

# Mapping the phase space of disordered lanthanide MOFs with simulation as a compass

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Disorder in metal-organic frameworks (MOFs) has a key role in their properties [1]. The recent discovery of correlated disorder in the lanthanide MOF UoB-100(Tb) [2] raises the question, what synthetic or compositional choices could modify this order? I use monte carlo and quantum mechanical simulations to answer this question, with comparison to measured data.

[1] Meekel, E.G., Partridge, P., Paraoan, R.A.I. *et al.* (2024). *Nat. Mater.* **23**, 1245–1251

[2] Griffin, S.L., Meekel, E.G., Bulled, J.M. *et al.* (2025). *Nat Commun* **16**, 3209