

## **Self-Assembly of Magnetic Nanostructures and Related Enabling Technologies**

One of the most important problems facing in nanomaterials and nanotechnology is synthesizing well-defined, stable nanostructures. Our team has worked on synthesizing magnetic nanoparticles with different particle sizes and different coatings. To understand structures in these materials and phase separation behavior, computer simulations of structure formations in magnetic fluids and amphiphilic self-assembly were carried out. At the meantime, encapsulation of self-assembled magnetic nano-beads has been studied as well to explore the medical application as drug delivering agent.

### **1. Synthesis of magnetic nanoparticles (Luo's group).**

Magnetic nanoparticles of  $\text{Fe}_3\text{O}_4$  with different diameters were synthesized. The sizes were determined by TEM to be 6nm-10nm. The temperature, PH value, and concentration of surfactants were adjusted to achieve optimum coating based on the maximum grafting number.

### **2. Self-assembled magnetic nanostructures and its encapsulations (Rosenzweig's and Luo's group).**

Magnetic nanostructures consisting of self-assembled magnetic nanoparticles were synthesized in Kerosene and water. They were then encapsulated by liposomes. The more stable structures were obtained by encapsulating the self-assembly in polymerization mixture of EGDMA and MMA.

### **3. Computer simulations**

#### **a) structures in self-assembled magnetic nanostructures (Tomanek's group)**

The ground state configuration of finite-size magnetic dipoles in a viscous suspension, modeling a ferrofluid, was studied. Our previous studies have shown the ring and chain to be the most stable structures for systems containing less than 25 particles. Here, we build up on these geometries for much larger systems, and investigate the multi-ring, multi-chain, coil structures, and torus geometries, up to several thousand particles. The numerical energy formulas for these systems were studied. Of particular interest are multi-ring, coil and multi-chain assemblies. The structural transitions between these particular structures were found from energy curve as a function of length scale of the structures.

#### **b) Pattern Formation through Surfactant-Colloid Self-Assembly (Bhattacharya's Group)**

Our theoretical input in this grand plan is to carry out, first Monte Carlo (MC) and then

Molecular dynamics (MD) simulation of colloid- amphiphilic system, in general, for various length scales of each species. A very important ingredient in achieving this goal is to have a code, that can incorporate various *geometric attributes* of the amphiphiles making the model more realistic and closer to experiments. With this aim in mind, we have added the following new features to our two dimensional off-lattice Monte Carlo(MC) code. We have incorporated certain finer geometric attributes to the model amphiphiles. The results show the *generalized kink-jump*, and this particular *generalized reptation* algorithm of our choice (which is more cost-effective for the computer), indeed produce micelles, and the total energy steadily goes down toward its final equilibrium value.

#### **4. New coating layer for magnetic particles (Belfield and Luo's group)**

Beside short surfactant, we also used polymers and bilayers of amphiphilic as surfactants to stabilize the magnetic colloids.

a) A polydimethylsiloxane (PDMS) - poly (3-cyanopropyl) methylsiloxane (PCPMS)- polydimethylsiloxane (PDMS) family of the tri-block copolymers with controlled block lengths was synthesized by anionic living polymerization.

Stable magnetic fluids of  $\text{Fe}_3\text{O}_4$  were prepared in water using 2.5 k - 5 k – 2.5 k, 26 k - 6 k – 26 and 8.8 k - 10 k – 8.8 k these three tri-block copolymers as stabilizers, and iron (II) chloride and iron (III) chloride as precursors. The dispersions can be dispersed well in a polyacrylamide gel.

b) In order to make self-assembled magneto-surfactant nano- and meso-structures as we proposed, DOPE/DDAB vesicles were prepared with the sonication method. The preparations were carried out at different pH values and temperatures. The mean size of vesicles is 310 nm by AFM characterization. Vesicles with magnetic cores were also prepared and the mean size is comparable to that of DOPE/DDAB vesicles.

#### *References*

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“Preparation of magneto-vesicles with DOPE/DDAB layers.” Kezheng Chen and Weili Luo, to be published in *European Cells and Materials*.