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# Self-Assembled Chiral Structures of Discoid Organic Molecule on Au(111)

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Using both experimentaland theoretical methods, we have investigated the structural and electronic properties of self-assembled two-dimensional organic molecule (hexaaza-triphenylene-hexacarbonitrile, HATCN), which is used as an efficient OLED hole injection material, on Au(111) surfaces. Low-temperature scanning tunneling microscope (STM) measurements revealed that self-assembled linear and hexagonal porous structures are formed at atomic steps and terraces of Au(111), respectively. We also found that the hexagonal porous structure have chirality and forms only small (< 1,000 nm2) phase-separated chiral domains that can easily change their chiral phase in subsequence STM images at 80 K. To explain these observations, we calculated the molecular-molecular and molecule-surface interaction energies by using first-principles density functional theory method. We found that the change of their chiral phase resulted from the competition between the two energies. These results have not only verified our experimental observations, but also revealed the delicate balance between different interactions that caused the self-assembed structures at the surface.

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