Poster Presentation

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Synthesis, structure and water sorption in Zr metal-organic frameworks

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Metal-organic frameworks (MOFs) based on zirconium secondary building units (SBUs) have proven to have great thermal and chemical stability,[1,2] which make them ideal for their use in different applications. We have prepared a series of six new MOFs made from the $Zr_6O_4(OH)_4(\text{-}CO_2)_n$ secondary building units (n = 6, 8, 10, or 12) and variously shaped carboxyl organic linkers to make extended porous frameworks, with the aim of studying their performance as water adsorbents. Thus, we have evaluated the water adsorption properties of these new MOFs and other reported porous materials to identify the compounds with the most promising materials for use in applications such as thermal batteries or delivery of drinking water in remote areas. An X-ray single-crystal and a powder neutron diffraction study reveal the position of the water adsorption sites in one of the best performing materials, and highlight the importance of the intermolecular interactions between adsorbed water molecules within the pores.

[1] *J. H. Cavka, S. Jakobsen, U. Olsbye, et al. Journal of the American Chemical Society, 2008, 130, 13850.,* ***[2]*** *W. Morris, B. Volosskiy, S. Demir, et al Inorganic Chemistry 2012, 51, 6443.*

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