Supplementary Material

In silico design of a new Zn – triazole based Metal-Organic Framework for CO_2 and H_2O adsorption [§]

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List of the Figures

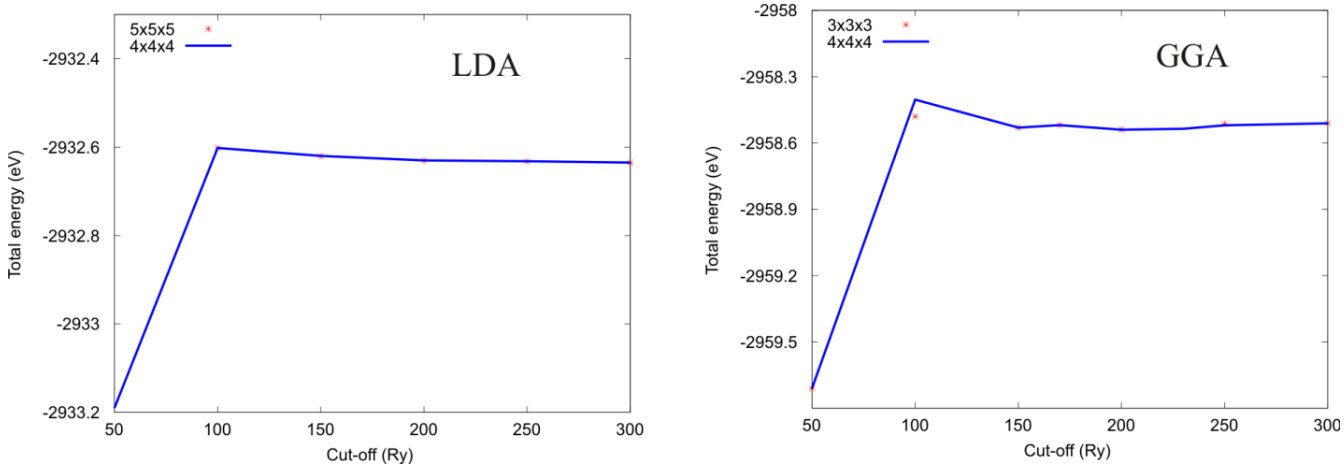

Figure S1: Convergence of the total energy with plane wave cut-off and k point sampling mesh for MAF-66.

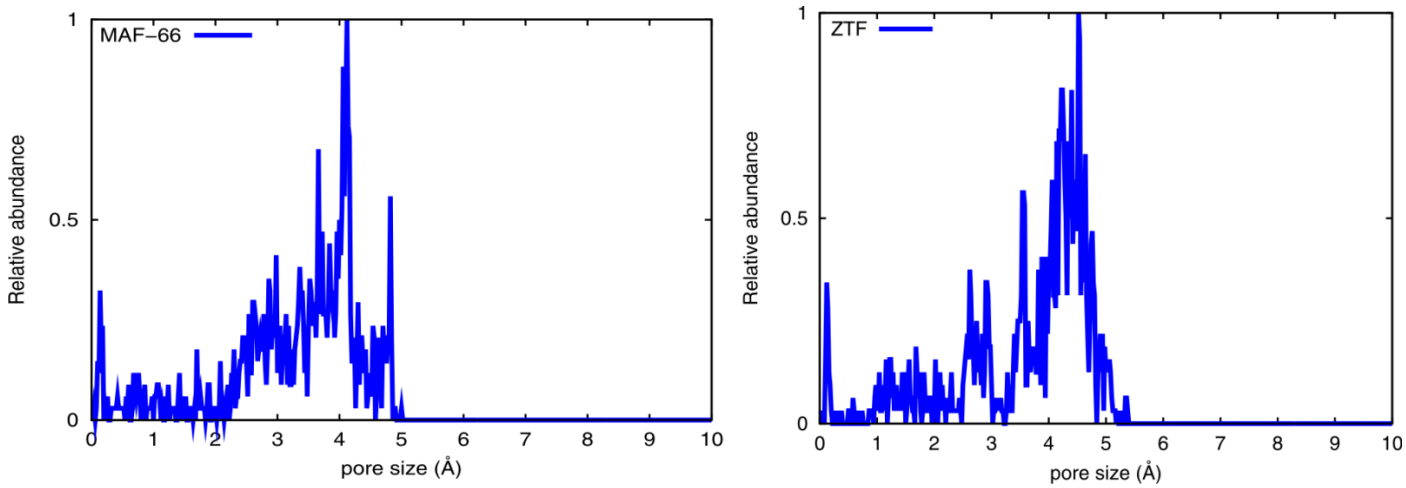

Figure S2: Pore size distributions of MAF-66 (left) and ZTF (right).

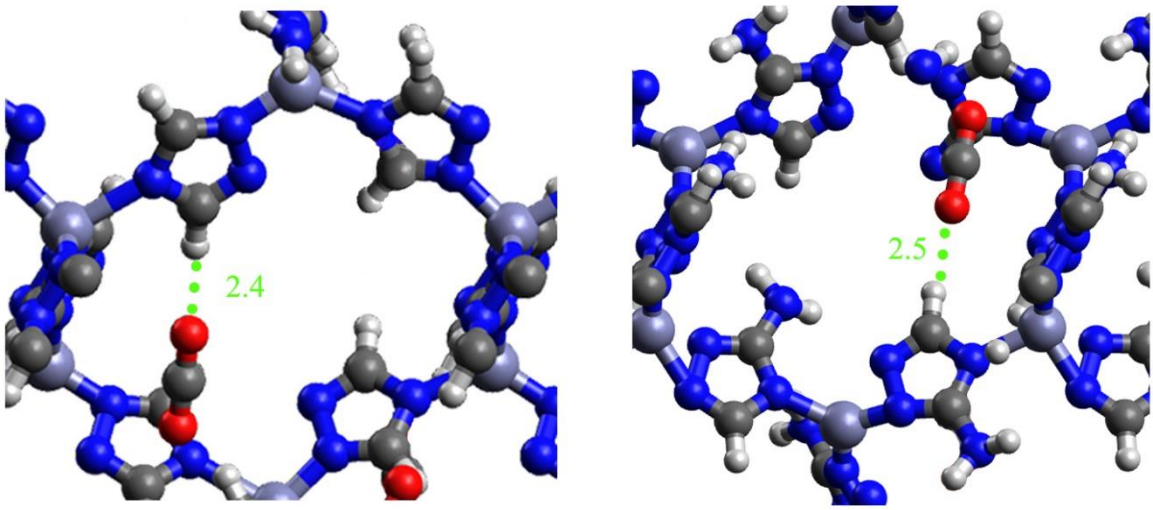

Figure S3: DFT optimized structures of parts of the supercells of ZTF (left) and MAF-66 (right) with one CO_2 molecule inside.

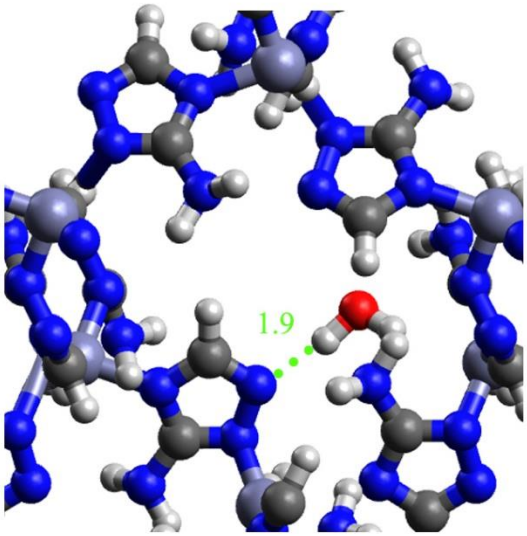

Figure S4: DFT optimized structure of parts of the supercell of MOF-66 with of one water molecule inside.