Critical Role of Defects in UiO-66 Nanocrystals for Catalysis and Water Remediation

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Metal−organic frameworks (MOFs) have emerged as a promising class of porous crystalline materials with outstanding physical and chemical properties. The significantly high surface area, permanent porosity, and wide chemical variety of its building blocks resulted in the development of thousands of MOF structures covering a wide array of applications. UiO-66, a zirconium subfamily of MOFs ($Zr_6O_4(OH)_4(BDC)_6$ BDC = benzene dicarboxylate), has been especially attractive due to its high chemical and thermal stability when compared to other MOFs. The discovery of defects in UiO-66 nanostructures revealed their critical role in the efficiency of UiO-66, especially in catalytic and adsorptive water treatment applications. This began many studies on understanding, controlling, and using a higher density of defects in UiO-66 nanocrystals. The presence of defects, their density, and distribution in the UiO-66 structure were proven to be a very powerful tool to tune the physical and chemical properties of UiO-66 without altering the main building blocks of the structure. The ability to control defect nanoregions in the UiO-66 structure, namely defect engineering, opened the door to an arising design strategy that allowed tuning of its surface area, porosity, pore size distribution, and the density and distribution of active sites. In this review, defects in UiO-66 are briefly introduced to explain their nature, origin, and effects on the UiO-66 structure's properties. Then the different methodologies by which these defects could be controlled, created, and activated are thoroughly reviewed. Next, two sections are devoted to discussing studies in catalysis and wastewater treatment that essentially relied on defects in UiO-66 nanocrystals as active or adsorptive sites. This review is presented as a practical and valuable guide on why and how to use defects in UiO-66 as a powerful tool to boost the performance of UiO-66 in the different fields in general and catalysis and adsorptive water treatment specifically.