Scientific Area	Multiscale Systems		
Project Title	Multiscale computational approaches for wetting on soft surfaces		
Recruiting Institution	The Cyprus Institute. Nicosia, Cyprus		
PhD awarding Institution	The Cyprus Institute. Nicosia, Cyprus	**PhD Duration**	36 Months
Supervisor/Institution	Asst. Prof. Nikos Savva, The Cyprus Institute		
Co-Supervisor/Institution	Prof. Dr. Marcus Müller, Georg-August Universität, Göttingen, Germany Prof. V. Harmandaris, The Cyprus Institute		
Secondment(s)	Goodyear; Universität Göttingen		

Project Description

The project aims towards the development of synergistic modelling, computational and data-driven methodologies to investigate the displacement of a liquid by another immiscible liquid on a soft polymer surface. It entails large-scale atomistic simulations to probe into the interface of liquid-polymer systems, and the development of coarse-grained computational models at the mesoscale to uncover their pertinent macroscopic material properties. Additionally, data-driven methodologies will be invoked to develop parsimonious constitutive laws at the continuum level, which are able to balance accuracy with complexity, thus informing the appropriate conditions to be used in macroscale simulations of the system. It is envisaged that through this coupling of macroscale and molecular-scale physics, a novel systematic multiscale framework will be introduced, which will consist of predictive tools that are capable of accurately simulating the wetting dynamics on soft polymer surfaces.

During the 3-year duration of the project, secondments will be undertaken at

- Goodyear – Application of wetting phenomena in industrial processes
- Universität Göttingen – Mesoscopic simulations

Project Objectives

- Acquire skills in
  - atomistic simulation;
  - computational fluid dynamics;
  - coarse-graining and multiscale methodologies;
  - data-driven modelling approaches.
- Develop a hierarchical multiscale modelling approach for the constitutive modelling and simulation of wetting systems.
- Develop and deploy computer codes for the simulation of wetting systems across different scales.

Required Candidate Qualifications

- MSc (or equivalent) in physics, applied mathematics, engineering with emphasis on scientific computing
- Proven computational and numerical skills; knowledge of a modern programming language, e.g. Python.
- Excellent oral and written communication skills in English.

Desirable qualifications

- Strong background in computational fluid dynamics, soft condensed matter or polymer science.
- Experience in high-performance computing