A chemometric view of ultrafast spectroscopy and super-resolution imaging

Cyril Ruckebusch

Laboratoire de Spectrochimie Infrarouge et Raman, Université de Lille, Villeneuve d'Ascq, Francia

cyril.ruckebusch@univ-lille.fr

Chemometrics, a component of data science in chemistry, can be seen as an ensemble of methods and data-driven approaches aiming at converting raw measurement into useful information. These methods are designed to suit the intrinsic physical or chemical nature of the measurement. In this seminar, we will focus on two advanced spectroscopic techniques and illustrate what a chemometric approach can bring to process unraveling and image resolution.

Time-resolved transient absorption spectroscopy is a pump-probe laser technique that allows measuring fast photoinduced processes occurring in the excited electronic state of molecules. It provides difference spectra that reveal information about the elementary molecular processes in photochemical and photobiological systems. We will show how spectral and kinetic information can be obtained to unravel information about the number of short-lived intermediates during fast chemical reactions, their nature and their dynamics. We will explain how multivariate curve resolution approaches can be designed to rationalize the reaction mechanisms. We will present results obtained on salicylidene-anilines which are photochromic compounds of interest for advanced functionalized materials.

Super-resolution wide-field fluorescence microscopy can provide structural information at the nanoscale and dynamic insight about biological processes in live cells. However, to obtain a high spatial resolution on short time sampling, and potentially probe dynamic processes, this principle must be extended to the analysis of high-density of emitters distributed over a few tens of movies frames only. As many emitters are simultaneously active, their emissions strongly overlap and single-emitter fitting methods collapse. Thus, for dynamic imaging and faster super-resolution, new methods are still required. We will present our approach for sparse image deconvolution and reconstruction. We will show that better contrasted, better resolved and more accurate estimates of the final super-resolution images of cellular structures can be obtained.

[1] Sparse deconvolution of high-density super-resolution images, S. Hugelier, J. De Rooi, R. Bernex, S. Duwé, O. Devos, M. Sliwa, P. Dedecker, P.H.C. Eilers, C. Ruckebusch, Sci. Rep. 6 (2016)

[2] Improved superresolution microscopy imaging by sparse deconvolution with an interframe penalty, S. Hugelier, P.H.C. Eilers, O. Devos, C. Ruckebusch, J. Chemometr. 31 (2017)

[3] Correcting for photodestruction in super-resolution optical fluctuation imaging, Y. Peeters, W. Vandenberg, S. Duwé, A. Bouwens, T. Lukeš, C. Ruckebusch, T. Lasser, P. Dedecker Sci. Rep. 7 (2017)