Master 2 Internship

Title: Charged aqueous interfaces studied by Second Harmonic Generation
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PhD funding (if any): Possible- ANR

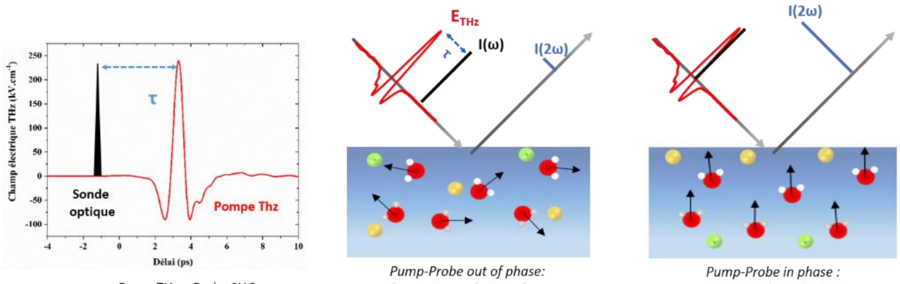
Project:

Interfaces of water and aqueous solutions play a prominent role in many technological and natural processes. The liquid/solid interface is the main driver for many electrochemical reactions. Water being present everywhere, the fields of applications are numerous.

Water interfaces are the most commonly used platforms for chemistry and biological processes, but the current understanding **at the molecular level and ultrashort timescales** is uncharted territory.

The main idea is then to structure and charge water interfaces, without adding any chemical compound, by intense terahertz (THz) pulses. This original idea is based on the fact that the coupling between the permanent dipole moment of the water molecules and the THz field should result in the re-orientation of the dipole moment which in turn should affect the arrangement of water molecules in the bulk and at the interface. This re-arrangement will be then revealed by performing **time-resolved** THz pump/SHG (second Hamonic Generation) probe experiments.

Our goal is to develop a hybridized SHG/ SFG spectroscopies to study vibrational modes for aqueous interfaces. More precisely, we intend to develop a method based on terahertz field-induced surface charging and study its consequent interface dynamics through SFG/SHG spectroscopies.



Pump THz – Probe SHG *Pump-Probe out of phase: Properties at the interface* *Pump-Probe in phase : Properties from the bulk*

To prove that we can structure a charged interface with THz, we shall start this project by measuring, as mentioned previously, the surface nonlinear signal for a charged interface and control the surface charge thanks to an intense THz field focused at the interface. We already built an SHG optical setup and implemented the THz beam. During the project, you will first study the water structure dynamics through SHG measurements. The second step will be the SFG setup implementation, i.e. adding an IR beam light. You will then be able to study the microscopic water structure, deduce the vibrational spectra of the Stern layer at the air/water interface as a function of electric field *for the first time* without adding any chemical, providing microscopic insight into the interfacial bonding structure at the air/water interface.

During this internship you will be working closely with a postdoc.

References

Wen, Y.-C.; Zha, S.; Liu, X.; Yang, S.; Guo, P.; Shi, G.; Fang, H.; Shen, Y. R.; Tian, C., Unveiling Microscopic Structures of Charged Water Interfaces by Surface-Specific Vibrational Spectroscopy. *Physical Review Letters* 2016, *116*, 016101.

Dalstein, L.; Chiang, K.-Y.; Wen, Y.-C., Direct Quantification of Water Surface Charge by Phase-Sensitive Second Harmonic Spectroscopy. *The Journal of Physical Chemistry Letters* 2019, *10*,5200-5205.