

Proposition de Financement Doctorale UPMC – Paris 6 pour la rentrée 2016-2017

Titre de la thèse :

Pump - probe photoelectron spectroscopy of proton transfer reactions

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Recent and rapid emergence of intense and ultrashort light sources together with the development of liquid micro-jet technologies open new opportunities in femtochemistry. In this context, the aim of the project is to theoretically investigate the mechanism of proton transfer reactions such as tautomerization in gas phase as well as in solution initiated by infrared pulses and probed with photoelectron spectroscopy. Such original pump-probe scheme should provide considerable insights in the reaction dynamics. The PhD candidate will develop methods and the associated numerical tools for simulating the electronic and nuclear dynamics during proton transfer triggered by an infrared pump pulse as well as for computing the probe photoelectron spectra. The codes will be employed to study first the tautomeric dynamics of acetylacetone molecule in different solvents. Further systems will then be investigated.

Mots clés : Electronic structure calculations, quantum dynamics, theoretical spectroscopy