Philosophy

Compact MSc projects with clear goals and strategy

Expandable projects (there is a “safe minimum” that satisfy the thesis requirements but any project can be easily expanded or/and made more ambitious if the student demands so)

I take into account limited time Skoltech students have for the thesis project and the tangible goals (e.g. desire to publish, direct interactions with experimental/industrial collaborators etc)

I try to work directly with each MSc student myself as much as I can

Sudden prolonged absence not tolerated; if you just disappear, I will make every effort to get rid of you.

It is your work. If you fail, you fail

Monte Carlo modeling of phase behavior of polyelectrolyte solutions

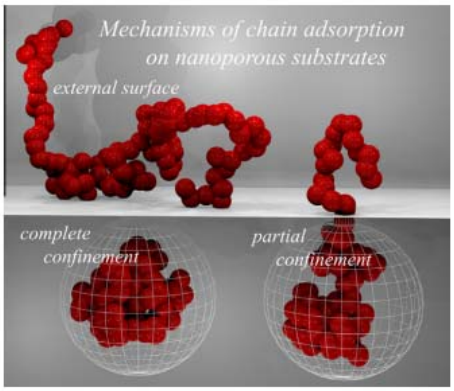


Figure: Cimino et al JCIS 481 181 (2016)

Modeling of polymer solutions by means of statistical mechanics resulted in critical insights in industrial processes of a great practical importance (polymer synthesis via polycondensation, separations of polymer solutions, polymer chromatography). A set of Monte Carlo modeling techniques have been developed in the literature for simulations of structure and properties of polymers, but often they are not applicable to polyelectrolytes. The goal of the MSc thesis projects in this field is to extend available techniques of MC simulation to polyelectrolyte solutions and gels.

This topic contains demanding but rewarding tasks (likely to require mastering concepts & language but pretty much publishable if you succeed). The students will need to study fundamentals of statistical mechanics and thermodynamics of polymer solutions and research literature on Monte Carlo simulations of polymers, extend existing simulation methods to polyelectrolytes. As a result, the students will get and extensive, hands-on experience in mathematical modeling of physical processes of practical importance, scientific programming and scientific writing, will learn to independently in an inter-discipline collaborative environment.

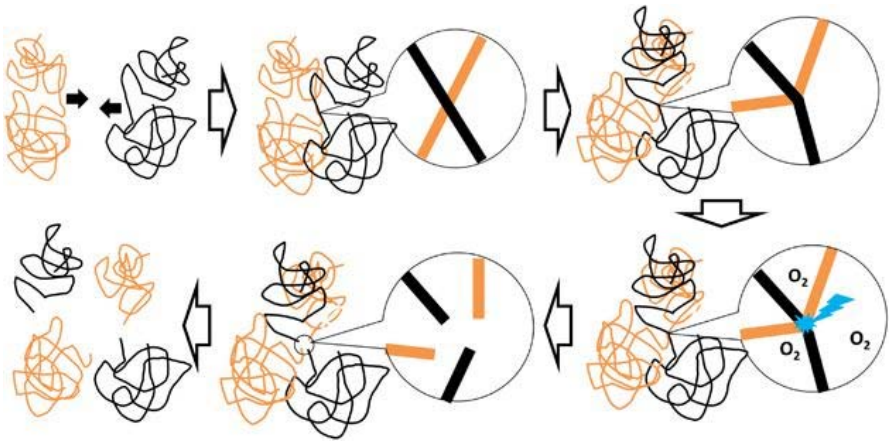
Track: CSE

Background required: probability theory (a must), programming (a must, C or Fortran preferred), general thermodynamics (a must), polymer physics & colloid chemistry (would be helpful but not required)

Keywords: statistical mechanics, Monte Carlo methods, polyelectrolytes, phase equilibria, polymer chromatography

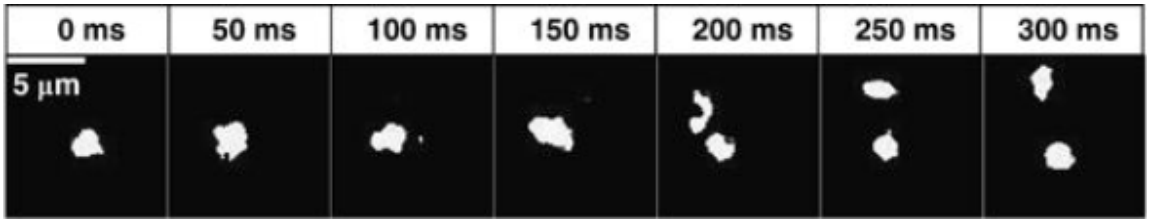
Polymer dynamics studied by coarse-grained simulations.

Because of the size of polymer molecules, their atomistic modeling of often prohibitively expensive. For that reason, simulation often relies on coarse-graining: individual atoms and molecules are “lumped together” and represented by quasiparticles (beads). Although coarse-grained modeling methods are well-established, only recently progress in molecular imaging enabled direct comparison between simulated and experimental dynamics of polymers in solutions. The simulation methodology will be applied to recently discovered effects of entanglement caused polymer scission.



Figures: Scheblykin et al 2014-2018

The scope and difficulty of is topic enables projects of different levels: from easy introductory simulations using standard simulation packages to ambitious and demanding master thesis projects that will require understanding of statistical mechanics and polymer physics. The students will construct coarse-grained models of polymers using approaches from the literature, perform simulations with open-source software packages, write trajectory analysis programs to characterize polymer dynamics, compare results with experiments (which will not be so evident!), model dynamics of macromolecules with Fokker-Planck equation.



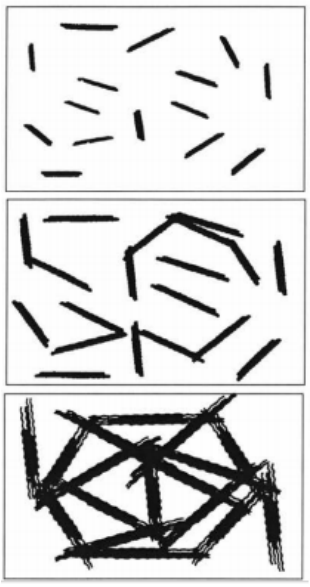
This is a more or less academic project with a potentially very much outcome that involves collaboration with experimentalists from Lund University, Sweden

Track: CSE

Background required: differential equations (a must), reasonable level in programming (a must), basics of thermo- and hydro-dynamics (a must)

Keywords: molecular dynamics, polymers, Fokker-Planck equation

Modeling gelation in waxy oils



“Waxes” is one of the main components of crude oil. Wax molecules are very long paraffin chains. Waxy crudes are known for gelation caused by partial crystallization of waxes. The project aims at designing a coarse-grained model able to describe the phenomena and the effect of other components, first of all asphaltenes.

Background required: probability theory (a must), programming (a must, C or Fortran preferred), basic thermo- and hydro-dynamics (a must).

Track: CSE

Keywords: crude oil, wax, crystallization, gelation

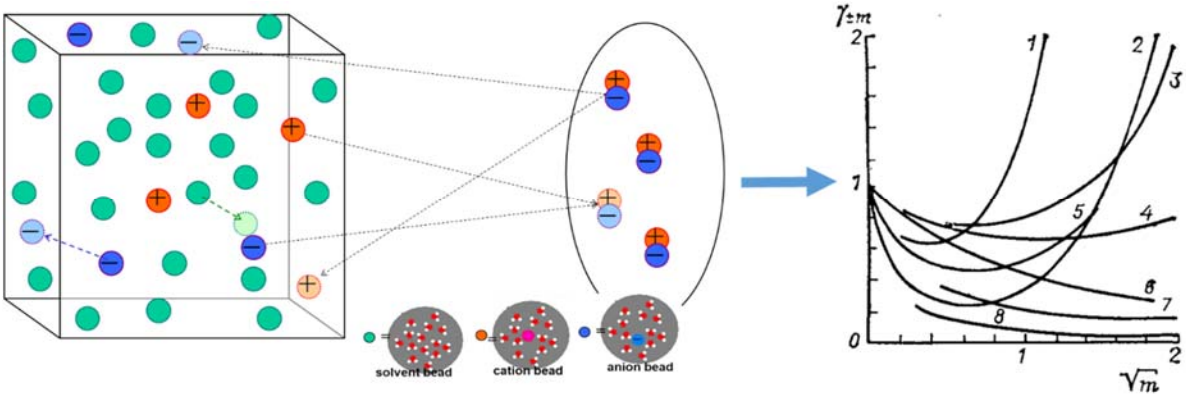
Soft-core models of electrolyte solutions

Because of the size of polymer molecules, their atomistic modeling of often prohibitively expensive. For that reason, simulation often relies on coarse-graining: individual atoms and molecules are “lumped together” and represented by quasiparticles (beads). In so called soft-core models the beads interact with short and soft forces (allowed to overlap) which provides a superb computational efficiency but restricts the model applicability. Simulations of [poly]electrolytes require charged beads with the charged smeared-out over the bead volume. Although this approach is rapidly gaining popularity, parameterization of soft-core electrolyte models is very much questionable since it is not clear how parameters are related to structural and thermodynamic properties of the solution. Establishing these relationships is the aim of the project.

The students will need to study fundamentals of statistical mechanics and thermodynamics of electrolyte solutions, explore the research literature, write Monte Carlo codes. As a result, the students will get and extensive, hands-on experience in mathematical modeling of physical processes of practical importance, scientific programming and scientific writing. This is more academic, technical project type with potentially publishable results.

Background required: probability theory (a must), programming (a must, C or Fortran preferred), general thermodynamics (a must).

Keywords: statistical mechanics, Monte Carlo modeling, electrolytes, Debye-Huckel theory.

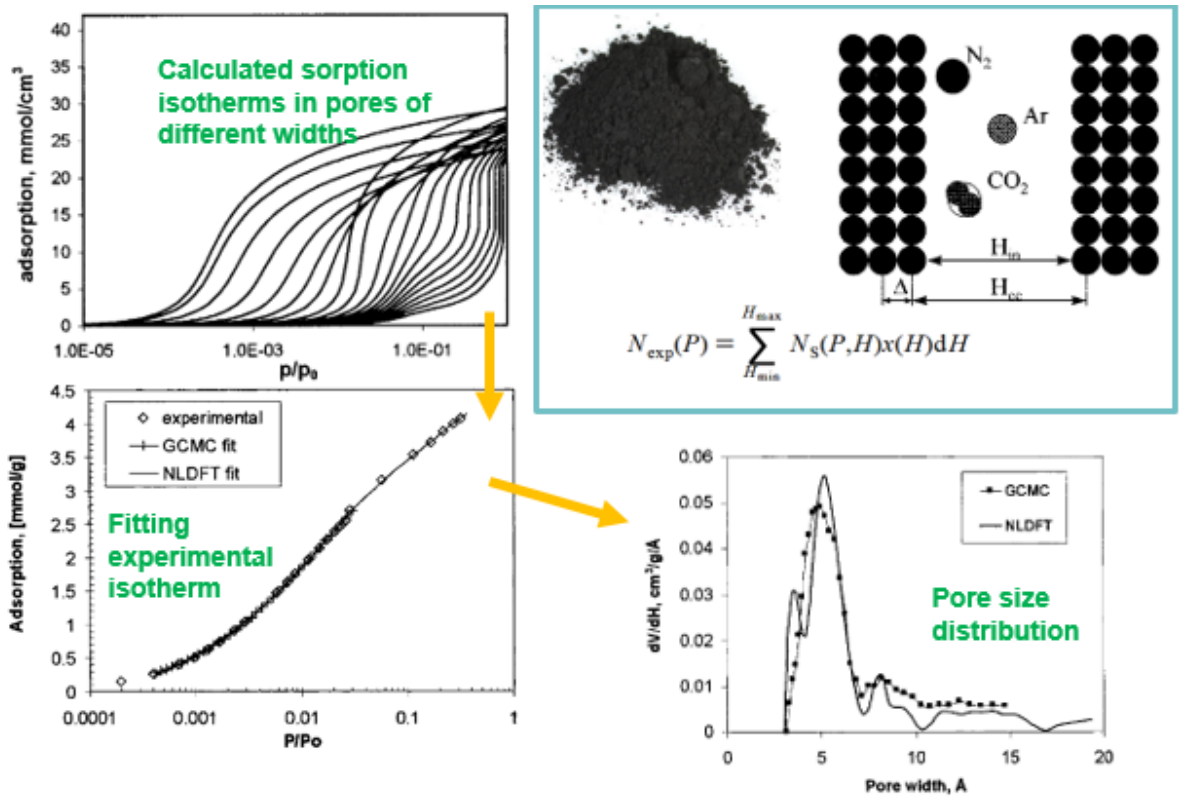


Inverse problem in adsorption characterization of heterogeneous porous solids

Vapour adsorption is a well-established inexpensive method for characterization of porous solids. Modern techniques of sorption characterization involve solving of an inverse problem: the surface and pore structure of a solid is deciphered by presenting experimental sorption isotherm as a weighted sum of isotherms theoretically calculated for pores of particular size, shape or surface chemistry. The aim of this work is extending this approach to very heterogeneous solids which may include components with qualitatively different chemistry and sorption mechanisms. Examples include geological samples encountered in oil/gas recovery, composite materials and pharmaceuticals. The components of such solids may feature both linear and non-linear transport-controlled sorption behavior. The tangible goal of the master thesis project is developing a solver for the inverse problem applicable to characterization of reference heterogeneous materials containing several precisely known reference ingredients.

Skills required: Numerical linear algebra

Keywords: inverse problems, optimization, SVD, adsorption, pore characterization, geological solids, composites



Modeling non-linear sorption in geological organic matter

Porous solids with isolated voids separated by permeable “matrix” materials are common both in nature and chemical technology. If the material is in thermodynamic equilibrium with a bulk sorbate of a certain temperature, the total amount of the fluid in the material can be presented as a sum if linear term (absorption of the sorbate by the amorphous matrix proportional to the outside bulk pressure) and a non-linear term that describes adsorption in the voids. Form the dynamic point of view, sorption in such medium with isolated voids can be defines as diffusion-limited, at diffusion controlled, due to low mobility of the adsorbate in the matrix.
An example of such material is naturally occurring organic matter insoluble in water or hydrocarbons, kerogen, is an amorphous complex mixture of mainly paraffin hydrocarbons. The structure and composition of kerogen supposedly control natural gas release in hydrocarbon recovery. Kerogen of different stages of maturity has different distributions of void sizes and matrix composition. The proposed master thesis project aims at development a mathematical model of diffusion-controlled sorption in complex porous media and application of this model to the sorption different compounds (methane, water, and CO2, hydrocarbons in kerogen of different stages of maturity. We may both use a 1D solution taking the porosity in account implicitly, or explicitly solve diffusion equation on a large 3D grid.
This is a practically oriented project in collaboration with CHR and application in oil recovery

Skills required: PDE, NLA

Keywords: petroleum, kerogen,

Aggregation of microparticle suspension in polymer solutions: application to additive manufacturing

The project involved modeling the dynamics of aggregation of solid particle in polymer solution, which serves as a precursor to a porous matrix that can be 3D printed in additive manufacturing technologies. Aggregation from liquid emulsions result in different porous ceramic materials (Figure 1). Additive manufacturing (AM) cannot however handle liquid suspension but handle polymer-particle "slurries". The hot slurry is ejected from a nozzle. Cooling initiates aggregation, and at some point, the structure is photopolymerized and thus "freezes". In this project we will model the aggregation with Langevin dynamics applying polymer-mediated forces to the particles. Special attention will be paid to non-pairwise nature of the polymer-mediated forces and their effect on the aggregation dynamics and the resulting structure. The multi-body forces will be derived from explicit-polymer simulations via machine learning.

This is a fundamental project with potentially publishable results.

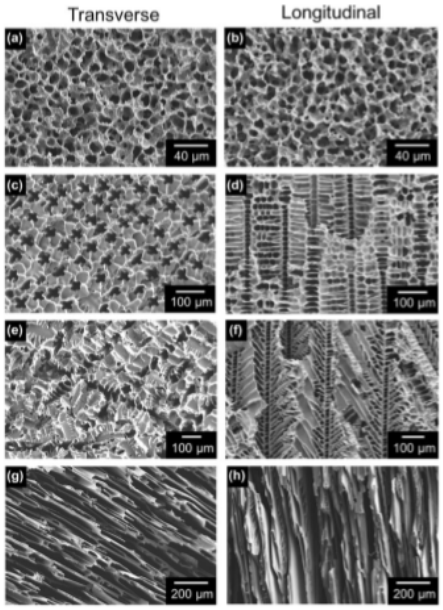


Figure 2. Examples of ceramic materials of different morphologies obtained via free-casting from ceramic suspensions [1]

Background required: programming (a must, C or Fortran preferred), general thermodynamics (a must).

Keywords: Brownian dynamics, polymer suspension.

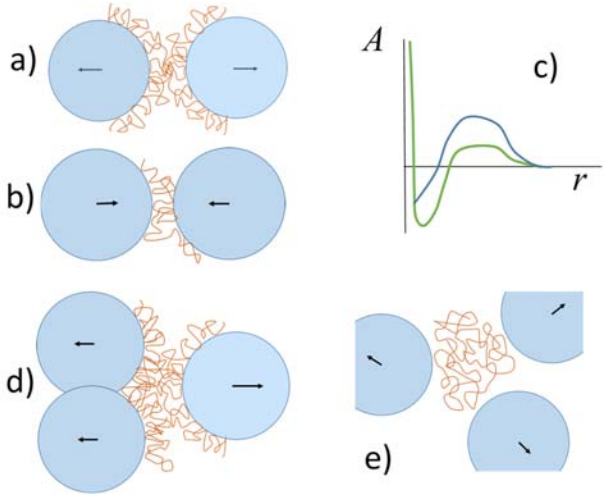


Figure 2. Multi-body effects in microparticle suspension in polymer solutions. Adsorbed polymers form a "corona", which causes entropic repulsion when two coronas overlap (a). The repulsion changes to attraction when a single polymers chain is adsorbed on two particles (b) resulting in a classical free energy dependence on distance with a barrier (green curve on graph (c)). If two particles sinter, the corona become denser due to reduced area (d) and the barrier for a third particle to approach strengthens (blue curve on graph (c)), note that this effect may quite strong even if the particle size is much larger than the effective polymer coil size. Panel (e) schematically shows the repulsive effect of a non-adsorbing coil confined between three particles that cannot be reduced to pairwise interactions.