<div align="center">

Oral presentation

A lanthanide MOF with nanostructured node disorder

</div>

<div align="center">

J. M. Bulled[1], S. Griffin[2], S. Canossa[3], N. Champness[2], E. G. Meekel[4]

[1]ESRF, Grenoble, France, [2] University of Birmingham, UK, [3]ETH, Zurich, Switzerland, [4]Kyoto University, Japan

johnathan.bulled@esrf.fr

</div>

The presence of disorder in MOFs is a field of growing importance, with a profound impact on their pore networks [1,2]. Correlations in this disorder cannot be measured by traditional crystallography, requiring local probes such as diffuse scattering [3,4]. We report the recent synthesis and characterisation of a dysprosium MOF, which contains both disordered nodes and linkers. This disorder is understood as the superposition of two geometries, which can be represented as hexapole moments [Fig. 1a]. In this way, we build a coarse-grained model of the system which quantitively reproduces the observed diffuse scattering [Fig. 1b] and 3D- PDF [Fig. 1c]. The correlated disorder of the linkers and the disordered pore structures present in the material are discussed.
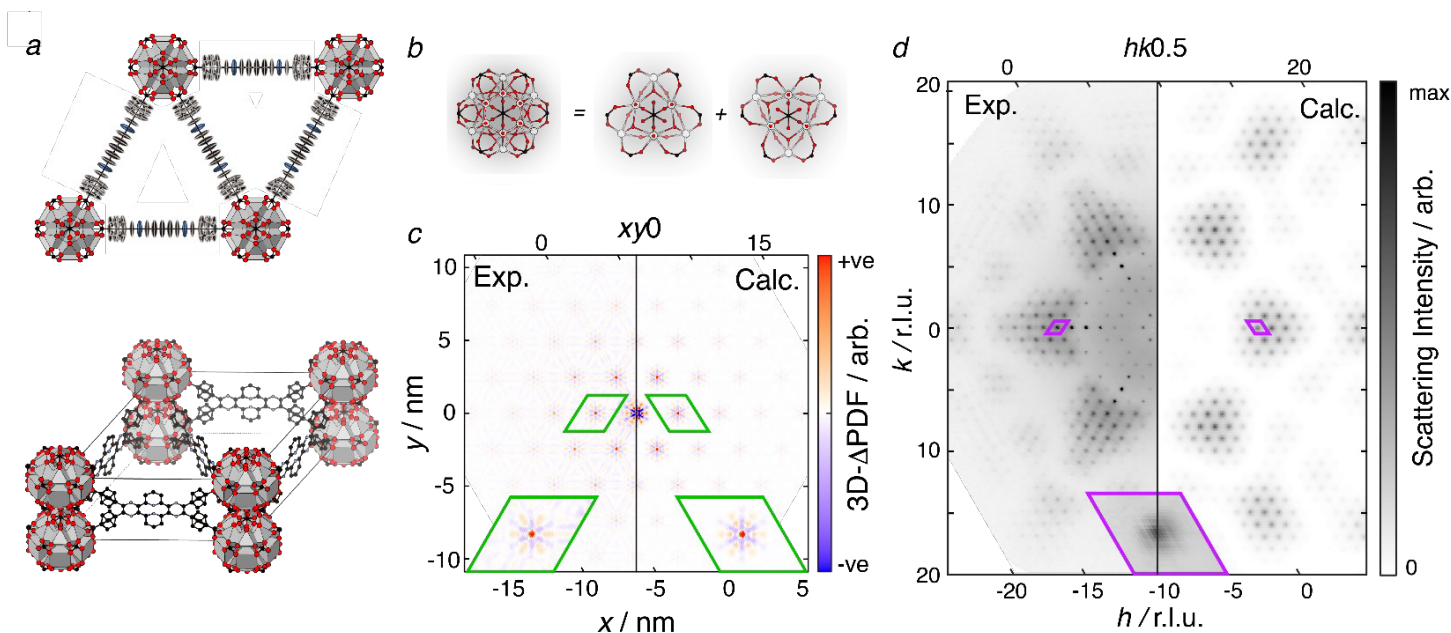

Figure 1: *a* Average crystal structure shown from above (i.e. along the *c*-axis) and the side. Color scheme: Dy = gray polyhedra, C = black, O = red, N = blue. Linker in the top image is shown with ellipsoids at 50% probability. *b* The average structure of the Dy node can be understood as a superposition of two nonanuclear clusters at a different orientation *c-d* Comparison of DS and 3D-ΔPDF obtained from experiment (left of each pane) and the best fit of the Monte Carlo model described in the text (right). The purple rhombuses shows the region bounded by used for fitting, and the inset shows this region enlarged.

[1] Meekel, E. G. *et al.* (2023) *Science* **379**, 357.

[2] Meekel, E. G & Goodwin, A. L. (2021) CrystEngComm, **23**, 2915.

[3] Goodwin, A. L. & Keen, D. A, (2015) *Nature* **521**, 7552, 303.

[4] Billinge S. J. L. & Levin, I., (2007) *Science* **316**, 5824, 561.