Bachelor and Master Projects SMB
November 2023
List of brief descriptions
"Die Qual der Wahl"

Note: Theoretical and Computational projects are indicated with the letter T. Most theoretical projects can be made to fit a dual Applied Physics and Mathematics & Computer Science research project.

Alexey Lyulin: A1 (T)
Novel polyelectrolyte membranes for flow and fuel cells. Atomistic molecular-dynamics computer simulations of Nafion/graphene oxide nanocomposites using Gromacs and LAMMPS software packages. The goal is the connection between the heterogeneous structure and the details of the proton transport in these devices. Contact: a.v.lyulin@tue.nl.

Alexey Lyulin/ Maarten Boomstra: A2 (T)
Novel phase change materials for optimal thermal energy storage. Atomistic molecular-dynamics computer simulations of paraffine/CNT/graphene nanocomposites using Gromacs and/or LAMMPS software packages. The goal is to provide insights into the mechanisms of the (still) very low thermal conductivity in these amorphous compounds. Contact: a.v.lyulin@tue.nl.

Alexey Lyulin/Frederik Wurm (U Twente) (T) Molecular Modelling of Ion Permeability and Transport in Polyphosphoester Membranes}

In this Project the student will carry out atomistic large-scale molecular-dynamics simulations to unravel the connection between the microscopic structure and structural changes in PPE membrane that explain their cation conductivity characteristics. The project is in close collaboration with the group of prof. F. Wurm (Twente) where the synthesis of the PPE membranes will be performed. The main task will be to carry out molecular simulations, and to perform the analysis of their results. The Gromacs/LAMMPS MD software package will be used for these purposes.

Paul van der Schoot/Alexey Lyulin/Saskia Lindhoud (U Twente): PAS1 (T)
Physics of membrane-less cell organelles. Membrane-less organelles play an important role in how biological cells cope with environmental stresses, but are also involved in neurodegenerative diseases including Alzheimer's. Aim is to model organelles consisting of oppositely charged polymer molecules, and study their internal structure and interaction with proteins. Specific focus is on the structure of the complexes near embedded model proteins, the role of excluded volume interactions. Analytical, numerical and computer simulation projects are possible. Contact: p.p.a.m.v.d.schoot@tue.nl.

Alexey Lyulin: A3 (T)
Glassy structure and segmental mobility in free-standing thin polymer films. Atomistic molecular dynamics computer simulations of dense polymers in thin films in absence of a substrate using an in-house developed software package. Contact: a.v.lyulin@tue.nl.

Alexey Lyulin/Nikos Sigalas: A4 (T)
Molecular dynamics of multilayer single polymer films. In this project we undertake multiscale simulations of semi-crystalline morphology development upon high-strain mechanical deformation of polyethylene and polypropylene to understand the mechanisms controlling crystallization, toughness, permeability, determine optimization design strategies and provide a molecular basis for finite-element simulations. Contact: a.v.lyulin@tue.nl.

Alexey Lyulin/Kees Storm/RIVM: SL1 (T)
Molecular Dynamics studies of the release of chemicals from solid matrices. The project is part of a larger research effort of the RIVM concerning dermal exposure to (toxic) chemicals. The project focusses on the use of molecular dynamics (MD) as a means of estimating parameters that relate to the dermal exposure such as diffusion coefficients and partition coefficients. These parameters are calculated for substances dissolved in material matrices that may come into contact with human skin, e.g. polymers, rubber, paint. Contact: a.v.lyulin@tue.nl.

Alexey Lyulin/Bernard Geurts (U Twente, CCER)/Kevin Redosado (U Twente, CCER): LGR (T)

Heat transport in perspective novel phase change materials. The project is part of the large NOW project involving different groups at both TU/e and U Twente. Using Direct Numerical Simulations (DNS) on system scales, the effective conductivity as function of network and paraffin properties can be predicted. Model parameters for coarsened system-scale descriptions are extracted from the atomistic modelling, thereby creating a coherent multiscale approach. The impact of cyclic melting/solidification of *Wax*$^{+}$ materials on the thermal conduction will be investigated. The goal is to provide insights into the mechanisms of the (still) very low thermal conductivity in these amorphous compounds. Contact: a.v.lyulin@tue.nl.

Wouter Ellenbroek/Alexey Lyulin: WA1 (T)
Optimizing the performance of filler particles for bioplastics. Hard rod-shaped particles can greatly improve the strength and stiffness of plastics, but only if they mix well with the polymers. Can we improve this mixing by modifying the surface of the fillers? Contact: w.g.ellenbroek@tue.nl.

Alexey Lyulin/Bernard Geurts (U Twente, CCER): LG (T)
All-organic non-aqueous redox flow batteries (NARFBs) offer a potential solution to scalable, low-cost and multi-hour energy storage, but suffers from low efficiency due to high permeability of redox-active species across the battery's membrane. In this project project we will computationally design new polypropylene-based separator that combines excellent mechanical and chemical stability and microporosity with selective anion-exchange capacity for NARFBs. The physical mechanisms which connect the chemical structure of the grafted substances, conductivity and membrane efficiency will be explained by multiscale molecular modelling. Using Direct Numerical Simulations (DNS) on the system scale, the effective conductivity as function of separator functionalization, tortuosity and porosity will be simulated. Close interaction with the group of Dr. Forner-Cuence (Chemistry and Chemical Engineering dept, TU/e) is expected. Contact: a.v.lyulin@tue.nl.

Wouter Ellenbroek/Alexey Lyulin/Kerstin Blank (Potsdam): WAK1 (T)
Collagen-like peptide unfolding. Collagen is what you are made of. Mostly. Its deepest-level structure is a peptide triple helix that now has many synthetic mimics that are being used to design novel materials. The formation and unfolding kinetics of these synthetic triple helices is not quite understood. Molecular Dynamics will help. Contact: w.g.ellenbroek@tue.nl