Advanced methods for the study of chemical systems by X-ray Absorption Spectroscopy

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In the last years a growing number of studies have been devoted, both experimentally and theoretically, to understanding the structural properties of disorder systems and chemical processes occurring in solution and more clear pictures are emerging. This was possible by the improvements of the experimental techniques and the development of more sophisticated and reliable theoretical models. As we will detail in this presentation, experimentally in the last years X-ray absorption spectroscopy (XAS) played a major role in unravelling many structural aspects of disordered systems and it was exploited to gain unprecedent information on chemical reactions occurring in solution. This was possible by coupling experiments with theoretical simulations and multivariate analysis, and by better exploiting the X-ray absorption near edge spectroscopy (XANES) that is very sensitive to three-dimensional structures. Here, we will show specific applications to several liquid systems and chemical reaction occurring in the ms time scale. Aqueous solutions containing lanthanoid and actinoid ions are analysed with the aim of providing a unified description of the hydration properties of these series. We will show how the combined approach using XAS and molecular dynamics simulations can be applied to the study of complex systems such as ionic liquids and deep eutectic solvents, that represent an innovative research field. Lastly, we will show how it is possible to shed light into mechanistic properties of bimolecular reactions in solution by combining XANES, UV-Vis with multivariate data analysis.

Keywords: XAS, XANES, Data Analysis, Chemical Systems