

## **Magnetic Properties of Albumin coated Mn ferrite Nanoclusters**

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Organic coating of magnetic nanoparticles attracts considerable attention for designing novel multi-functional nanomaterials. The role of surface coating has been regarded as highly important to achieve physical and chemical stability and to control the magnetic properties of nanoparticles and their assemblies. Notably, it has been demonstrated that the coating process can also affect the assembly's morphology by inducing particle clustering and thus can modify the magnetic behaviour of the nanoparticles system.

In view of this, we perform a systematic study of the magnetic behaviour of ultra-small Mn ferrite nanoparticles entrapped in bovine serum albumin (BSA) which is known as an environmentally friendly surfactant. The albumin coating process generates a change in the actual size and shape distribution of clusters of exchange coupled particles, giving rise to a large distribution of blocking temperatures. In addition, this protein binding to nanoparticles' surface modifies both their magnetization and the surface anisotropy while the ultra-small size induces strong interface/surface effects.

For the study of the system, we have developed a multi-scale modeling to calculate the atomic scale parameters of the coated nanoparticle via DFT calculations and the mesoscopic magnetic behaviour of the nanoparticles' clusters via Monte Carlo simulations. We have investigated the complex interplay among the intra-particle interactions, the dipolar inter-particle interactions and the exchange intra-cluster interactions acting between partially covered nanoparticles forming large isolated clusters.

Our numerical results are in good qualitative agreement with the experimental data. Importantly, our work suggests tailoring and optimization of the magnetic properties of nanoparticles' assemblies by properly selecting not only the organic coating but also the coating procedure.