

## 1 year Postdoc position

### Ab initio modelling of nanomaterials for Raman characterization

Supervisor: Prof. M. Calatayud [calatayu@lct.jussieu.fr](mailto:calatayu@lct.jussieu.fr)  
Laboratoire de Chimie Théorique, Sorbonne Université  
4, Place Jussieu 75252 Paris Cedex 05, France.

starting date: Apr 2021  
(12 months)

salary: ~2000 E/month net

Funding scheme: H2020 RIA CHARISMA 952921 (4.9 M EUR)

Keywords: DFT, nanomaterials, Raman spectroscopy, surface reactivity, standardization

Raman spectroscopy is a key tool for the characterization of a variety of complex system, from molecules to nanomaterials, and its use has spread in many technological applications. The diversity in the data acquisition, treatment and analysis needs spectra calibration and harmonization in order to be interoperable among equipments and conditions. Computational modelling is a powerful tool to obtain experiment-free spectroscopic features to interpret, assess and predict experimental response. The goal of the CHARISMA project is to harmonize Raman spectra through a combination of reference samples, standardized conditions and theoretical modelling, enabling its optimal use in selected industrial processes.

#### Main tasks and milestones.

- Selection of a set of relevant materials (calculable and representative) through extensive literature search and consortium input
- Building of relevant models for the selected materials: molecules, solids (crystalline and amorphous), surfaces, nanoparticles
- Production of calculated physico-chemical properties, in particular Raman spectra, to characterize and analyse the systems' electronic features and reactivity, according to the state of the art
- Interaction with the other partners of the project by sharing information, communicating and discussing results, participating in training activities such as workshops, mentoring students, dissemination

**Requirements:** PhD in theoretical chemistry or physics.

Prior knowledge of quantum chemistry programs (VASP, Quantum Espresso) and surface science, nanomaterials chemical reactivity, as well as literature search tools is mandatory. Basic programming skills (scripting)

Knowledge of conceptual DFT, QSAR analysis, databases, machine learning is a plus.

Ability to work in autonomy and as part of a team

Fluent and efficient communication skills in English (oral, written)

**Working conditions:** the candidate will integrate the Materials for Environment and Energy group in the Laboratoire de Chimie Théorique, Sorbonne Université campus PMC (4, Place Jussieu 75005 Paris). He/she will have access to the lab and campus facilities: local and national supercomputing centers, libraries, and a rich scientific and living area in the city center.

**Income:** ~2000 € (net) per month; the candidate will be hired by Sorbonne Université as full-time researcher for the period. He/she will benefit of the French social security, unemployment allowance after the end of the contract.

Application: Please send your CV, two recommendation letters to Monica Calatayud ([calatayu@lct.jussieu.fr](mailto:calatayu@lct.jussieu.fr)) specifying "postdoc CHARISMA" in the subject.