Application of Multiscale Computational Techniques to the study of Magnetic Nanoparticle Systems

Marianna Vasilakaki, Nikolaos Ntallis, Kalliopi Trohidou
Institute of Nanoscience and Nanotechnology, NCSR 'Demokritos'
Athens, Greece
k.trohidou@inn.demokritos.gr

We have employed a multiscale modeling approach that combines ab-initio electronic structure calculations with atomic and mesoscopic scale modelling to describe the magnetic behavior of assemblies of magnetic nano-paricles (MNPs) with core/surface morphology. Our modeling is based on the calculated atomistic parameters and we rescale them after the reduction of the simulated number of the NPs atomic spins to the minimum necessary to represent theirâĂŹ magnetic structure in the assemblies. Monte Carlo simulations are them performed to study their macroscopic magnetic behaviour. We apply our model to a) CoFe2O4 NPs coated with two different surfactants and b) bovine serum albumin-coated MnFe2O4 MNPs' clusters. Our approach overcomes current computational limitations. The numerical results produced are in excellent agreement with the experimental findings illustrating the potentials of our strategy to simulate the magnetic behaviour of complex magnetic nanoparticle systems and to optimize their magnetic properties for advanced energy and biotechnology nanomaterial applications.

Keywords: multiscale modeling, magnetic nanoparticles, DFT calculations, Monte Carlo simulations.