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In situ pXRD monitoring of compliant MOFs under combined mechanical and gas pressure

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Compliant MOFs are known to respond to external stimuli, such as pressure, temperature, and adsorbed guests by undergoing remarkable structural changes [1]. Here, the coupling of two or more stimuli presents the opportunity of tuning a process like gas separation, affording control over the underlying framework's state [2]. However, structural information of materials undergoing combined guest adsorption and mechanical pressure application has been insofar limited to closed-system diamond anvil cells [3].

We here detail a unique clamped diamond window cell prototype specially developed for use with soft porous materials. For the first time, uniaxial mechanical pressure (up to 0.5 GPa) and gas dosing (up to 20 bar) were combined in an in-operando PXRD experiment, where the two stimuli can be decoupled and independently controlled. The cell was first validated using reference materials (NaCl and SiO2), followed by a study of a CO2 sorption under pressure in the metal-organic framework MIL-53, known to undergo "breathing"compliance under both stimuli [3,4]. The cell allowed a direct observation of MIL-53 phase existence throughout a gas-mechanical pressure space. In particular, it was possible to obtain tentative evidence that mechanical pressure can maintain this material's pores in a closed state throughout gas adsorption, confirming previous experimental and computational results [2].

References
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