ID: MSCA-19-Tielens03

Discipline: Chemistry

Title: Characterization of Bio-organic Self Assembled Monolayer on Metal Surfaces

Abstract: The formation of nanostructured bio-organic interfaces has attracted a lot of attention recently in surface science worldwide because of its promise in fields in need of biocompatible materials, such as biosensors and biomaterials, but also in molecular electronics devices. Furthermore, the understanding of processes such as biofouling has direct applications, e.g. looking for adapted coatings to avoid the adsorption of biological material on trade vessels crossing seas and oceans. But also in the elaboration of anti-corrosion coatings and other “smart” electronically connected devices.

The prototype molecules for self-assembly on metals are thiols, which have been investigated at both the theoretical and experimental level. From there, the step was made to amino acids, which are now seen as the ideal test case for three reasons: firstly, they are small enough to allow for calculations with high accuracy to model the chemisorption of bio-functional molecules. Secondly, forming the building blocks of peptides and proteins, they are a good representation of such complex molecules and their interaction with the surface of interest, a crucial point for issues related to biocompatibility. Finally, since amino acids are chiral, they can transfer this chirality onto an achiral surface, which has important applications in enantioselective catalysis, a key process in modern chemistry and particularly important in the field of pharmaceutics.

The holy grail for this field, from the molecular modelling point of view, is the simulation of an entire protein in realistic conditions, which is computationally too expensive at the DFT/ab initio level at the moment. However, in order to model the interactions, present in these systems, it is important to fully understand the behaviour of their building blocks, the amino acids, and to make the step to slightly more complex systems such as peptides.

Supervisors: Frederik Tielens, frederik.tielens@vub.be

Website: http://we.vub.ac.be/en/general-chemistry

To apply: https://www.vub.ac.be/en/european-liaison-office#apply-msca-if