In 2012-2013, Professor John Shaw came to Pau for a year-long sabbatical (TOTAL and UPPA). One of the positive consequences of this visit was a collaborative project between the University of Alberta in Edmonton and UPPA. The primary objective of the project, which began in 2014, was to identify the chemical composition of the constituents of petroleum fractions, and in particular of a fraction called asphaltene.

Global environmental challenges have lead us, in recent years, to rethink our relationship with energy, and, to rethink the use of fossil fuels, which are the world's primary energy resource, followed by nuclear energy, and are non-renewable. In 2017, no scenario or projection can reasonably imagine a future where petroleum resources have no role, which highlights the necessity for leading-edge research to improve current industrial extraction and refining processes.

Diminishing light crude resources have lead to greater use of heavier fractions of crude oil, with the introduction of desulfurization stages in industrial oil distillation. Further, the improvement of these processes relies more on the improved quality of the distillation products (through more adapted desulfurization procedures), than on the the distillation of heavier and heavier of crude oil, which allows for a more sustainable use of fossil energy.

It is thus crucial to understand that improving these processes requires a better understanding of the chemical composition of the different crude oil distillation products. It is not enough to simply derive them from the extraction and refining methods commonly used for lighter fractions of crude oil: treating heavier fractions requires looking more precisely at the chemical nature of the molecules to understand the resulting physical properties and to be able to develop innovative procedures to guarantee the efficient refining of a growing number of crude oil fractions.

Quite logically, it is also indispensable to study both the chemical composition of the "exploitable" constituents of heavy fractions and the "non-exploitable" constituents, whose physico-chemical behavior is the cause of many difficulties throughout the various phases of industrially petroleum exploitation. Asphaltenes, the object of the collaboration between the two universities, belong to the latter category. The current lack of understanding of these systems is the cause of severe restrictions, from lower output to pipeline obstructions. Characterizing asphaltenes is therefore a very important problem.

For the UPPA theoretical chemistry team, solving this problem begins with fundamental research. In particular, one of the goals of the collaboration with the Canadian teams is to take on the challenge of quantum treatment of the complex chemical systems which characterize asphaltenes. Like the recent Nobel Prize winner in chemistry, computational
chemistry, which is also used in this project, has revolutionized the way that researchers understand molecular structure and reactivity. Simulation has become essential part of scientific progress. Because of the nature and complexity of asphaltenes, it is impossible to characterize them using only experimental data. Simulation, in this case, is a necessity.

Our current work concentrates on the simultaneous study of

* molecular configuration,
* intermolecular interactions and
* the stability and aggregation phenomena of asphaltenes.

In particular, the joint project with the University of Alberta is focused on the development and implementation of theoretical chemistry methodologies for calculating vibrational spectrums, which are the real fingerprints that allow us to elucidate the composition of these complex chemical systems.