Tuning the local structure of isoreticular porous materials

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The concept of isoreticular chemistry has been key in the design of porous framework materials, enabling the tailoring of functionality and pore size whilst preserving the topology [1]. However, subtle variations in the local structure of such isoreticular materials – including the orientation of low-symmetry building blocks, defect distribution, and dynamic disorder – can profoundly influence material properties in ways that are often overlooked [2].

In this talk, I will present a number of case studies on porous materials, including the metal-organic frameworks (MOFs) TRUMOF-1 [3] and UoB-100 [4], which share identical underlying networks yet exhibit distinct local structural deviations. By combining synthetic approaches with X-ray total scattering techniques, such as diffuse scattering and three-dimensional difference pair distribution function (3D-ΔPDF) analysis, I will show how these local variations can be controlled and discuss their impact on chemical properties.

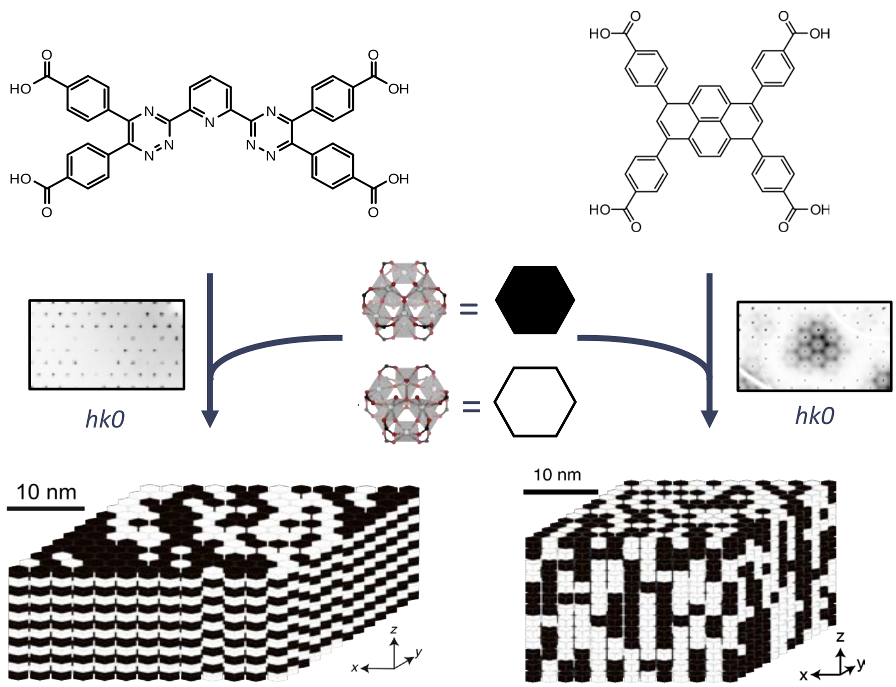

Figure 1. Schematic illustrating how the linker type influences correlations between two orientations of the metal cluster in UoB-100 (left) and CU-10 (right), leading to distinct diffuse scattering features, in turn indicating the formation of different nanodomains.

[1] Yaghi, O., O'Keeffe, M., Ockwig, N. *et al*. Reticular synthesis and the design of new materials. *Nature* **423**, 705–714 (2003)

[2] Meekel, E. G. and Goodwin, A. L. Correlated disorder in metal–organic frameworks, *CrystEngComm* **23**, 2915-2922 (2021)

[3] Meekel, E. G. *et al.* Truchet-tile structure of a topologically aperiodic metal–organic framework. *Science* **379**, 357-361(2023)

[4] Griffin, S.L., Meekel, E.G., Bulled, J.M. *et al*. A lanthanide MOF with nanostructured node disorder. *Nat Commun* **16**, 3209 (2025)