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Adsorptions and Dissociations of Nitric Oxides at Metalloporphyrin Molecules on Metal Surfaces: Scanning Tunneling Microscopy and Spectroscopy Study

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Organometallic complexes containing unpaired spins, such as metalloporphyrin or metallophthalocyanine, have extensively studied with increasing interests of their promising model systems in spintronic applications. Additionally, the use of these complexes as an acceptor molecule in chemical sensors has recently received great attentions.

In this presentation, we have investigated adsorption of nitric oxide (NO) molecules at Co-porphyrin molecules on Au(111) surfaces with scanning tunneling microscopy and spectroscopy at low temperature. At the location of Co atom in Co-porphyrin molecules, we could observe a Kondo resonance state near Fermi energy in density of states (DOS) before exposing NO molecules and the Kondo resonance state was disappeared after NO exposing because the electronic spin structure of Co-porphyrin were modified by forming a cobalt-NO bonding. Furthermore, we could locally control the chemical reaction of NO dissociations from NO-CoTPP by electron injections via STM probe. After dissociation of NO molecules, the Kondo resonance state was recovered in density of state.

With a help of density functional theory (DFT) calculations, we could understand that the modified electronic structures for NO-Co-porphyrin could be occurred by metal-ligand hybridization and the dissociation mechanisms of NO can be explained in terms of the resonant tunneling process via molecular orbitals.

Keywords: organometallic complexes, scanning tunneling microscopy, chemical reaction