Towards a clean atmosphere: The physics and chemistry of molecular fragmentation

One of the main challenge for humanity in the coming decades is to find an answer to the problem of the emission of pollutants, chiefly hydrocarbons and VOCs, that are toxic to human health and that can cause the global warming of the Earth. It is a duty of fundamental and applied sciences to investigate new options and propose novel ideas to tackle the issue. The solution we explore at Paris-Sud University consists of fragmenting (breaking) the pollutant molecules using the high-energy electrons and excited species produced in non-thermal equilibrium plasmas of atmospheric gases. This promising technology is still confronted with several issues related to fundamental questions in physics and chemistry and to its actual technical implementation.

The way in which an excited molecule will decay by fragmentation is not yet well understood, as chemistry is mostly concerned by the science of *building* molecules. However, nuclear physicists have studied in details the fragmentation of nuclei. At the CSNSM (my laboratory: the Center for Nuclear Sciences and Matter Sciences), we are developing a new statistical physics model, following a scheme used to model nuclear fragmentation, that allows predicting to which fragments (smaller molecules) a pollutant molecule will decay after being excited at a given energy. The PhD student will participate in the reflection and elaboration of this theoretical model and to its implementation as a computer code. Thus, the theoretical part of the doctoral research will take place at the CSNSM.

The second part of the project will be dedicated to the experimental study of the fragmentation of pollutant molecules (e.g. acetone) excited in a plasma. The DIREBIO (Décharges Impulsionnelles, REactivités à haute pression, et interfaces plasma-BIOlogie) group at the LPGP (Laboratory for the Physics of Gas and Plasma) is pioneer in the realization of large volume homogenous plasmas of pulse discharges making use of the photo-triggering technique. The PhD student will study the process of pollutant fragmentation, varying the electrical parameters of the photo-triggered discharge and the gas mixture composition in order to understand the energy transfers to the molecules and determine the optimum operating mode. Finally, the molecular composition of the residual gas will be analyzed using gas chromatography and the newly developed high-resolution mass spectrometers of the LCP (Laboratory of Chemical Physics). The experimental results will be examined in conjunction with the theoretical predictions in order, on the one hand, to validate the theory and, on the other, to determine the distribution of excitation energy deposited by the plasma in the molecules. The final objective of the method is to reject non-polluting fragment molecules only, spending as little energy as possible.

Who we are

We are physicists and chemists working on the Orsay campus of Paris-Sud University (http://www.u-psud.fr/en/), a member of the new Paris-Saclay University (http://www.epps.fr/en/a-global-cluster/), 35 minutes from downtown Paris.
Paris-Sud is ranked:

- First university in France in the Shanghai ranking for Physics
http://www.shanghairanking.com/SubjectPhysics2014.html
- First university in Europe (with LMU Munchen) by the CHE ranking for Physics
http://www.excellenceranking.org/eusid/EUSID?module=Hitliste&do=show_l1&esb=4&order_left=1#res

Who you are
You are a good student in Physics, with broad interests in environmental issues, in theoretical and applied Physics, in Physical chemistry and in computer sciences.

Three-year doctoral program schedule
• 12 to 18 months at the CSNSM dedicated to bibliographical research, theoretical modeling and computer code implementation
• 6 to 12 months at the LPGP for plasma experiments
• 12 months at the LCP to study residual gas characterization and thesis and publication manuscript writing.

References
(these articles might be difficult for you to understand; this is normal)

• "Statistical nature of nuclear multifragmentation"
A.S. Botvina, D.H.E. Gross, Phys. Rev. C 58, R23(R)

• "Kinetics of organic molecules in pulsed plasmas of nitrogen or N2/O2 mixtures at near atmospheric pressure"
S. Pasquiers, N. Blin-Simiand, L. Magne
Plasma Physics and Controlled Fusion, 55 (2013) 124023 (10 pages).

• "Role of quenching of metastable states in acetaldehyde decomposition by a non-equilibrium nitrogen plasma at sub-atmospheric pressure"
W. Faider, S. Pasquiers, N. Blin-Simiand, L. Magne, Journal of Physics D: Applied Physics, 46 (2013) 105202 (16 pages).