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Incorporation of N-heterocyclic carbene moieties into MOFs

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Metal-organic frameworks (MOFs) are a class of porous materials that can be synthesised through judicious combination of metal salts and organic linkers. MOFs are constructed from a bottom up approach, where variation of the starting materials can yield a vast array of structures with varying pore sizes, shapes, and chemistry. The high versatility of MOFs makes them a highly desirable target in the fields of gas storage and separation, as well as catalysis. Recently, there has been significant interest in incorporating N-heterocyclic carbene (NHC) precursors into MOFs for use in catalysis. NHCs can be readily synthetically modified, making them an interesting functional group to incorporate into MOFs in order to develop new catalysts, or fine tune existing molecular catalysts.

In this contribution, a series of MOFs incorporating a substituted NHC precursor as the organic linker will be reported. By choice of the starting metal salt different MOFs may be accessed, in which NHC precursor azolium linkers are retained or substituted NHC complexes are generated. For example, reactions with Zn(II) (and an added Cu(I) source) and Cu(II) give MOF materials with concomitant Cu(I) metalation of the NHC moiety. The degree of metalation is currently being studied by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) and Single Crystal X-Ray Diffraction (SCXRD). The chemistry of these and several other related NHC MOFs will be presented in this contribution.

Keywords

metal organic framework, N-heterocyclic carbene, porous material, catalysis

Primary author: Mr CAPON, Patrick (The University of Adelaide)

Co-authors: Dr BURGUN, Alexandre (University of Adelaide); Prof. SUMBY, Chris (University of Adelaide)

Presenter: Mr CAPON, Patrick (The University of Adelaide)

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