Multiscale models of ferrofluids with reference to magnetic nanoparticle hyperthermia

Roy Chantrell

School of Physics, Engineering and Technology, The University of York, UK

Early in the development of Ferrofluids, magnetic hyperthermia was proposed as a potentially important medical application. Only over the last decade or so has this become a reality, along with the concept of magnetic particle imaging (MPI) which offers possible exciting theranostic applications. Along with the important experimental developments which have driven the field, supporting computational models have also advanced. I will outline some developments, particularly in relation to 'multiscale' modelling. This has 2 facets, perhaps the most developed one being the linkage of timescales using the numerical integration of the Landau-Lifshitz-Gilbert-equation, practically limited to microsecond timescale, with that of the kinetic Monte Carlo method which is computationally more efficient at longer timescales and for systems of interacting particles. The model is used to investigate the dynamical orientation of nanoparticle easy axes in alternating field environments. I will also briefly outline the importance of developing atomistic level models, firstly for understanding the complex energy surfaces which can arise from mixed cubic and shape anisotropies and secondly for understanding the heat generation and transfer processes involved in MNH.