Post-Doctoral position in **chemical physics or physical chemistry**

Molecular Modelling of hyperpolarizability of interfaces to interpret **SHG** experiments for **liquid/liquid interfaces**

In tight collaboration, **ICSM in Marcoule** and **UMR PASTEUR at ENS Paris** open a postdoctoral position in **modelling**. The project consists in modelling Second Harmonic Generation (SHG) experiments for liquid/liquid interfaces from a molecular approach.

Knowledge of the **interface between two liquids** is fundamental for the development of numerous processes, such as **solvent extraction** which is the most important method for separating and recycling metals. However, very few data and experimental methods are available. The **second harmonic generation** method (SHG) is in this context a **method of choice** because it is **interface specific**, with volume terms cancelling each other out on average, but there is no procedure to interpret the results directly at the molecular level. For the first time, we propose to do this within the framework of liquid-liquid interfaces of separative chemistry using **molecular simulation**. The idea is to start from a **multi-scale approach** we recently proposed in order to move away from the concept of individual hyperpolarizability, which is not relevant for flexible molecules. Practically, first, classical dynamics calculations describing the interface will be performed. Then, we will calculate directly the SHG signal on the entire simulation box from quantum calculations by choosing a representative set of system states. A complementary methodology based on a fluctuation method will also be introduced. If successful, this post-doctoral work should have a **very significant impact** on the study of interfaces because this coupling between SHG and molecular simulation will provide a **new probe at the molecular level for liquid/liquid interface**

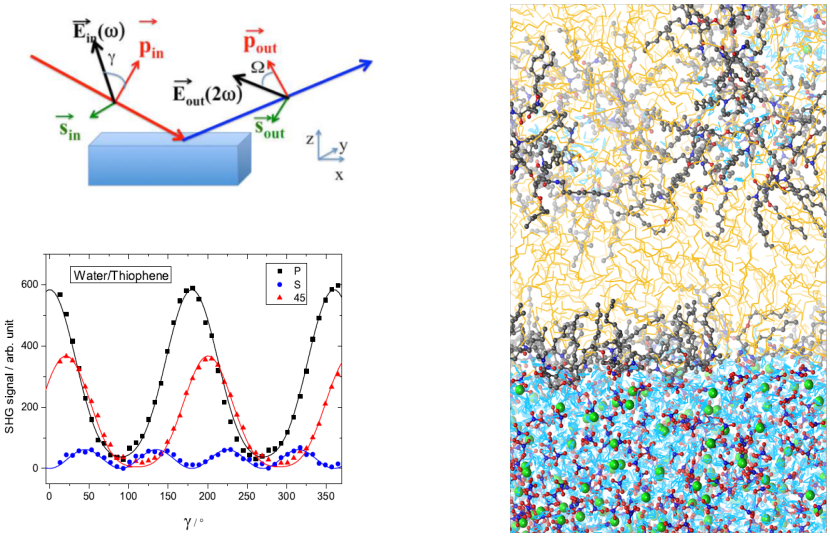

Figure: SHG experiment (top left) and the resulting measured SHG signal for a water/thiophene interface system (bottom left). Molecular dynamics simulations of water/oil interfaces in solvent extraction (right)

Profile: Theoreticist with a PhD in physical chemistry or chemical physics. A knowledge of classical or *ab initio* molecular simulations will be appreciated.

Scientific teams: The researcher will be located either in ICSM in Marcoule or in UMR PASTEUR in ENS Paris, and he/she will interact with then two teams together with experimentalists.

ICSM: the Institut de Chimie Séparative de Marcoule (Joint Research Unit CEA – CNRS – Univ. Montpellier – ENSCM) is an international institute involved in the research and the development of new and innovative separation processes for energy and sustainable development. The project is affiliated to the modelling group headed by J.-F. Dufrêche in collaboration the experimentalists devices developed by the group of O. Diat.
PASTEUR: is a joint laboratory (UMR) from ENS Paris/PSL Research university, CNRS and Sorbonne Université. The researcher will be affiliated to the Theoretical Chemistry group, which is an internationally recognised group focussing on chemical reactivity in condensed and complex media.
The SHG experiments and the molecular interfacial model is developed at ICSM. Quantum calculations of hyperpolarizabilities will be performed at UMR PASTEUR.

Details: The position is funded by CEA (bottom-up SHG futur project) for (at least) 1 year, starting in 2019 as soon as a suitable candidate is selected. The researcher will be located either in ICSM in Marcoule or in UMR PASTEUR in ENS Paris, and he/she will interact with then two teams together with the experimentalists.

How to apply: Interested candidates should email their CV and a (short) application letter to:

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- Pr. Rodolphe Vuilleumier, PASTEUR rodolphe.vuilleumier@ens.fr