First-principles study of tilted binding and precession motion of diatomic NO adsorbed to Co-porphyrin on Au(111) YUNHEE CHANG, Graduate School of Nanoscience and Technology, KAIST, HOWON KIM, SE-JONG KAHNG, Department of Physics, Korea University, YONG-HYUN KIM, Graduate School of Nanoscience and Technology, KAIST — To understand the bright square ring structures observed in scanning tunneling microscopy (STM) experiments of NO adsorption to CoTPP on Au(111), we performed first-principles calculations within the spin-polarized DFT formulation and DFT-D method; which includes the van der Waals interaction between CoTPP and Au(111). With the correction, the calculated electronic structures of NO adsorbed CoTPP/Au(111) are well consistent with STM and scanning tunneling spectroscopy (STS) results. Upon NO exposure, three-lobed structures of CoTPP were transformed to bright square ring shapes on Au(111). The adsorbed NO molecule is tilted away from the axial direction. Due to the symmetry of the CoTPP, the adsorbed NO molecule have a precession motion with the energy barrier of 33 meV. This energy barrier is small enough to allow a fast precession motion of the NO molecule even in cryogenic temperatures as low as 80 K. We will discuss details about NO adsorption mechanisms and electronic structures.

Yunhee Chang
Graduate School of Nanoscience and Technology, KAIST

Date submitted: 09 Nov 2012 Electronic form version 1.4