Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Magnetic Anisotropy of an Fe-Porphyrin Complex on Au(111) Surface[1] WEIHUA WANG, BING LIU, HUIXIA FU, SHUYA XING, SHENG MENG, JIANDONG GUO, Institute of Physics, Chinese Academy of Sciences — By a combined study of low temperature scanning tunnelling microscopy (STM) and density functional theory (DFT) calculations, we have investigated the magnetic properties of an Fe-TPyP complex (i-FeTPyP) in the initial stage of metalation reaction on Au(111) substrate. The inelastic electron tunneling spectroscopy of i-FeTPyP showed typical zero-field excitation energy of 18 meV for the first excited state. Modeling the spin excitation energy in magnetic fields by spin Hamiltonian gave an easy-axis anisotropy perpendicular to the molecular plane. DFT calculations reveal that the Fe atom in i-FeTPyP is lifted from Au substrate and surrounded by elongated Fe-N bonds, and has an orbital angular momentum of $\boldsymbol{L}$=2 and spin angular momentum of $\boldsymbol{S}$=2. The orbital angular momentum not only contributes to the large magnetic anisotropy by spin-orbital coupling interaction, but also the in-plane orbital motion causes the easy-axis anisotropy, in agreement with experimental results. Our experiment demonstrate a new method to achieve large magnetic anisotropy by ligand fields realized in on-surface metalation reaction, and again highlights the crucial role of ligand field in determining the magnetic property of $3d$ magnetic atoms.

[1]This project was supported by the Hundred Talents Program of the Chinese Academy of Sciences.

Weihua Wang
Institute of Physics, Chinese Academy of Sciences

Date submitted: 20 Oct 2016 Electronic form version 1.4