Seminário do Grupo de Física Estatística

3ª feira, 22/11/2016 - 15:00 horas
Sala 201 – Ala I

"Multi-scale atomistic simulation of complex materials for energy and infrastructure applications"

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- **Resumo:** With emergence of nanotechnology, it is possible to control interfaces and flow at nanoscale. In this scenario, the properties of fluids confined in porous media can differ from the bulk case due to the combined effects of confinement and interactions with the surface. Currently, our group is exploring the phenomena of interfacial and confined fluids in a porous media for applications in energy (Oil and Gas industry) and infrastructure (cement and asphalt). By using an integrated multiscale computational approach ranging from quantum mechanics calculations, molecular dynamics and Lattice Boltzmann modeling, we have been able to systematically model and characterize complex materials at nanoscale and the implications for energy and infrastructure applications. In this talk, I will summarize some of our findings based on multiscale molecular simulations to i) displace more oil by controlling the chemical environment of oil/brine/rock interfaces using functionalized nanoparticles, ii) characterize and understand the interfacial effects of oil and water confined in porous media (calcite slites and silica nanoporous) through NMR spin relaxation and Hydrogen bond analysis, and iii) our first attempts to propose fully atomistic models of asphalt and cement.