***Multi-scale Modelling of nanoparticles***

**A. Atomistic simulations of nanoparticles: from the atom to the nanoparticle**

Aim: understanding the differences between the bulk and the nano

Systems: gold and silver nanocrystals coated by thiolates

Methods: Molecular dynamics and Monte Carlo at atomic level, massive parallelism, DFT

**B. Simulation of nanoparticle assembly: from one nanoparticle to thousands**

Aim: using nanoparticles as LEGO bricks

Systems: supercrystals made of gold, silver, maghemite and cobalt nanoparticles

Methods: Molecular dynamics and Monte Carlo at atomic and particle level, Flory-type solubility theories

 **C. Theory of mesostructures made of magnetic nanoparticles:** **from 100 nm upward**

Aim: understanding and prediction of new mesostructures

Systems: patterns made of cobalt and maghemite nanoparticles, cracks in nanoparticle films, super spin and spin glasses

Methods: free energy approaches, Brownian dynamics and Monte Carlo simulations at particle level, bundle-spring block models for cracks, parallel tempering