



## **PhD subjects at Interdisciplinary Center for Advanced Science and Technology at the University of Split**

**ICAST** is an interdisciplinary initiative in nanoscience, including nanobiology, structured optical and catalytical materials for biosensing, fuel and solar cells. Research projects at ICAST are based on multi-disciplinary approach to the scientific topics that unifies advanced computer simulations, which are the expertise of the ICAST scientific team, with the experiments at the scientific frontiers that are realized through the cooperation with a number of Universities in Europe and in the US. Director of ICAST, Prof. Dr.Dr.h.c. Vlasta Bonačić-Koutecký, is an internationally recognised scientist in the fields of theoretical chemistry, nanocluster physics, photochemistry and femtochemistry. PhD subjects described below will be carried through under her supervision.

### **1. Development of new generation of nanostructured biosensing materials**

- A. The objective of the PhD dissertation at ICAST is to investigate the absorption, photoemission and energy transfer processes in metal nanoclusters-protein hybrid systems by advanced theoretical modelling of optical resonance and ultrafast dynamics. The goal is to develop a new generation of hybrid nanostructured materials for label-free biochips. The project will be carried out in the cooperation with the University of Birmingham.
- B. The objective of the PhD dissertation is to use optimal quantum control with shaped laser fields to increase sensitivity and reproducibility of nanostructured biochips. For this purpose, the electric field induced molecular dynamics will be used and experimental validation will be performed with advanced shaped light sources in cooperation with the University of Geneva.

### **2. Metal clusters for optical detection of biological aging**

The fluorescent markers are a commonly used technique for detection of protein carbonylation, which is a measure of biological aging. The subject of the PhD dissertation at ICAST is to investigate how to significantly increase the performance of such markers by exploiting metal clusters enhancement of absorption and fluorescence. For this purpose theoretical modelling will be used to design efficient markers and the results will be validated in the collaboration with the experimental group at the University of Lyon.

### **3. Development of new materials for solar cells**

The subject of the PhD dissertation at ICAST is theoretical investigation of optical properties of liganded porphyrins in cooperation with the experimental group at the University of Colorado. An example of possible application that can be envisaged readily is to prepare a porphene sheet carrying electron donors on one side and acceptors on the other, and to use the spectral properties of the ligands or of porphene itself for the capture of solar photons and their conversion into spatially separated electron-hole pairs. Since the electrons would all be on one side and holes

all on the other side of the porphene sheet, the structure would resemble a well-defined p-n junction. Electrodes, possibly represented by additional parallel porphene sheets if they are conductive enough, or possibly by graphene sheets, could be located very close for efficient removal of the photogenerated charges to an outside circuit.

#### **4. Design of new catalytic materials for fuel cell feed gas purification**

The objective of the PhD dissertation at ICAST is to advance the catalysts that selectively remove CO from the hydrogen rich feed gas used for the polymer electrolyte membrane fuel cells (PEMFCs) and thus lower the poisoning of the cell. The research will focus on the catalytic methanation reactions mediated by ruthenium clusters. The ruthenium particle size effects and metal charging effects are expected to be crucial for sensitivity of these reactions. Advanced computational simulations at ICAST will be used to reveal molecular aspects of metal catalyzed reaction mechanism and will be the basis for the advancement of the efficiency of fuel cell technology as a green technology of the future. Experimental verification will be carried out in cooperation with the University of Ulm.