

### THREE-YEAR PHD PROJECT

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Support :

3-year financial support (doctoral contract) from fall 2012.

Project title : Study of the electronic processes induced by ion impact on molecular targets : development and application to H<sub>2</sub>O.

The understanding of the electronic processes occurring in the course of atomic and molecular collisions is of great importance for the description of phenomena observed in complex systems as atmospheric, astrophysics, plasma and biologic media. The modelling of the electronic structures induced by ion impact on complex molecules is still a major challenge, due to (i) the multicentric feature of the target, (ii) the large number of electrons implied in the process and therefore also (iii) the number of open channels, even for simple molecules as H<sub>2</sub>O.

In this context, the present project especially concerns the theoretical and numerical description of electron transfer and ionization processes occurring in A<sup>q+</sup>-H<sub>2</sub>O keV/u collisions, leaving (multi-) ionized molecular targets which can further dissociate into neutral and ionic fragments. This collision system has been the subject of numerous experimental studies which require further analysis. The aim will be therefore to develop a new non-perturbative methodology based on the "coupled-channel" - typed resolution of the time-dependent Schrödinger equation. It will involve an important effort of computation and code-writing for the extension of existing computer codes. The results and their interpretations should represent new benchmarks to test the validity of the simple models used presently in the community (monoelectronic, independent particles, quasi-atomic target, ...).

3 related publications :

A. Dubois, S. Carniato, P.D. Fainstein and A. Dubois, *Phys. Rev. A* **84**, 012708 (2011).  
N. Sisourat, I. Pilskog and A. Dubois, *Phys. Rev. A* **84**, 052722 (2011).  
J. Caillat, N. Sisourat, A. Dubois, I. Sundvor, and J. P. Hansen, *Phys. Rev. A* **73**, 014701 (2006).