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 $\pi$ and $\sigma$ 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.