



School of Nano Science



IPM Condensed Matter &
Statistical Physics Group

Weekly Seminar

Colloidal Hard Sphere Crystals and their Interfaces in Density Functional Theory

Invited Speaker:

Dr. Mohammad Hossein Yamani

Abstract:

Colloidal hard spheres are an intensely studied model system for addressing nucleation of crystals from metastable liquids. Understanding nucleation requires a precise knowledge about equilibrium crystal structures and free energies. The research presented in this talk addresses necessary equilibrium information for understanding of homogeneous and heterogeneous nucleation in the hard sphere system. Classical density functional theory (DFT) of fundamental measure type (FMT) is used to evaluate the fully minimized crystal density profiles and their interfaces.

Equilibrating fcc, hcp and bcc crystal densities and evaluating their free energies in FMT and comparing results with other theoretical and simulational approaches enables us to explain the stability of different crystal structures. At a hard, flat and unstructured substrate, the crystalline phase completely wets the substrate. Heterogeneous nucleation for the hard sphere fluid at unstructured hard walls has not been found neither in simulation methods nor in DFT approaches. Besides equilibrium crystal structures, the hard sphere fluid in the vicinity of soft substrates are studied in search of a variable nonzero contact angle which could allow studying heterogeneous nucleation.

Wednesday, 6th of Bahman(1395) (January 25th, 2017), 14:00-15:00

Farmaniyeh seminar room