

Functionalization of ferrite nanoparticles with organic coatings

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Recent studies have demonstrated that organic coatings on the surface of magnetic nanoparticles modify their magnetic and the electric properties (i.e. the charge, electrostatic potential). Their effect depends on the type of the magnetic nanoparticle, the type of coating and the amount of coverage.

Here we present our results for the magnetic and electrostatic behavior of maghemite and Co ferrite ultrasmall nanoparticles of size ~ 2 nm in order to investigate the effect of the coating when they are covered with oleic acid (OA), diethylene glycol (DEG) and OH. The coverage concentration was varied from 0% to 20% on the surface of the nanoparticles.

We have performed DFT calculations for the magnetocrystalline anisotropy, the magnetic moments, the charge and the electrostatic potential of the nanoparticles. Our findings demonstrate that the OA results to the decrease of the mean magnetic moment for both particles as the coating increases. The magnetocrystalline anisotropy shows different behavior, as it increases for maghemite and decreases for Co ferrite with the increase of the coating. This is attributed to different types of ions being attached to the coated molecules. For DEG and OH no significant variance is observed neither in the magnetic moment nor in the magnetic anisotropy since the DEG and OH coatings show a weaker attachment on the surface than OA molecules by almost 1eV. The latter is attributed to the different functional groups of the coatings, COOH for OA and OH for the others. COOH shows a larger percentage of covalent bonding rather than OH. The charge calculation was performed with the implementation of the Bader charge analysis and we identified the ionic state of each atom. Then from the solution of the Poisson equation we extract the average electrostatic potential outside the particle's surface. As COOH shows a larger percentage of covalent bonding than OH larger amount of charge is transferred to both particles when OA is attached on their surface rather than DEG or OH. Overall a larger increase of the charge was found in the Co ferrite particles that leads to a larger tail of the electrostatic potential outside the particle resulting to the increase of the colloidal stability of Co particles compared to that of the maghemite nanoparticles with the same type and percentage of coverage.