



## Lauren Macreadie

University of New South Wales (UNSW), Sydney, Australia

### Title | Reimagining MOF Design with Three-Dimensional Linkers: Expanding Pore Chemistry and Flexibility

**Abstract** | Aromatic ligands with polycarboxylate or multitopic functionalities have long been the cornerstone of metal–organic framework (MOF) design. Their rigidity, availability, and versatile coordination modes have enabled the creation of an extensive library of MOFs. Yet, their reliance on phenyl-based interactions can limit chemical diversity within pore environments and constrain functional tunability. Our research introduces three-dimensional (3D) linkers, such as cubane-1,4-dicarboxylic acid ( $H_2cdc$ ), bicyclo [1.1.1] pentane-1,3-dicarboxylic acid ( $H_2pdc$ ), and p-carborane-1,12-dicarboxylic acid ( $H_2pcarb$ ), as alternatives to benzene-1,4-dicarboxylic acid ( $H_2bdc$ ). These 3D linkers allow the construction of MOF analogues that retain structural similarity while offering new opportunities to modulate pore chemistry and probe host–guest interactions.<sup>1-3</sup>

To maximize their potential in gas storage and separation, MOFs must exhibit both responsiveness and flexibility.<sup>4</sup> We demonstrate strategies to control localized flexibility, such as negative thermal expansion (NTE), and global framework flexibility, including breathing behavior in response to guest molecules. Using aliphatic linkers, we tune thermal expansion coefficients and uncover the influence of hybridization on framework dynamics. In complementary studies, we design pillared zinc triazolate MOFs with bulky 3D linkers that resist collapse and display enhanced flexibility under gas loading. Coupling gas adsorption with in situ powder X-ray diffraction (PXRD) provides a powerful asynchronous approach to track structural evolution during sorption (Figure 1). Together, these studies highlight how incorporating 3D linkers expands the design space of MOFs, enabling new pathways to control flexibility, stability, and guest responsiveness. These features are essential for advancing their applications in adsorption, storage, and separation technologies.

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**Bio** | Dr [Lauren Macreadie](#) is a Scientia Fellow and Senior Lecturer in the School of Chemistry at UNSW Sydney. Her research focuses on the design and understanding of porous materials, particularly metal–organic frameworks (MOFs), to address challenges in carbon capture, water harvesting, and chemical separations. Her group specialises in the use of advanced X-ray diffraction techniques to probe how external stimuli influence the structure and stability of these materials, with the goal of linking fundamental behaviour to real-world applications. Lauren completed her PhD through a joint program with CSIRO and Monash University in 2016. She subsequently held research positions at Trinity College Dublin, working on MOFs for water splitting, and at CSIRO in Melbourne, where she investigated MOFs for use in respiratory protection in collaboration with the Defence Science and Technology Group. She began her independent career as a lecturer at Massey University in 2020, before undertaking a DECRA fellowship at the University of Sydney in 2021. In 2022, she joined UNSW as a Scientia Senior Lecturer.