

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Ligand effects on the electronic structure and magnetism of magnetite surfaces KATARZYNA BRYMORA, FLORENT CALVAYRAC, Universite du Maine, Le Mans, France — We address the effect of functionalization on the electronic and magnetic properties of magnetite surface as an indicator of the same properties in nanoparticles too big for a direct ab-initio approach. Using well-established methods and references (namely LDA+U on magnetite surfaces) we could verify the validity of our approach, and using two typical ligands, dopamine and citrate, namely π and σ electron donors, we could predict that those ligands would induce a different change in the electronic properties of the systems, but in both cases an enhancement of magnetization.

Katarzyna Brymora
Universite du Maine, Le Mans, France

Date submitted: 23 Oct 2012

Electronic form version 1.4