Studying metal speciation in non-conventional solvents through X-ray absorption spectroscopy and molecular dynamics

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Metal speciation in liquid media is central in solution chemistry, because of its relevance in a large number of physicochemical processes in nature, industrial technologies and living organisms. In particular, a topic of great interest in the last few decades has been the understanding of the coordination properties of metal cations in non-conventional solvents, such as ionic liquids (IL), mixtures of IL with more conventional solvents or deep eutectic solvents (DES). There are well known difficulties in obtaining reliable structural information on disordered systems and identifying solvation complexes in liquid media. An invaluable tool for this task is the X-ray absorption spectroscopy (XAS), which can provide accurate structural information on the metal solvation complexes due to its unique short-range-order sensitivity and chemical selectivity. Furthermore, the reliability of such information can be enhanced by combining XAS with molecular dynamics (MD) simulations. Through the synergic use of XAS and MD techniques one can experimentally check the validity of the forcefield used in the simulations, while having at the same time reliable structural models to be used in the analysis of the experimental data.

Here we will show how the XAS-MD approach can be applied to study the coordination properties of metal cations in challenging non-conventional solvents, as well as the tools and strategies that can be developed and used to further improve the information obtainable from this powerful combined method.