Invited Lecture

The use of the Pair distribution function in Metal-Organic Framework composites

C. Castillo-Blas[1], A. M. Chester[1], R.P. Cosquer[2], A. F. Sapnik[1], L. Corti[2], R. Sajzew[3], G. Robertson[1], F. Blanc[2], L. Wondraczek[2], D. A. Keen[4], T. D. Bennett[1]

[1]Department fo Materials Science and Metallurgy, University of Cambridge, UK, [2]Department of Chemistry, University of Liverpool, Liverpool, UK, [3] Otto Schott Institute of Materials Research, University of Jena, Jena, Germany, [4] ISIS Facility, Didcot, UK.

cc2078@cam.ac.uk

The knowledge of the interface between different components in composites is crucial to understanding and predicting all the exciting chemical and physical properties of these materials. However, the structural study of the interface regions within a MOF composite is extremely challenging, given the low volume of interaction and the consequent need for characterisation to be carried out at the local atomic scale. Here we investigate the potential interactions at the glass-MOF interface of a MOF-glass composite. This material containing a metal-organic framework (MOF) embedded within an inorganic glass was synthesised via the dispersal of crystalline zeolitic imidazolate framework (ZIF-8), within a phosphate-base glass matrix. Treatment at a suitable working temperature allowed the glass matrix to flow around the MOF particles. The local structure of this material was analysed in detail by pair distribution function methods, and potential interactions at the glass-ZIF interface identified from different data analysis approaches, including, differential PDF, Principal Component Analysis and Multilinear Regression Analysis [1,2]. This study was also combined with multinuclear multidimensional magic angle spinning nuclear magnetic resonance correlations spectroscopy. These demonstrated potential glass-ZIF atom-atom correlations. These new methodologies have opened new avenues to characterise the interface at local structure in other MOF-composite materials.

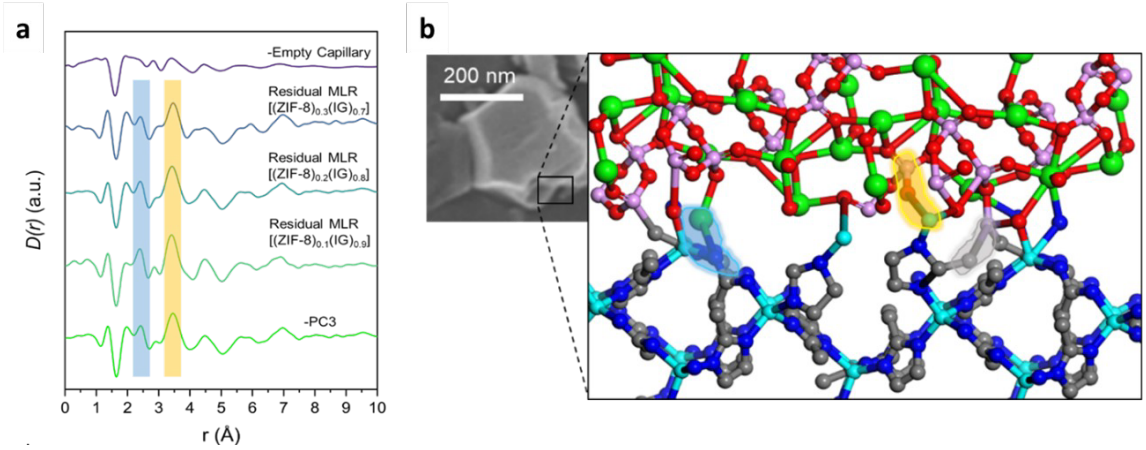

Figure 1. **a**. Comparison between scaled borosilicate capillary, residuals of the multilinear regression and negative PC3, exhibit similar fea-tures. New correlations at 2.45 and 3.35 Å at PC3 and residuals are high-lighted in blue and yellow, respectively. **b**. SEM image and schematic depiction of the interaction at the interface glass-ZIF-8 with the spatial proximities for H···P (grey highlights) and new potential interactions for Na···N (blue highlights) and Zn···O···P (orange highlights). Zn (cyan), C (grey), N (blue), Na (violet), O (red), P (green). Hydrogens were omitted for clarity.

[1] C. Castillo-Blas, F. Blanc, D.A. Keen, T.D. Bennett, et al. (2023) *J.Am.Chem.Soc.* **145**, 42, 22913–22924.

[2] A.M. Chester, C. Castillo-Blas, D.Keen, T.D. Bennett, et al. (2023). *Chem. Sci.*, **14**, 11737-11748.