



Contribution ID: 78

Type: Oral presentation

Insights into dissipative and oscillatory chemical reactions by combining X-ray absorption and NMR/UV-Vis spectroscopies

Thursday, 15 September 2022 11:45 (15 minutes)

Chemical reactions mainly occur in solution and the use of different techniques to monitor the advancement of a chemical process in the liquid phase is often a powerful tool to gain a satisfactory understanding of the underlying reaction mechanism. Among the spectroscopic techniques that have been applied to follow chemical reactions occurring in solution, X-ray absorption spectroscopy (XAS) is a unique method that allows one to follow the variations in both the local electronic and structural configuration of a selected photoabsorbing atom. An advancement of this experimental approach is to combine XAS with ¹H-NMR and/or UV-Vis spectroscopies. Indeed, XAS and the conventional spectroscopic methods can be considered complementary. On the one hand, XAS allows one to quantitatively monitor the evolution of species often silent to conventional detections with an unrivaled degree of accuracy. On the other hand, the fate of the organic components of the reaction, namely ligands and reagents, can be tracked by ¹H-NMR/UV-Vis measurements. Notably, a multivariate and theoretical analysis of the XAS data may further complement the information acquired on the chemistry of the given reactive system.

In this presentation, we apply our method to gain a comprehensive view on: (i) a prototypical reaction involving the dissipative translocation of the Zn(II) cation from two different organic ligands (see Figure 1) [1], and (ii) the evolution of the main Bromine-related species during the classic cerium ion catalyzed Belousov-Zhabotinskii reaction [2].

Through our combined experimental and theoretical approach we gain insights into the nature, concentration time evolution and structures of the key metal and non-metal reaction species. Our method may prove to be useful in the toolbox necessary to reach a full mechanistic picture of reactive processes in solution.

Figure 1. Time evolution of the Zn K-edge XANES spectra measured during the dissipative translocation of the Zn(II) cation between the hexaaza-16-crown-8 and terpyridine ligands.

[1] F. Fratello, F. Tavani, M. Di Berto Mancini, D. Del Giudice, G. Capocasa, I. Kieffer, O. Lanzalunga, S. Di Stefano, P. D'Angelo, *J. Phys. Chem. Lett.* 2022, *accepted*.

[2] R. J. Field, E. Körös, R. M. Noyes *J. Am. Chem. Soc.* 1972, 94, 8649–8664.

Primary author: TAVANI, Francesco (Università La Sapienza di Roma)

Co-authors: Dr FRATELLORETO, Federico (Università La Sapienza di Roma); Dr DI BERTO MANCINI, Marika (Università La Sapienza di Roma); Dr DEL GIUDICE, Daniele (Università La Sapienza di Roma); BUSATO, Matteo ("Sapienza" University of Rome); Dr CAPOCASA, Giorgio (Università La Sapienza di Roma); Prof. LANZALUNGA, Osvaldo (Università La Sapienza di Roma); Prof. DI STEFANO, Stefano (Università La Sapienza di Roma); Prof. D'ANGELO, Paola (Università degli Studi Sapienza Roma)

Presenter: TAVANI, Francesco (Università La Sapienza di Roma)

Session Classification: MS

Track Classification: Nanostructured Materials