Direct Functionalization of Metal-Organic Framework Node: Targeting Diamine Grafting for Removing Toxic Chemicals in Humid Environment

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Zirconium-based metal-organic framework (Zr-MOF) and its functionalized analogues have been widely investigated to efficiently remove chemical warfare agents and simulant as well as industrial toxic gas due to their chemical and thermal stability comparing other MOFs. Herein, we have developed a selective functionalization of Zr-bridging hydroxo species on Zr-nodes in Zr-MOFs with a triethylenediamine (TEDA) through gas phase acid-base reaction, successfully leading to formation of ionic frameworks. Remarkably, TEDA grafted MOF-808 show exceptional performance for removal of toxic chemicals, such as CK, DMMP and ammonia in humid conditions. *In situ* analyses demonstrate how the TEDA is selectively deposited on Zr-bridging hydroxo sites (μ_3-OH) in Zr-MOFs and also *operando* FT-IR spectra show why TEDA grafted MOF-808 has superior sorption characteristics. This work highlights the advantages of diamine-grafted MOFs for the preparation of versatile adsorbents, extending their scope to catalytic applications.