Scientific Area	Multiscale Systems		
Project Title	Modelling and basic understanding of natural molecules with surfaces and nanoparticles		
Recruiting Institution	Foundation for Research and Technology (FORTH)		
PhD awarding Institution	The Cyprus Institute (CyI)	**PhD Duration**	36 Months
Supervisor/Institution	Prof. Vangelis Harmandaris / CyI		
Co-Supervisor/Institution	Dr. Evangelia Kalligannaki / FORTH		
Secondment(s)	Applications of multi-scale modelling in nanotechnologies –NovaMechanics and FORTH		

Project Description

Functionalized bio-derived surfaces and biopolymer nanocomposites are very important materials towards the transition to a more circular economy. To design and formulate new bio-based functionalized products, with the desired properties, it is necessary to predict their properties from the molecular structure. The main goal of the project is to provide a fundamental understanding of bio-based materials via computational modeling, involving advanced molecular simulation approaches and data-analytics algorithms. We propose hierarchical multi-scale modelling approaches, based on large-scale atomistic simulations and systematic coarse-grained models, for predicting structure-property relationships of biomolecules interacting with specific surfaces and of bio(polymers)-based nanocomposites. Different systems of biomolecules (proteins, peptides, biopolymers) in contact with surfaces, as well as biopolymer-based nanocomposites, such as poly-lactic acid/silica nanoparticle (NP), will be studied via atomistic molecular simulations. Then, via data-driven algorithms, the atomistic results are used to derive proper coarse-grained models for biomolecules. The latter will allow the study of larger systems for longer spatio-temporal scales. A main part of the project also refers to the creation of a detailed "(bio)-nanocomposite material database" involving molecular structure characteristics and macroscopic properties of biopolymer nanocomposites. The database will be employed by data mining tools to propose hidden correlations between molecular fingerprints and structure.

Project Objectives

- Develop hierarchical multi-scale modelling and simulation methodologies for obtaining a basic understanding of biopolymers and proteins interaction with specific nanoparticles (NPs);
- Obtain microscopic structure – macroscopic properties relations for various systems;
- Predict structure, conformations, and dynamics of biolpolymers/NPs model systems, as a function of polymer/NP interaction, temperature, concentration etc.

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, applied mathematics, engineering or a related field;
- Computational and programming skills;
- Candidates with a strong background in computational soft condensed matter and materials science will be favoured.