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Ultrahigh surface area zirconium MOFs and insights into the applicability of the BET theory.

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Streszczenie

An isoreticular series of metal–organic frameworks (MOFs) with the ftw topology based on zirconium oxoclusters and tetracarboxylate linkers with a planar core (NU-1101 through NU-1104) has been synthesized employing a linker expansion approach. In this series, NU-1103 has a pore volume of 2.91 cc g–1 and a geometrically calculated surface area of 5646 m2 g–1, which is the highest value reported to date for a zirconium-based MOF and among the largest that have been reported for any porous material. Successful activation of the MOFs was proven based on the agreement of pore volumes and BET areas obtained from simulated and experimental isotherms. Critical for practical applications, NU-1103 combines for the first time ultrahigh surface area and water stability, where this material retained complete structural integrity after soaking in water. Pressure range selection for the BET calculations on these materials was guided by the four so-called “consistency criteria”. The experimental BET area of NU-1103 was 6550 m2 g–1. Insights obtained from molecular simulation suggest that, as a consequence of pore-filling contamination, the BET method overestimates the monolayer loading of NU-1103 by ∼16%.

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