Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Magnetocrystalline anisotropy of 3d transition metal atoms on graphen JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA 92697-4575 — Graphene has attracted most attention in the field of condensed matter physics, chemistry and material science since the first day when it was produced in lab. It's an ideal material for two-dimensional electron gas (2DEG). Most intriguingly, the electronic and magnetic properties can be easily engineered by decorating with external elemental atoms ranging from non-metal to transition metal. Especially, graphene is attractive for spintronics due to its long spin life time and high mobility. So far, ultrathin Co films have been deposited on graphene which exhibit perpendicular magnetic anisotropy. In this work, first-principles calculations are performed to systematically study the magnetic properties of graphene decorated by 3d transition metal atoms with several covering patterns. We find that Fe/graphene always exhibits in-plane anisotropy regardless the coverage, while Mn/graphene and Co/graphene tend to have perpendicular easy axis for most range of coverage. The spin moments of Ni atoms are largely quenched for Ni/graphene. Moreover, the Mn atoms on graphene prefer ferromagnetic exchange coupling which are totally different from the pure counterpart without graphene support. The strong hybridization between 3d orbitals of transition metal atoms and pi states of graphene are responsible for the modification of magnetic properties. **Acknowledgement.** This work was supported by DOE Grant DE-FG02-05ER46237.

Jun Hu
Department of Physics and Astronomy,
University of California, Irvine, CA 92697-4575

Date submitted: 28 Nov 2011 Electronic form version 1.4