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Combining X-ray scattering and spectroscopy as structure resolving tool

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Modern applications and basic research in medicine, biotechnology and materials are often concerned with hybrid (organic-inorganic) and synergetic systems. In other words, systems that brings enhanced properties and performances. The challenge is now in the understanding of the complex interactions leading to their assembly and operation. Due to their inherent chemical and structural complexities a combination of several techniques is necessary to determine unambiguously the molecular mechanisms of assembly and operation. [1, 2] To address this need, we have implemented a simultaneous measurement platform called SURF [3] that consists of SAXS, UV-Vis, Raman and fluorescence techniques. The SURF platform provides simultaneous measurements on the same sample volume and a multivariate framework to associate the spectroscopic and X-ray scattering information. Convex constraint analysis (CCA) and two dimensional correlation analyses (2DCOS and 2DHCOS) had been introduced to enhance the interpretation and integration of the data from the different techniques producing self-consistent models and resolving complex behaviour details (structure and chemistry). Additional benefits of the SURF are sample quality control and “on line” diagnostics. In this contribution, we illustrate the benefits of the SURF approach on selected examples. Acknowledgements: The SURF set-up has been mainly financial supported by MAX IV laboratory. S. Haas has a postdoctoral grant of MAX IV lab. S Canton and Q. Zhu are acknowledged for fruitful discussions.

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