X-ray and Auger spectroscopies in liquids: a theoretical study

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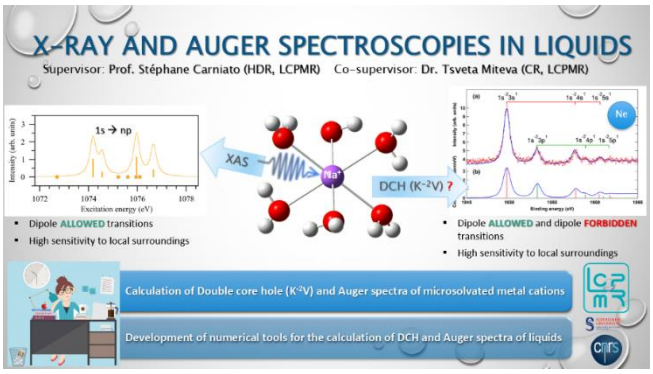
Application deadline: **July 31**, 2020
Starting date: **October 1**, 2020

Scientific context

In 2013[1] our group proposed "a novel spectroscopy" called $K^{-2}V$ (simultaneous core ionization and excitation) opening up new possibilities for the study of molecules in the gas phase compared to traditional X-ray spectroscopies, such as X-ray Photoelectron Spectroscopy (XPS) (involving simple core ionization) or X-ray Absorption Spectroscopy (XAS) (involving simple core excitation).

The project



The main goal of this project is to develop a theoretical model for the simulation of X-ray spectra, $K^{-2}V$ and Auger, in liquids. The model will be further applied to compute the X-ray spectra of solvated metal cations, such as Na^+, K^+, Mg^{2+} and Ca^{2+}. More generally, we would like to understand how the nature of the solvent influences the simultaneous inner-shell excitation and ionization. To this end, the analysis of the spectra will focus on specific electronic transitions, called forbidden dipolar transitions, which are only accessible through $K^{-2}V$ transitions. Moreover, we will also investigate the effect of the solvent on the ultrafast delocalization of the excited electron preceding Auger decay of the core hole.

To achieve the above mentioned goals, the PhD student will therefore have to adapt the computational tools currently available in our group to the simulation of the spectra of solvated metal cations. The latter simulation also requires the computation of the lifetimes of core-excited/ionized states which will be carried out with the Fano-CI method developed and implemented in our group.

Finally, LCPMR represents the ideal environment for the successful accomplishment of the goals of the project. Apart from having a deep understanding of the theoretical description of inner-shell spectroscopies, LCPMR also hosts experimental groups who work in the development of experimental set-ups dedicated to the study of liquids in collaboration with synchrotron SOLEIL. The PhD student will therefore have the exceptional opportunity to collaborate not only with other theoreticians in the group but also with the experimental groups at LCPMR.

The candidate

The candidate should have a strong background in theoretical chemistry with particular interest in the description of light-matter interactions. The subject requires good knowledge in one or both programming languages Fortran and Python.

If this is your dream PhD, please send us your application including a detailed CV, a letter of motivation in line with the research proposal, a detailed academic record and 2 recommendation letters or contacts.

[1] Nakano et al., Phys. Rev. Lett., **111**, 123001 (2013) https:/doi.org/10.1103/PhysRevLett.111.123001