

## 第 6 回機能物質化学講演会

講演日時：2011 年 10 月 21 日（金）14 時～15 時半

場所：J 棟 505 室

講演者：Cyril Ruckebusch

所属：Lasir, CNRS, University Lille1

身分：Associate Professor

演題：Chemometrics in time-resolved spectroscopy: data, models and applications

講演要旨：This presentation will provide an overview of state of the art chemometric methods for a scientific and meaningful description of time-resolved spectroscopy data. The importance of data structure will be highlighted first. We will then focus on the relationship between models and the multivariate or multi-way nature of the data.



Emphasis will be on multivariate curve resolution methods for the bilinear description of two-way data matrices, with possible extension to multiple sets of data of different structures. Of particular interest for applications is the possibility to input knowledge in very different and flexible manners in MCR, such as under the form of constraints corresponding to chemical or mathematical properties the solutions should obey, but not only. Applications will be mainly chosen in femtosecond transient absorption spectroscopy where a comprehensive understanding of the photodynamics of complex molecular processes requires extensive data analysis. As in many other fields, the extraction of detailed information regarding the characterization of the chemical process is expected here, e.g. number of transient species, kinetics, pure spectra and connectivity between species. As we will see, specific chemometric procedures are also required since experimental conditions and instrument characteristics strongly alter the data structure in any ultrafast measurement.