone molecules on a metallic surface are studied using scanning tunneling microscope (STM) under ultrahigh-vacuum conditions. When we deposited anthraquinone molecules on Au(111) substrate, the molecules formed three different phases (Chevron type, tetragon type and disordered type) on the surface. Based on our STM measurements, we proposed models for the observed molecular structures. Chevrons are consisted of several molecular chains, which make well-ordered two-dimensional islands by some weak interrow interactions and we could observe tetragon structures which make array of (111) metallic surface. each molecular rows in the chevrons are stabilized by two parallel O-H hydrogen bonds and disordered structures are observed 1-dimensional phase with hydrogen bond. First-principles calculations based on density functional theory are performed to reproduce the proposed models. Distances and energy gains for each intermolecular bond are estimated. In this presentation, we explain possible origins of these molecular structures in terms of hydrogen bonds, Van der Waals interactions and molecule-substrate interactions.

Keywords: Supramolecular chemistry, Self-assembly, Chevron, Tetragon, 1D structure, Hydrogen bonds, Scanning tunneling microscopy