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Correlated defects in group 4 metal-organic frameworks

M. Cliffe¹, W. Wan², X. Zou², F. Coudert³, A. Goodwin¹

¹University of Oxford, Department of Chemistry, Oxford, UK, ²Stockholm University, Department of Materials and Environmental Chemistry, Stockholm, Sweden, ³CNRS and Chimie ParisTech, Paris, France

The importance of defects for inorganic functional framework materials is well established, being crucial for properties from relaxor ferroelectricity to superconductivity. The corresponding study of defects in metal-organic frameworks (MOFs) is still however in its infancy. Recent studies have established that ligand-absence defects can be controllably introduced into frameworks and that these defects can drastically improve the material properties, but have so far shown no evidence of correlation between defects. Much of this research has focussed on UiO-66, a zirconium dicarboxylate MOF that was amongst the first very stable MOFs to be discovered.[1] As a result of its stability, it and its derivatives have been investigated for a wide range of properties including photo- and Brønsted acid catalysis, sensing and gas sorption properties. The ability to introduce defects has been demonstrated to substantially enhance both the sorption and catalytic properties of UiO-66.[2][3] We have demonstrated, using a combination of powder X-ray diffraction, total scattering and electron diffraction measurements, that UiO-66 can be engineered, under the appropriate synthetic conditions, to accommodate correlated defect nanodomains. These correlations offer exciting opportunities for manipulating the physical properties, including mass transport, chemical activity and mechanical flexibility.

[1] J. H. Cavka, S. Jakobsen, et al., *J. Am. Chem. Soc.* 2008, 130, 13850, [2] F. Vermoortele, B. Bueken, et al., *J. Am. Chem. Soc.* 2013, 135, 11465, [3] H. Wu, Y. S. Chua, et al., *J. Am. Chem. Soc.* 2013, 135, 10525



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