

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Magnetic and structural behaviors of transitional metallo-porphines monolayer and bilayer on Ag(111) X.Q. TIAN, J.B. XU, DEPT OF ELEC ENGI AND MSRC, THE CHINESE UNIVERSITY OF HONG KONG TEAM, CHEMISTRY DEPT, PRINCETON UNIVERSITY COLLABORATION — Five monolayers and bilayers of transitional metallo-porphine(MP) (Mn, Fe, Co, Ni, Cu) on Ag(111) substrate are investigated by *ab initio* calculation. The strong coupling of FeP and CoP MP/Ag(111) interface leads to magnetic-nonmagnetic transition. The competition mechanism between intermolecular ferromagnetic exchange interaction and coupling of FeP/Ag(111) prevents the magnetic-nonmagnetic transition of interface. The top layer of all 5 bilayers keeps their intrinsic magnetic properties and planar structures, so the bottom layer of the bilayer serves the role of buffer layer. These theoretical results could be used to explain the recent STM and XPS experiments. A new interfacial magnetic competition mechanism has been proposed and hopefully it will influence the construction and design of future molecular spintronics.

X.Q. Tian

Date submitted: 29 Nov 2008

Electronic form version 1.4