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Mechanical-pressure induced response of the MOF Al-MIL-53-TDC

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Abstract

The mechanical behavior of the recently synthesized flexible metal organic framework [Al(OH)(TDC)] with the well-known MIL-53 topology, built of 2,5-thiophenedicarboxylate (TDC²⁻), OH⁻ and Al³⁺ ions, named Al-MIL-53-TDC, has been explored using a combination of advanced characterization tools including mercury intrusion and high-pressure synchrotron X-ray powder diffraction, supported by Density Functional Theory calculations. This hybrid porous material was shown to exhibit a pressure-induced reversible structural contraction at ~275 MPa associated with a unit cell volume change of ~28.1% and a hysteresis loop once the pressure is released. This leads to an unprecedented energy work of 79 J.g⁻¹ that can be stored during one compression/decompression cycle for such a class of porous solids presenting a large-pore form ↔ closed-pore form phase transition. As such Al-MIL-53-TDC is at this time the best candidate of the MIL-53's family for a future potential application where a nano-damper is required.

1. Introduction

Metal organic frameworks (MOF) are one of the most recent classes of porous materials [1-4]. This family of hybrid porous solids constructed by the assembly of a wide range of metal centers and organic linkers has attracted a huge interest for a series of potential applications in the fields of adsorption/separation, catalysis, electronic/magnetism, drug delivery and so on... [5-8]. In addition, in the recent years, the mechanical properties of MOFs appeal a growing

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