Electronic Supplementary Information

Relevance of hydrogen bonding in CO_2 capture enhancement within InOF-1: an energy and vibrational analysis

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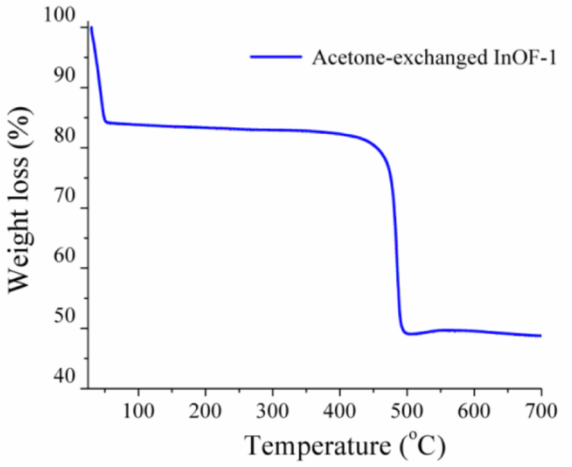

Fig S1. TGA analysis of InOF-1 (acetone-exchanged).

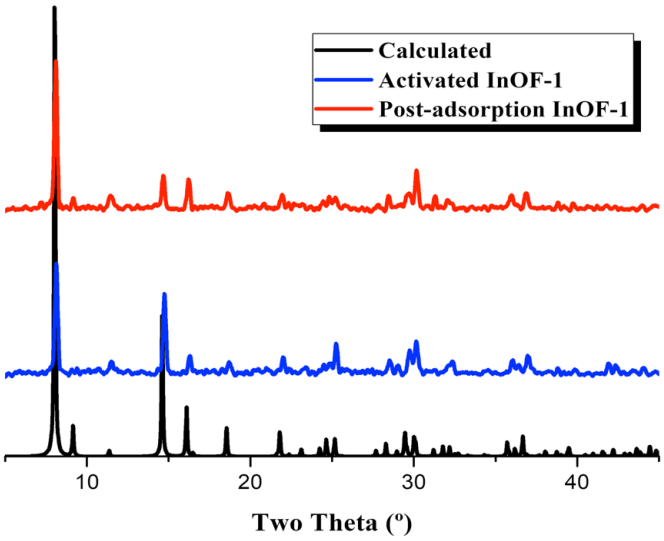

Fig S2. Powder X-ray diffraction patterns of calculated (black), activated (blue) and post-adsorption (red) InOF-1.

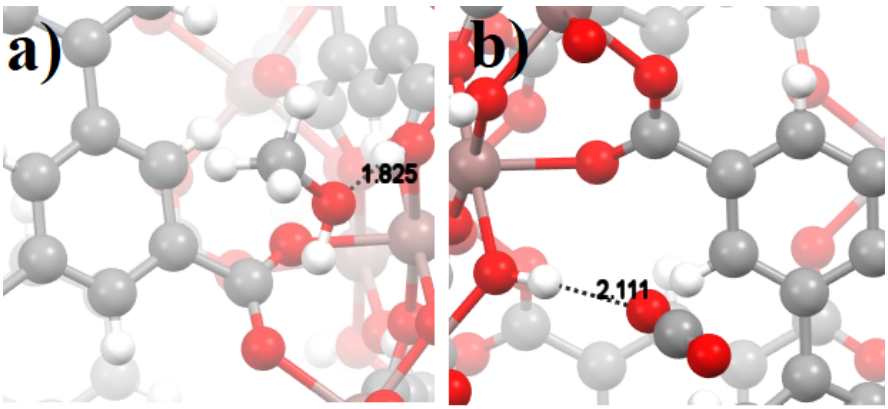

Fig S3. Optimized geometry of a) MeOH and b) CO_2 adsorbed in InOF-1 via a hydrogen bond formed with the μ_2-OH functional group of the MOF.

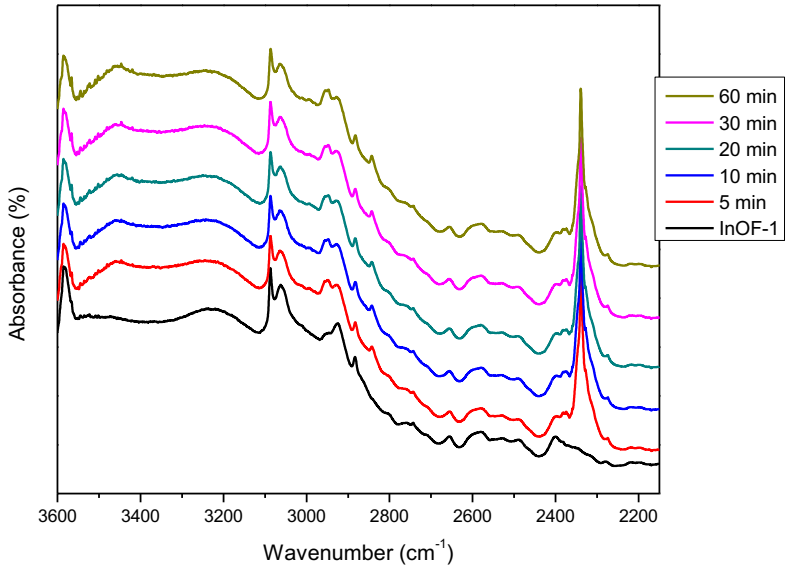

Fig. S4 DRIFTS spectra collected at different times without any flux at 30 °C. Stability of the established hydrogen-bonds among InOF-1, MeOH and CO_2.