Crystallochemistry underneath function: *in situ* powder diffraction at work

Simona Galli

Dipartimento di Scienza e Alta Tecnologia, Università degli Studi dell'Insubria, Como, Italy

simona.galli@uninsubria.it

The development of next-generation adsorbents with optimized, application-tailored functional behaviour inherently relies on the (combined) usage of cutting-edge solid-state characterization techniques [1–3]. Such an approach is essential to uncover key atomic-level details that are crucial to rationalizing the functional performance of the adsorbent materials under investigation. As a matter of fact, the recurse to complementary techniques such as (in *situ* and *operando*) X-ray diffraction, X-ray absorption, electronic absorption spectroscopy, luminescence spectroscopy, and solid-state NMR does provide deep insight into fundamental features such as primary adsorption sites, adsorbent–adsorbate interactions, the role of unsaturated metal centers or linker moieties, local and long-range structural dynamics, and enables the extraction of thermodynamics parameters therefrom. This comprehensive understanding is vital for guiding advancement in material design and functionality.

In this context, the present lecture will showcase a selection of case studies [4–9] from the research group in Structural chemistry of advanced materials, Università dell'Insubria, where the application of a multi-technique strategy – including (*in-situ* synchrotron-radiation) powder X-ray diffraction – proved essential in unraveling the atomic-level features (Fig. 1) underlying the observed bulk functional properties of metal-organic frameworks [10] and covalent organic frameworks [11].

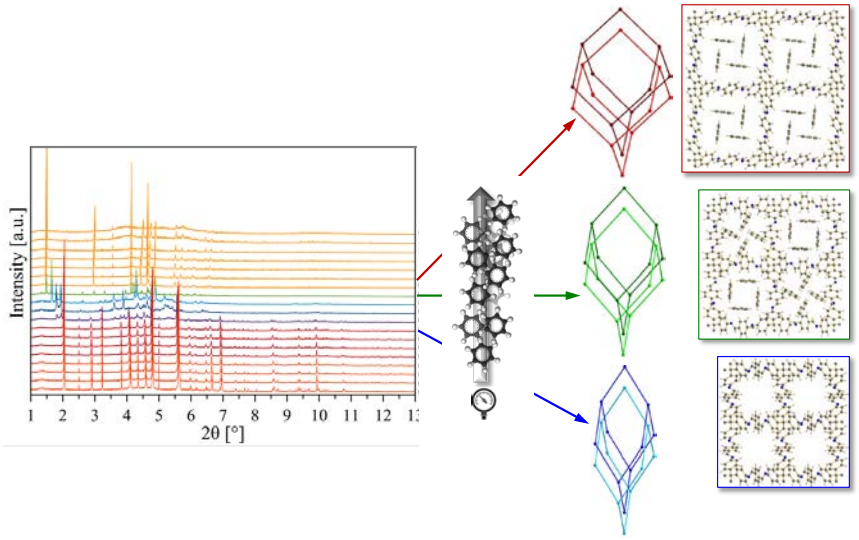

Figure 1. Pictorial representation of the current potential of synchrotron-radiation *in-situ* PXRD. Pictures adapted from [4].

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