Contribution ID: **121** Type: **Oral Presentation**

Monte Carlo Simulations of Magnetite Nanoparticles Stabilised With Sebaccic Acid and 1, 10-Decanediol Surfactants

Friday, 15 July 2011 08:45 (15 minutes)

<p>Iron oxide-based nanomagnets, such as maghemite (Fe2O3) and magnetite (Fe3O4), have attracted a great deal of attention in nanomedicine over the past decade. On the nanoscale, superparamagnetic iron oxide nanoparticles can only be magnetized in the presence of an external magnetic field. This property makes these nanoparticles capable of forming stable colloids in a physio-biological medium. Their superparamagnetic property, together with other intrinsic properties, such as low cytotoxicity, colloidal stability and bioactive-conjugation, makes such nanomagnets ideal for both in vitro and in vivo biomedical applications. Several methods for the synthesis of iron oxide nanoparticles have been developed. The most common ones for contrast agent synthesis are based on the precipitation of magnetite nanoparticles from solutions containing stabilizing agents such as synthetic or natural polymers; or adsorption of stabilizing agents on the magnetite particle surface after synthesis. The first method often leads to the formation of multicore particles, while the second one demands coating stabilisation by cross-linking, that can lead to particle aggregation. For this reason the stabilising properties of two surfactants, sebaccic acid (with carboxylic acid groups on the peripheries) and 1, 10-decanediol (with hydroxyl groups on the peripheries), were investigated and compared theoretically. DFT adsorbance simulations were run and the average total energies of the two ligands adsorbed onto the magnetite nanoparticles were compared. XRD measurements also revealed a change in crystal structure for the Fe3O4 nanoparticles when stabilised with the different ligands.

Level (Hons, MSc,
   PhD, other)?

PhD

Consider for a student
   award (Yes / No)?

No

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

No

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Session Classification: CMPMS1

Track Classification: Track A - Condensed Matter Physics and Material Science