Scientific Area	Multiscale Systems		
Project Title	Hierarchical multi-scale modeling of macromolecular systems at interfaces		
Recruiting Institution	Max Planck Institute for Polymer Research, Germany		
PhD awarding Institution	University of Mainz, Germany	**PhD Duration**	36 Months
Supervisor/Institution	Prof. Dr. Kurt Kremer, Theory Group, MPIP		
Co-Supervisor/Institution	Prof. Vangelis Harmandaris / The Cyprus Institute		
Secondment(s)	HPC Training MPCDF Garching or JSC Jülich Training on optimizing back-mapping algorithms – CyI		

Project Description

The study of polymer thin films, free standing or supported, is extremely important both from the scientific and technological point of view. This project concerns a computational approach for providing a fundamental understanding of polymer films, over a variety of spatiotemporal scales, as well as for predicting their structure-property relations in order to guide the design of such systems. While the behaviour of low molecular weight polymers at interfaces is well-studied and can be resolved, e.g. with detailed atomistic simulations, the behaviour of high molecular weight polymer films, is still poorly understood, especially since they often do not reach thermodynamic equilibrium and become trapped in long-lived, metastable states. To address these challenges, the current project proposes a hierarchical multi-scale simulation methodology combining atomistic and coarse-grained particle models of polymer films. Key in the proposed approach is the development of generic blob-based mesoscopic models, for polymers of specific chemistry, forming free standing films and adsorbed on substrates. These models will be parametrized using data from detailed atomistic simulations of specific polymer/substrate systems. Moreover, systematic back-mapping strategies on coarse-grained configuration will be optimized to obtain high-molecular-weight all-atom polymer liquids in order to predict properties of long polymer chains at liquid/vapor and liquid/solid interfaces.

"Efficient equilibration of confined and free-standing films of highly entangled polymer melts", Hsu HP, Kremer K, J. Chem. Phys. 153, 144902 (2020)

"Hierarchical modelling of polystyrene melts: from soft blobs to atomistic resolution", Zhang, GJ; Chazirakis, A; Harmandaris, VA; Stuehn, T; Daoulas, KC; Kremer, K, Soft Matter, 15, 289-302 (2019)

Project Objectives

- Develop a hierarchical computational approach that involves detailed atomistic and mesoscopic blob-based models for specific chemistry polymer/substrate systems;
- Provide a fundamental understanding concerning the structure, morphology and dynamics of polymer thin films at liquid/vapor and liquid/solid interfaces;
- Develop systematic back-mapping data-driven algorithms for re-inserting atomic detail into on coarse-grained configurations of high molecular weight polymers;
- Apply the computational methods to selected systems and examples, to explore metastable states and kinetic phenomena of high molecular weight polymer chains adsorbed on solid surfaces

Required Candidate Qualifications

- MSc (or equivalent) in physics, chemistry, applied mathematics, engineering, computational science/informatics, or a related field
- Proven computational and numerical skills; knowledge of a modern programming language; experience in high-performance computing (using e.g., GPU-acceleration) is desirable.
- Excellent communication skills (oral and written) in English
- Candidates with a strong background in computational soft matter or polymer science will be favoured