

Guest induced structural deformation of metal-organic polyhedra

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Dynamic systems exhibiting structural transformations upon external stimuli are currently of high interest owing to the novel properties that these behaviors may lead to. In that field, coordination polymers or metal-organic frameworks (MOFs), which are infinite supramolecular architectures, has already shown such dynamics known as gate opening, swelling or shrinking effects upon guest inclusion/removal. These physical transformations are usually associated to cooperative effects within the frameworks built by strong coordination bonds. However, owing to their polymeric nature (1-, 2- or 3-D), these structural modifications are, to some extent, controlled by their intrinsic scaffold. In that sense, metal-organic polyhedral (MOP), which are 0D porous molecular cages and which can self-organize into highly ordered systems might be new materials displaying novel dynamic properties.

Here, we present new porous materials based on the assemblage of 0-D MOP, which show a stepwise sorption behavior correlated with dynamic structural transformations upon CO₂ sorption. A series of molecular cages of the lantern-type geometry based on paddlewheel metallic nodes (M₄L₄) were synthesized and harvested in the crystalline state yielding solids with highly ordered porous cages through van der Waals interaction. We further investigated their gas sorption properties and observed non-typical isotherms upon CO₂ sorption suggesting structural modification such as packing change during the all process. In addition, we also investigated the effect of surface functionalization and the nature of the metallic node and observed different behaviors regarding CO₂ sorption.

Keywords: [Metal-organic polyhedra](#), [Gate-opening pressure](#), [Structural transformation](#)