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Size effects on the magnetic performance of organic coated ferrite nanoparticles.

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At the nanoscale size dependent magnetic surface anisotropy and magnetic moment can affect the magnetic performance of a material [1]. Surface functionalization of magnetic nanoparticles can be achieved by organic coatings, that modify the magnetic and the electric properties (i.e the charge, electrostatic potential) of nanoparticles. Their effect depends on the type of the magnetic nanoparticle, the type of coating and the amount of coverage [2]. Moreover the size of the particles plays important role in their magnetic and electrostatic behavior as the surface modification (broken bonds, active sites) affects the binding energies of the attached ligands [3].
Here we present our results for the magnetic behavior, charge distribution and electrostatic potential of maghemite and Co ferrite nanoparticles, with diameter ~2nm to ~4nm in order to investigate the nanoparticles size effect. These nanoparticles are covered with oleic acid (OA), diethylene glycol (DEG) and OH. The coverage concentration was varied from 0% to 20% of the surface of the particles.
We perform DFT calculations for the magnetocrystalline anisotropy, the magnetic moments and charge of the nanoparticles. Our calculations show that as the size of the nanoparticle increases the metal-O bond lengths increase and more specifically 8% for Fe-O and 12% for Co-O providing a larger amount of ionic character of Co-O bonds. This makes the Co atoms more favorable to be attached by the ligands. In Co ferrite nanoparticles covered with OA the magnetic moment increases with the size whereas the magnetic anisotropy decreases. This effect leads to a reduction of the spin-orbit energy for Co by 0.01meV/atom and an increase of its magnetic moment by 0.3μB/atom. In the maghemite nanoparticles the opposite trend is found with the increase of the size. In this case the expansion of the bond lengths between Fe-O increases by ~15% and it leads to a decrease of the magnetic moment by 0.16μB/atom and also a small increase of spin orbit energy by 10^{-3}meV/atom.

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[3] B. Farkas, et al. Phys. Chem. Chem. Phys. 22 (2020) 985