Zirconium based metal organic frameworks for the capture of carbon dioxide and ethanol vapour. A comparative study.

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Supporting information.

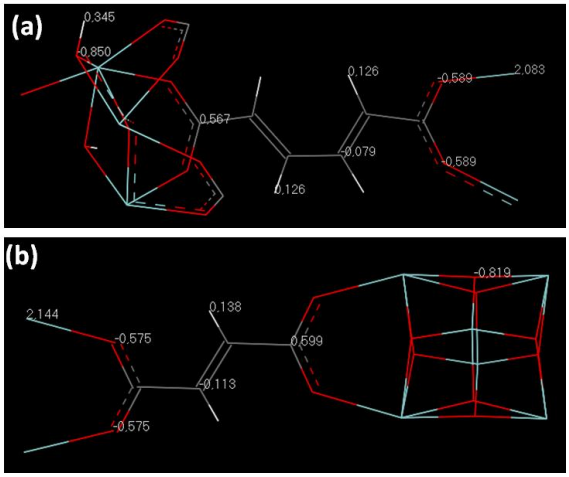

Figure S1. Partial charges extracted from DFT geometry-optimizations for Muc-Zr (a) and MOF-801 (b)

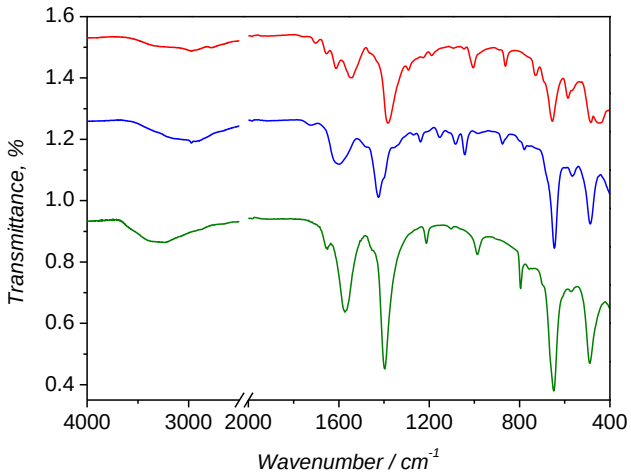

Figure S2. Transmittance infrared Spectra of the prepared materials. **(red)** MOF Zr-muconic, **(blue),** MOF MIP-202 and **(green)** MOF-801.

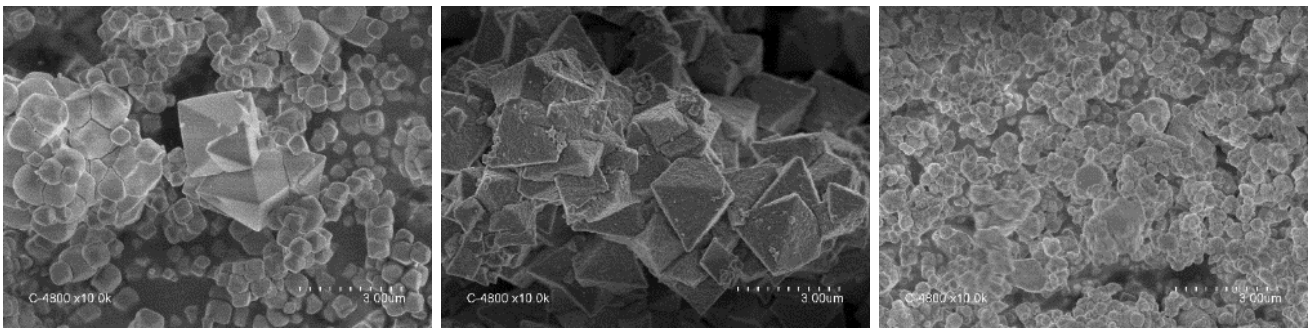

Figure S3. SEM image of MOFs: **(left)** MOF801 ,**(middle)** muc-Zr MOF, **(right)** MIP202.

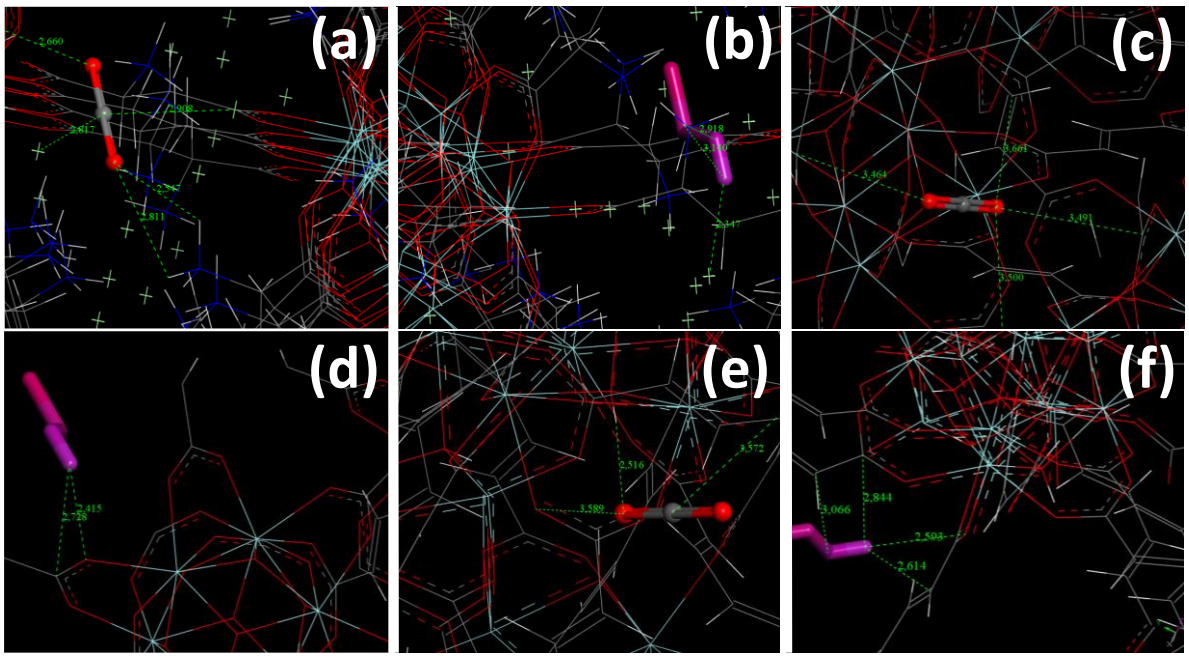

Figure S4. Snapshots obtained from Monte Carlo simulations and corresponding to the most probable adsorption sites for CO_2 and EtOH respectively in MIP-202 (a and b), MOF-80 (c and d) and Muc-Zr (e and f). The colors of the different atoms are C (grey), O (red), H (white), Cl (green), Zr (cyan), N (blue).