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Magnetic nanoparticles as polarity-sensors: a Molecular Dynamics study on the effect of solvent interactions with surface atoms on iron oxide nanoparticles' magnetization.

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Abstract content
   (Max 300 words)
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Iron oxide magnetic nanoparticles have unique physical and chemical properties due to their extremely small size and large specific area. Applications for these nanoparticles range from contrast agents in magnetic resonance imaging (MRI) in the biomedical field through to heating agents in hyperthermia for cancer therapy. In all of these applications the magnetic particles are coated with surfactants and polymers to enhance biocompatibility, prevent agglomeration and add functionality. However the surfactants interact with the surface atoms of the nanoparticles leading to the formation of a magnetically disordered layer, which in turn reduces the effective magnetic phase. The magnetic phase reduction can also be attributed to the interaction between the surfactant and the solvent.

In this study the interactions between the surfactant, iron oxide nanoparticle and the suspension media were investigated to understand their effect on magnetization of magnetic iron oxide nanoparticles. A molecular mechanics model was developed to investigate the mechanism that leads to the relative magnetic phase variation when suspending the oleic acid coated magnetite nanoparticles in three different solvents: heptanes, hexane and acetone. Various minimized system geometries were calculated and the optimized binding energy configurations were obtained for three iron oxide nanoparticles stabilized with oleic acid as surfactant. The potential application as a polarity sensor is discussed.

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