Scientific Area	Multiscale Systems		
Project Title	Single-Chain and Collective Dynamics of Polymer Materials		
Recruiting Institution	Georg-August Universität, Göttingen, Germany		
PhD awarding Institution	Georg-August Universität, Göttingen, Germany	**PhD Duration**	36 Months
Supervisor/Institution	Prof. Dr. Marcus Müller, Institute for Theoretical Physics		
Co-Supervisor/Institution	Institute for Theoretical Physics, Georg-August Universität, Göttingen, Germany		
Secondment(s)	Prof. V.A. Harmandaris, FORTH / CyI		

Project Description

Phase separation and/or self-assembly of multicomponent polymers is a route to nanoscale materials with intriguing functions and application potential. Whereas the equilibrium properties of model systems are rather well understood and can be predicted e.g., by self-consistent field theory, polymer materials often do not reach thermodynamic equilibrium but become trapped in long-lived, metastable states. Thus, processing often dictates application-relevant properties such as e.g., the domain morphology. For the rational design of materials via process-directed (self)-assembly it is crucial to predict and optimize the kinetics of structure formation. The overarching goal of this project consists in devising simulation models and techniques that establish a quantitative link between thermodynamics, single-chain dynamics, and the collective kinetics of order parameters such as the concentration field and in studying this correlation by the large-scale simulation of particle-based and field-theoretic models on supercomputers.

Project Objectives

- Develop a hierarchical multiscale modelling approach that bridges from a particle-based description to a field-theoretic one.
- Devise computational strategies to match the equilibrium properties of particle-based models (such as highly coarse-grained, soft bead-spring models) and continuum models (such as the standard Gaussian chain model for multicomponent polymer melts or extensions thereof)
- Study the coarse-graining of dynamics by comparing particle-based models with two different resolutions and particle-based and field-theoretic models; quantify the influence of single-chain dynamics on the collective kinetics of structure formation
- Explore techniques to describe the dynamics of structure formation, phase-separation or self-assembly in coarse-grained particle-based and field-theoretic models, accounting for memory effects induced by coarse-graining, dynamic asymmetry between components, and/or slow configurational properties
- Apply the modelling approaches to selected examples (e.g., solvent evaporation from a solvent-swollen polymer film or phase separation in dense multicomponent mixtures).

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 condensed matter or polymer science will be favoured

The University of Göttingen is an equal opportunities employer and places particular emphasis on fostering career opportunities for female scientists. Qualified women are therefore strongly encouraged to apply as they are underrepresented in this field. Disabled persons with equivalent aptitude for the position will be favored.