NATIONAL TECHNICAL UNIVERSITY OF ATHENS
SCHOOL OF CHEMICAL ENGINEERING
Department of Materials Science and Engineering
Computational Materials Science and Engineering (CoMSE) Group

Ph.D. positions available

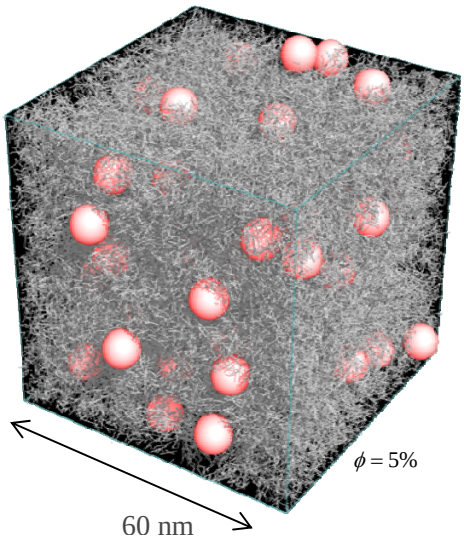
Two new doctoral candidate positions are available in the CoMSE Group at NTUA in the context of the research programme "Multiscale Simulations of Complex Polymer Systems" (MuSiComPS), carried out in collaboration with the University of Patras thanks to the generous support of the Limmat Foundation, Zurich, Switzerland. These new positions are available immediately (starting date 1 March 2015) for one year, with the possibility of extension for two additional years. The gross salary of each Ph.D. candidate will be 20,000 €/yr.

The projects to be undertaken by the two Ph.D.'s are outlined below.

Candidates holding a Diploma in Chemical Engineering, Materials Science and Engineering, or any other branch of Engineering, in Physics, or in Chemistry, with an excellent academic record, strong interest and demonstrated talent in computational research are encouraged to apply by sending a curriculum vitae and arranging for two letters of recommendation to be e-mailed directly to

Professor Doros N. Theodorou
School of Chemical Engineering
National Technical University of Athens
9 Heroon Polytechniou Street, Zografou Campus
157 80 Athens, Greece
doros@central.ntua.gr
http://comse.chemeng.ntua.gr

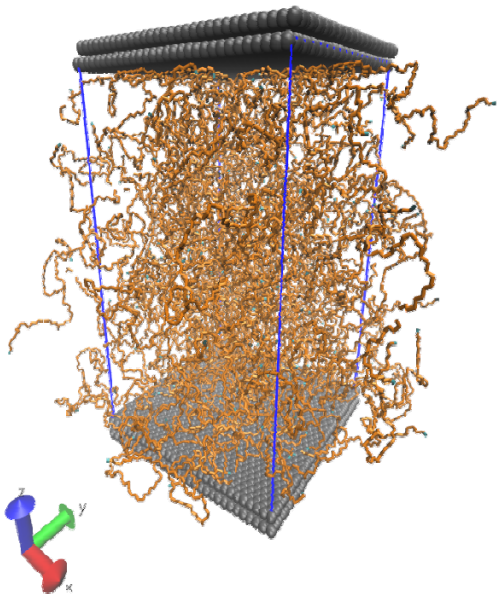
Position NTUAPhD1: **Self-Consistent Field/Finite Element Method for predicting interactions among nanoparticles in molten polymers (SCF/FEM NANO)**



The state of dispersion of nanoparticles in polymers is key to the properties of polymer-matrix nanocomposites. In applicatioins one strives to achieve a good dispersion by judicious molecular engineering design of the polymer matrix and filler nanoparticles and of the processing conditions used to form the nanocomposite.

This project aims at the development and implementation of a novel mesoscopic approach, combining polymer self-consistent field theory (SCF) with the Finite Element method (FEM), for predicting the polymer-mediated interactions among nanoparticles from their size, shape, chemical constitution, the chemical constitution and molar mass distribution of matrix chains, and the chemical constitution, surface density, and molar mass distribution of surface grafted chains, if present, in a polymer nanocomposite at equilibrium. This approach, and the computer programme which implements it, will be valuable as a stepping stone towards property prediction and rational design of polymer-matrix nanocomposites.

Position NTUAPhD2: Atomistic and mesoscopic simulations of the interfacial dynamics of polymer melts (INTERF DYN)



The dynamics of polymers at interfaces plays a significant role in melt processing operations, such as extrusion and film blowing; in the performance of soft adhesives; in the mechanical properties of polymer-matrix nanocomposites, such as rubber tires; in friction, wear, and lubrication phenomena; and in the design of biocompatible surfaces.

This project aims at developing a multiscale simulation strategy for predicting the dynamics of long-chain, entangled polymer melts at interfaces under equilibrium and flow conditions. The approach will be tested and validated using polyethylene and atactic polystyrene as polymers, and graphite and silica as substrates.

The project will involve mapping atomistic simulations to a coarse-grained bead-spring model, with particular attention to the rates of bead adsorption and desorption at the solid substrate, as well as mesoscopic Brownian Dynamics/Kinetic Monte Carlo simulations of melt flow past the substrate. Results will be analyzed to determine the velocity profile and the shear stress, detect wall slip at the interface, and formulate an appropriate constitutive law for its description. In addition, changes in the molecular-level orientation and entanglement structure of the melt induced by flow will be analyzed and compared against available experimental evidence.