# PhD Proposal 2017

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| **School: École Centrale de Paris (CentraleSupélec)** | |
| **Laboratory: LGPM** | **Web site: www.spms.ecp.fr** |
| **Team: Martials and Bio-Martials** | **Head of the team: M-L. Giorgi** |
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| **Collaboration with other partner during this PhD:**<br>**In USA : Prof V. Kokoouline at University of Central Florida** | **In China: to be considered with the candidate** |

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| **Title: Hydrocarbon molecules databases for waste treatment applications.** |
| **Scientific field: Chemical physics, quantum physics, basis on mathematical modelling and simulation, applied physics, engineering sciences** |
| **Key words: hydrocarbon, molecular dynamics, rate coefficients, treatment** |

## Details for the subject:

These last years, Hydrocarbon molecules such as $CH_2$, $CH_3$, $C_2H$ and $C_xH_y$ in general have attracted considerable attention for the various manufacturing applications including elaboration of advanced carbon materials and nanostructures [1-3], in view of several key-applications, e.g., drugs sensors [4], stretchable conductors [5] or more generally electronic devices [6], optoelectronics [7], energy storage [8-11], flue gas treatment [12] and fuel conversion [13]. They are also produced in order to investigate the formation of the chondritic organic matter (COM), contributing substantially to our understanding of the mechanisms involved in the formation of the solar system [14-15]. Most of the studies carried out were restricted to application oriented issues. As a result, despite their large appeal, these molecules remain very poorly understood.

Usually plasma composed by hydrocarbon molecules shows a large dissociation degree and a composition that is totally different from the feed gas. In such cases, the plasma behaviour depends on the electron interaction with the secondary radicals and ions produced by electron-impact dissociation of the feed gas molecule or through plasma-surface interaction. This question, having never been considered, **need to be addressed through the investigation of the dynamics of the reactions** between the free **electrons and the primary and secondary radicals**.

## Research subject, work plan:

The aim of this project is to contribute to enrich **the cross sections** database for excitation of hydrocarbon molecules by electron impact. The cross sections and related rate-coefficients on a large energy range, temperature, will be evaluated **using molecular dynamics** via tow physical approaches: (i) time independent R-matrix, Multichannel Quantum Defect Theory (MQDT)[17] and/or (ii) time dependent standard wavepacket methods or Multi-Configuration Time Dependent Hartree (MCTDH). The obtained cross sections of collision processes will be introduced into databases used for modeling the dynamics hydrocarbon plasmas **especially for waste treatment and depollution applications.**

The PhD work consists of three main tasks:

**Task 1 –** As a first step of this work**,** we propose to determine the structure of small molecules such as $CH_2$ or $CH_3$ using molecular dynamics approach throughout the MOLPRO software. This later is a comprehensive system of *ab initio* programs for advanced molecular electronic structure calculations. The developed methodology can then generalized to larger molecules with treatment or depollution interests.

**Task 2 –** Once the structure of the molecules is determined, we propose to use the Quantemol software and the implemented the UK R-matrix formalism (Fig. 1) to determine ro-vibrational, electronic excitations and ionization cross sections for some hydrocarbon molecules. Cross sections for these processes are needed for modelling atmospheric plasma. For this purpose, the UK R-matrix formalism is an efficient method for calculating low-energy electron-molecule scattering cross sections.

**Take 3-** The above-mentioned calculations will be compared and validated with experiments performed in laboratory especially in collaboration with the group Materials at the "Université Paris-13 Villetaneuse". These data will be also included in the atomic and molecular databases for plasma modelling such as ADAS (http://open.adas.ac.uk/) and KIDA (http://kida.obs.u-bordeaux1.fr/).

**This work will be carried out with a strong collaboration with Prof V. Kokoouline at the University of Central Florida (UCF) and Prof Khalid Hassouni at "Université Paris-13 Villetaneuse". An exchange and long term stay at UCF is planned during the PhD.**

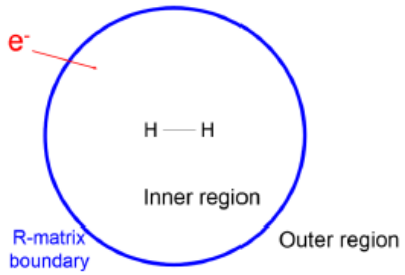


*Fig. 2: Schematic representation of the R-matrix formalism for electron $H_2$ collision. The inner region, inside the blue circle, where Schrödinger equation is solved and the outer region using the asymptotic expansion such as a long range multipolar interactions.*

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