Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Magnetic properties of 3d transition metal-phthalocyanine molecules on oxided Cu(110) surface JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 — After being extensively interesting topics in both fundamental researches and application practices for a decade, spintronics is now on its way of diversity. Molecular spintronics has attracted much attention in recent years, due to the accelerating miniaturization of electronic devices. In this work, based on first-principles calculations, we studied the electronic and magnetic properties of both isolated metal-phthalocyanines (commonly referred to as MPc) molecules (M=Mn, Fe and Co) and a single MPc molecule adsorbed on oxided Cu(110) [O-Cu(110)] surface. We find that the easy axis of FePc molecule switches from in-plane direction to perpendicular direction when it is adsorbed on O-Cu(110) surface. However, such a switch of direction of magnetization could not be observed for MnPc and CoPc molecules which are two neighbors of FePc with one electron less and more, respectively. Furthermore, we find that the magnetization of these MPc molecules on O-Cu(110) surface are rather stable, so they could not be altered by moderate hole/electron doping. The e_g orbitals (d_{xz} and d_{yz}) of MPc molecules are found to be crucial for their magnetization on O-Cu(110) surface. **Acknowledgement.** This work was supported by DOE Grant DE-FG02-05ER46237.

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Date submitted: 29 Nov 2011 Electronic form version 1.4