Scientific Area	Multiscale Systems		
Project Title	Multi-scale simulation methodologies of organic semiconductors for morphology control		
Recruiting Institution	The Cyprus Institute		
PhD awarding Institution	The Cyprus Institute	**PhD Duration**	36 Months
Supervisor/Institution	Prof. V. Harmandaris / The Cyprus Institute		
Co-Supervisor/Institution	Dr. K. Daoulas / MPIP		
Secondment(s)	Trained on the development of coarse-grained models for OS materials – MPIP; Trained on back-mapping algorithms, and on data mining and ML techniques for developing a 2D OS materials database – NovaMechanics		

Project Description

Two-dimensional (2D) materials are sheet-like macroscopic crystals with thickness of one or (maximum) a few atomistic or molecular building units. One prominent case is 2D crystals of organic semiconductors (OS), which have tremendous potential to serve as active layers of optoelectronic devices that benefit from a 2D architecture. This project focuses on developing and applying novel, quantitative, multi-scale simulation methodologies for studying 2D-OS, understand their molecular arrangement and develop design rules to formulate molecular-, system-, and process-design guidelines for manufacturing large-area single crystals. The project consists of the following tasks:

Task 1: Perform simulations based on all-atom models of 2D crystals of organic semiconductors. Clarify the kinetics of the self-assembly (nucleation/growth mechanism) and the structure of aggregates at the liquid/vapour interface, on length scales ranging from individual chemical bonds up to domains of 10–20 nm.

Task 2: Develop systematic mesoscopic (coarse-grained) model of OS, which can handle systems with dimensions between 100 and 500 nm, to provide information on materials, with device relevant dimensions.

Task 3: Create a detailed "2D-OS material database" involving molecular structure characteristics and macroscopic properties of 2D OS materials. The database will be employed by data mining tools to propose hidden correlations between molecular fingerprints, structure and properties.

Project Objectives

- Develop quantitative multi-scale simulation methodologies for studying organic semiconductor (OS) materials;
- Understand the molecular arrangement, including the structure and statistics of defects, in 2D-OS crystals, assembled at the liquid-vapour or liquid-solid interface;
- Develop design rules to formulate molecular-, system-, and process design guidelines for manufacturing large-area single crystals that are interesting for e.g. optoelectronics

Required Candidate Qualifications

- BSc (or equivalent) degree in Physics, Applied Mathematics, Engineering or a similar discipline;
- MSc (or equivalent) in computational science, soft condensed matter, or a related field;
- Computational and programming skills;
- Candidates with a strong background in computational soft condensed matter and materials science will be favoured.