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Metal-Organic Coordination Number Determined Charge Transfer Magnitude[1] HUNG-HSIANG YANG, YU-HSUN CHU, CHUN-I LU, TSUNG-HAN YANG, KAI-JHENG YANG, Department of Physics, National Taiwan University, Taipei, Taiwan, CHAO-CHENG KAUN, Research Center of Applied Sciences, Academia Sinica, Taipei, Taiwan, GERMAR HOFFMANN, Department of Physics, National Taiwan University, Taipei, Taiwan, MINN-TSONG LIN, Department of Physics, National Taiwan University, Taipei, Taiwan; Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan. — By the appropriate choice of head groups and molecular ligands, various metal-organic coordination geometries can be engineered. Such metal-organic structures provide different chemical environments for molecules and give us templates to study the charge redistribution within the metal-organic interface. We created various metal-organic bonding environment by growing self-assembly nanostructures of Fe-PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) chains and networks on a Au(111) surface. Bonding environment dependent frontier molecular orbital energies are acquired by low temperature scanning tunneling microscopy and scanning tunneling spectroscopy. By comparing the frontier energies with the molecular coordination environments, we conclude that the specific coordination affects the magnitude of charge transfer onto each PTCDA in the Fe-PTCDA hybridization system.

[1] H.-H. Yang, Y.-H. Chu, C.-I Lu, T.-H. Yang, K.-J. Yang, C.-C. Kaun, G. Hoffmann, and M.-T. Lin, ACS Nano 7, 2814 (2013)

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