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Abstract Submitted for the MAR17 Meeting of The American Physical Society

Molecular self assembly and chiral recognition of copper octacyanophthalocyanine on Au(111): Interplay of intermolecular and molecule-substrate interactions.¹ REJAUL SK², BARUN DHARA, Indian Institute of Science Education and Research, JOEL MILLER, University of Utah, APARNA DESHPANDE, Indian Institute of Science Education and Research — Submolecular resolution scanning tunneling microscopy (STM) of copper octacyanophthalocyanine, $CuPc(CN)_8$, at 77 K demonstrates that these achiral molecules form a two dimensional (2D) tetramer-based self-assembly upon evaporation onto an atomically flat Au(111) substrate. They assemble in two different structurally chiral configurations upon adsorption on Au(111). Scanning tunneling spectroscopy (STS), acquired at 77 K, unveils the HOMO and LUMO energy levels of this self-assembly. Voltage dependent STM images show that each molecule in both the structurally chiral configurations individually becomes chiral by breaking the mirror symmetry due to the enhanced intermolecular dipolar coupling interaction at the LUMO energy while the individual molecules remain achiral at the HOMO energy and within the HOMO-LUMO gap. At the LUMO energy, the handedness of the each chiral molecule is decided by the direction of the dipolar coupling interaction in the tetramer unit cell. This preference for LUMO energy indicates that this chirality is purely electronic in nature and it manifests on top of the organizational chirality that is present in the self-assembly independent of the orbital energy.

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