Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Density functional calculations of the absorption and magnetic properties of oxygen molecule on Au(110)[1] RUQIAN WU, YANNING ZHANG, JUEXIAN CAO, YING JIANG, WILSON HO — Studies of the Kondo effect in molecular magnets and molecular junctions capture extensive attention of experimentalists and theorists. Our low temperature STM experiments revealed fascinating features of O_2 on the reconstructed Au(110) surface. O_2 forms alternating zig-zag and ying-yang rows on Au(110) and displays sizeable Kondo effect. Density functional calculations were performed to understand the driving force for the unusual structure and magnetic properties. Using the fixed triplet state of O_2, the optimized atomic structure resembles the experimental topography well. The magnetization of O_2 is stable with regular density functional calculations, 1.97 μ_B from. We will discuss the pattern of Kondo clouds in view of molecular orbitals and density of states. Extensive experimental and theoretical data allow comprehensive understanding of the essence of spin polarization and spatial Kondo effect in molecular systems.

[1]The work was supported by DOE (Grant No. DE-FG02-04ER15611). The calculations were performed on the supercomputers at NERSC.

RUQIAN WU
University of California, Irvine

Date submitted: 19 Nov 2009 Electronic form version 1.4