Invited Lecture

Rationalizing the functional properties of porous materials: The role of *in situ* powder X-ray diffraction

S. Galli

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

simona.galli@uninsubria.it

Disclosure of crystallochemical information to rationalize the solid-state performance of bulk materials cannot prescind from the (combined) application of advanced characterization techniques, which is beneficial in both the short and long term. As a matter of fact, this strategy not only provides a comprehensive picture for the current case of study, but also paves the way to the development of new-generation substances with functionality optimized for the investigated applicative context.

In the context of a multi-technique approach, the title contribution will prove that *in situ* powder X-ray diffraction (PXRD) under non-ambient conditions does afford an essential and versatile portfolio of tools to disclose the structural features underneath an observed functional behaviour.

To the aim, the audience will be introduced into the vast realm of metal-organic frameworks (MOFs) [1] and covalent organic frameworks (COFs) [2]. In the past two decades, *in situ* PXRD methods have known an incessant development for the study of MOFs and COFs [3-5]. Since 2014, the research group in Structural Chemistry of Advanced Materials (SCAM) at the University of Insubria has actively concurred to this development. The involvement of the SCAM group into this expanding field will be highlighted through a selection of examples recently reported in the literature [6-9], overall showing the relevance of *in situ* PXRD, performed in house or at large scale facilities, in pinpointing those MOFs and COFs crystallochemical features - occurrence of framework modifications, identification of primary adsorption sites and adsorbent-adsorbate interactions, adsorbate quantification, influence of pore walls decoration - governing their functionality as solid-state adsorbents.

[1] *Metal-organic framework: from design to applications* (2020), edited by Bu, X.-H., Zaworotko, M. J., Zhang, Z., Springer.

[2] Geng, K., He, T., Liu, T. R., Dalapati, S., Tan, K. T., Li, Z., Tao, S., Gong, Y., Jiang, Q., Jiang, D. (2020). Chem. Rev. **120**, 8814.

[3] Petersen, H., Weidenthaler, C. (2022). Inorg. Chem. Front. **9**, 4244.

[4] Albalad, J., Sumby, C. J., Maspoch, D., Doonan, C. J. (2021). CrystEngComm **23**, 2185.

[5] Senkovska, I., Bon, V. *In Situ X-ray diffraction and XAS methods* in *The chemistry of metal–organic frameworks: synthesis, characterization, and applications* (2016), Volume 1, edited by Kaskel, S., Wiley-VCH.

[6] Mauri, A., Vismara, R., Moroni, M., Roldan-Molina, E., Navarro, J. A. R., Galli, S. (2024). Manuscript in preparation.

[7] Moroni, M., Nardo, L., Maspero, A., Vesco, G., Lamperti, M., Scapinello, L., Vismara, R., Navarro, J. A. R., Monticelli, D., Penoni, A., Mella, M., Galli, S. (2023). Chem. Mater. **35**, 2892.

[8] Moroni, M., Roldan-Molina, E., Vismara, R., Galli, S., Navarro, J. A. R. (2022). ACS Appl. Mater. Interfaces **14**, 40890.

[9] Giacobbe, C., Lavigna, E., Maspero, A., Galli, S. (2017). J. Mater. Chem. A **5**, 16964.