POSTDOC OFFERS

PROJECT

Acronym	SELPHY
Title	Correlating **S**tructural, **El**ectronic and **P**hotophysical Properties of Metal-based Nano-**Hy**brids
Coordinator's name	Dr. Ivan Rivalta
Lab name/team name	Laboratoire de Chimie (ENS Lyon) – Theoretical Chemistry Axe

Funding : iMUST
Gross Salary : 2685 €/month
Workplace: ENS Lyon – Laboratoire de Chimie
Beginning of the contract: Upon candidate availability
contract length : 12 months + 12 months

MISSIONS AND SCIENTIFIC PROGRAM

A computational protocol will be developed for multiscale simulations of the structural and photophysical properties of a promising class of nano-hybrid systems. The goal is to provide an atomistic interpretation and quantitatively characterize the charge and energy transfer phenomena induced by the photoactivation of the organic dyes grafted on gold nanoparticles, which will manifest as both quenching of the dyes luminescence and transient LSPR shift of the nanoparticles. The scientific program initially involves structural characterization of the supramolecular architecture of the gold nanohybrids by means of quantum-mechanical (periodic slab) calculations combined with classical molecular dynamics simulations. Refinement of existing force fields of the hybrid systems will be followed by MD simulations at different initial conditions, consistently with concurring experiments performed by the project's partners. A software interface will be created for the statistical analysis of the MD trajectories and the creation of inputs for the electronic structure calculations of the photosensible hybrid systems. Photophysical properties of the gold nanohybrids will be determined using cluster model approaches and by means of TD-DFT methods.

KNOWLEDGE AND SKILLS REQUIRED

The call is open to highly motivated applicants with previous experience with ab initio calculations and/or classical molecular dynamic approaches (preferentially both). The candidate must have a PhD in Theoretical Chemistry, Physical Chemistry or Physics. Programming skills (preferentially Python) are required. Experience in development and application of classical force fields for metals (gold in particular) is highly welcome. Advanced knowledge of the following codes will be an advantage: VASP and/or CRYSTAL, NAMD and/or GROMACS, MOLCAS, Gaussian09. Previous work experience on organic/inorganic interfaces and/or excited states will be a plus. Good communication skills (written and spoken English) are required for the collaborative teamwork.

The folder includes	To be forwarded to
CV – list of publications Motivations letter PhD thesis title and summary: Name and contact information of 2 or 3 referents	ivan.rivalta@ens-lyon.fr

WORKING ENVIRONMENT/CONTEXT

The project will be carried out in the Chemistry Laboratory of the ENS Lyon (Campus Site Monod), which is a joint unit operated by the CNRS, the École Normale Supérieure of Lyon and Université Lyon 1. The Chemistry Laboratory (http://www.ens-lyon.fr/CHIMIE) spans a range of specialities in chemistry and physical chemistry and it develops interdisciplinary research projects at the frontiers with biology, material sciences and physics. The candidate will work in the "Theoretical Chemistry Axe" of the Chemistry Laboratory (http://www.ens-lyon.fr/CHIMIE/recherche/Teams/Chimie_Theorique), in an international research environment and in strong collaboration with two experimental partners: the "Functional Materials and Photonics" team of the ENS-Lyon and the "FemtoNanoOptics" team of the Institut Lumière Matière (ILM-Lyon).