

## Sequential Phase Transformation of PCN-250 and its Impact on Methane Storage

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Metal-organic frameworks (MOFs) are an emerging class of porous materials with potential applications for gas storage and separation. With industrialization, MOFs inevitably encounter processing under mechanical pressure, whereas the behaviors of MOFs under such conditions are not commonly studied. PCN-250, a promising candidate for methane storage, to study the impact of uniaxial mechanical pressure on the MOFs' structures and properties as a model of an MOF extrusion process. A sequential phase transformation was observed and recorded by X-ray diffraction analysis, which involved N=N bond flipping and Fe–O bond bending. Furthermore, the effects of pressure on the CH<sub>4</sub> adsorption capacity of PCN-250 were investigated by experiments and simulations. The PCN-250 pellet processed under optimized conditions shows an improved volumetric CH<sub>4</sub> uptake of 21% without obvious loss of gravimetric performance.<sup>1,2</sup>

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