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# Influence of Fe(110) Substrate with strong On-site Coulomb Repulsion on the Electronic Structure of Single Cobalt Tetraphenylporphyrin: Scanning Tunneling Microscopy Study

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Scanning tunneling microscopy (STM) was used to study the electronic structure of cobalt(II) tetraphenylporphyrin (CoTPP) on the Fe/W(110) substrate. Clover-like conformation of CoTPP was observed and showed bias dependent STM images. The central Co(II) ion of this porphyrin was protruded on the positive biases, but it was depressed on the negative biases. On the positive biases, the phenyl rings of CoTPP appeared to be bright contrary to the invisible pyrrole rings. These results were compared the first-principles calculations using GGA and GGA+*U* to elucidate the influence of the Fe substrate. GGA+*U* results agreed well with the experimental results; however, GGA did not. These results show that proper treatment of the on-site Coulomb repulsion of the Fe ions is crucial to describe the electronic structure of this system. By the comparison between the GGA+*U* calculations on the Fe substrate and the gas phase calculations, it can be noted that chemical potential shift occurred accompanying charge transfer from the Fe ions of the substrate to the pyrrole ligand of the porphyrin.