Ultraporous, water stable, and breathing zirconium-based metal—organic frameworks with ftw topology.

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Streszczenie

“Breathing” metal–organic frameworks (MOFs) are an emerging class of soft porous crystals (SPCs) with potential for high working capacity for gas storage applications. However, most breathing MOFs have low stability and/or low surface area. Here we report a water-stable, high surface area, breathing MOF of ftw topology, NU-1105. While Zr6-oxo clusters as nodes introduce water stability in NU-1105, its high surface area and breathing character stem from its pyrene-based tetracarboxylate (Py-FP) linkers, in which the fluorene units (F) in the FP “arms” play a key role in promoting breathing behavior. During gas sorption studies, the “closed pore” (cp) ↔ “open pore” op) transition of NU-1105 occurs at a propane pressure of ∼3 bar. At 1 bar, NU-1105 is in its cp form and adsorbs less propane than it would in its op form, highlighting improved working capacity. In situ powder X-ray diffraction during propane sorption was used to track the cp ↔ op transition, and molecular modeling was used to elucidate the structure of the op and cp forms of NU-1105. According to TD-DFT calculations, the proposed conformations of the Py-FP linkers in the op and cp forms are consistent with the measured excitation and emission spectra of the op and cp forms of NU-1105. Similar structural transitions are also observed in the porphyrinic MOF NU-1104 depending on the identity of the porphyrin core; we observed breathing behavior if the constituent Por-PTP linker is nonmetalated.

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