Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Single molecule dissociation by tunneling electrons in NO-Co-Porphyrin complex on Au(111): A novel mechanics revealed by scanning tunneling spectroscopy and first-principles thermodynamic simulation YUNHEE CHANG, Graduate School of Nanoscience and Technology, KAIST, HOWON KIM, Dept. of Physics, Korea University, EUI-SUP LEE, Graduate School of Nanoscience and Technology, KAIST, WON-JUN JANG, Dept. of Physics, Korea University, YONG-HYUN KIM, Graduate School of Nanoscience and Technology, KAIST, SE-JONG KAHNG, Dept. of Physics, Korea University — To microscopically understand the mechanisms of electron-induced NO dissociations, we performed first-principles density-functional theory (DFT) calculations for NO-CoTPP on Au(111). We explain the scanning tunneling microscopy (STM) results that the dissociations of NO were induced by both positive and negative voltage pulses with threshold voltages, +0.68 V and 0.74 V, respectively, at 0.1 nA tunneling current, showing power law relations between tunneling current and dissociation yield. To evaluate first-principles thermodynamics of the NO dissociation, we considered not only adsorption-desorption energetics, zero-point energy, and vibrational free energy at experiment temperature from first-principles, but also the chemical potential of NO gas at the cryogenic ultra-high vacuum condition. Using first-principles thermodynamics for the NO dissociation, we argue that the dissociations are induced with inelastic electron tunneling through molecular orbital resonances.

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Date submitted: 14 Nov 2014 Electronic form version 1.4