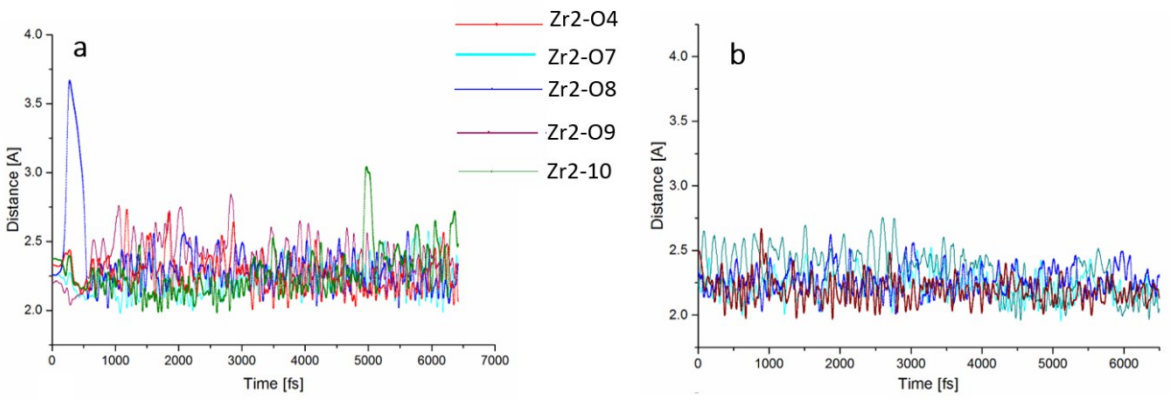

Figure S1. Zr2 ···O distance changes in defect-free structure (a) initial steps (b) after removal of surrounding water molecules at 383 K.

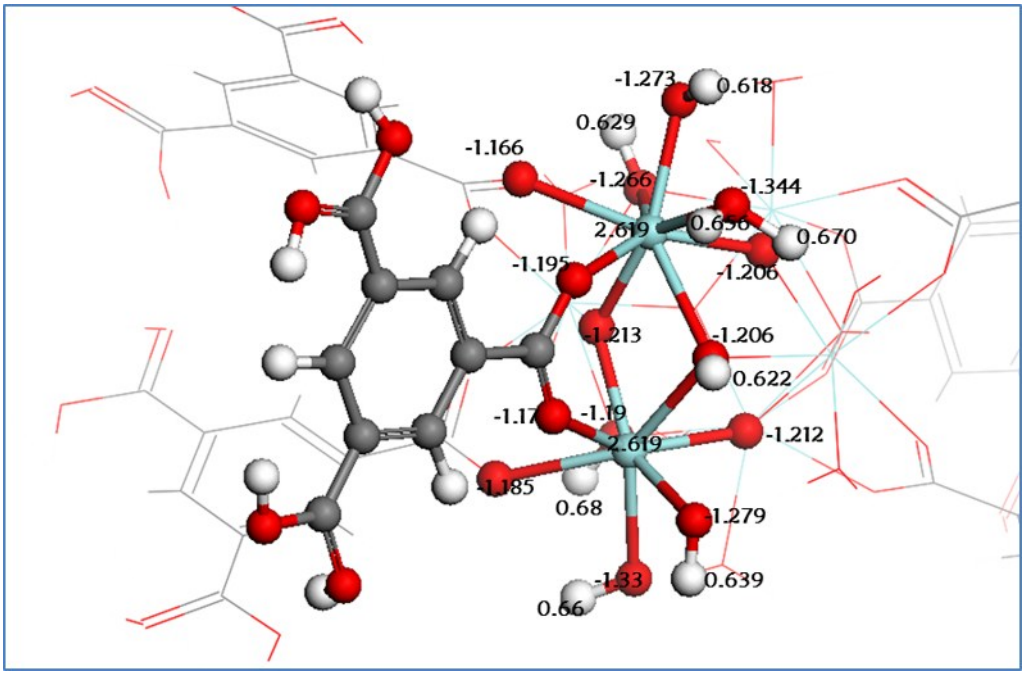

Figure S2. Bader charge of the initial defect-free cluster.

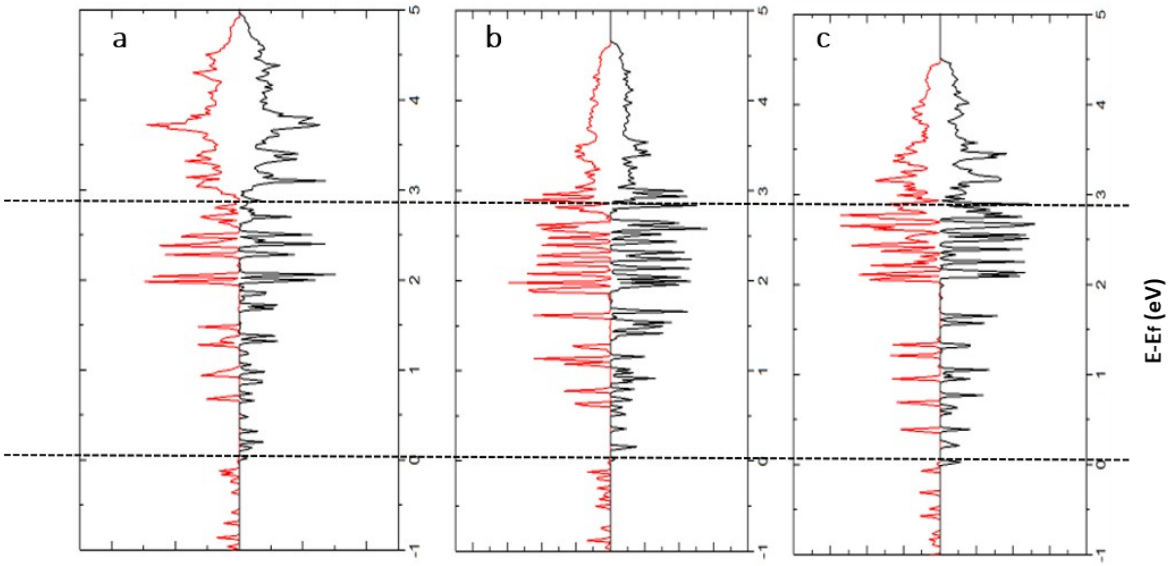

Figure S3. Total DOS of (a) hydroxylated-defect free, (b) dehydroxylated-defect free, and (c) dehydroxylated defect **MOF 808** structures. The defect-free MOF808 exhibits inherently six missing linker defects per cluster.

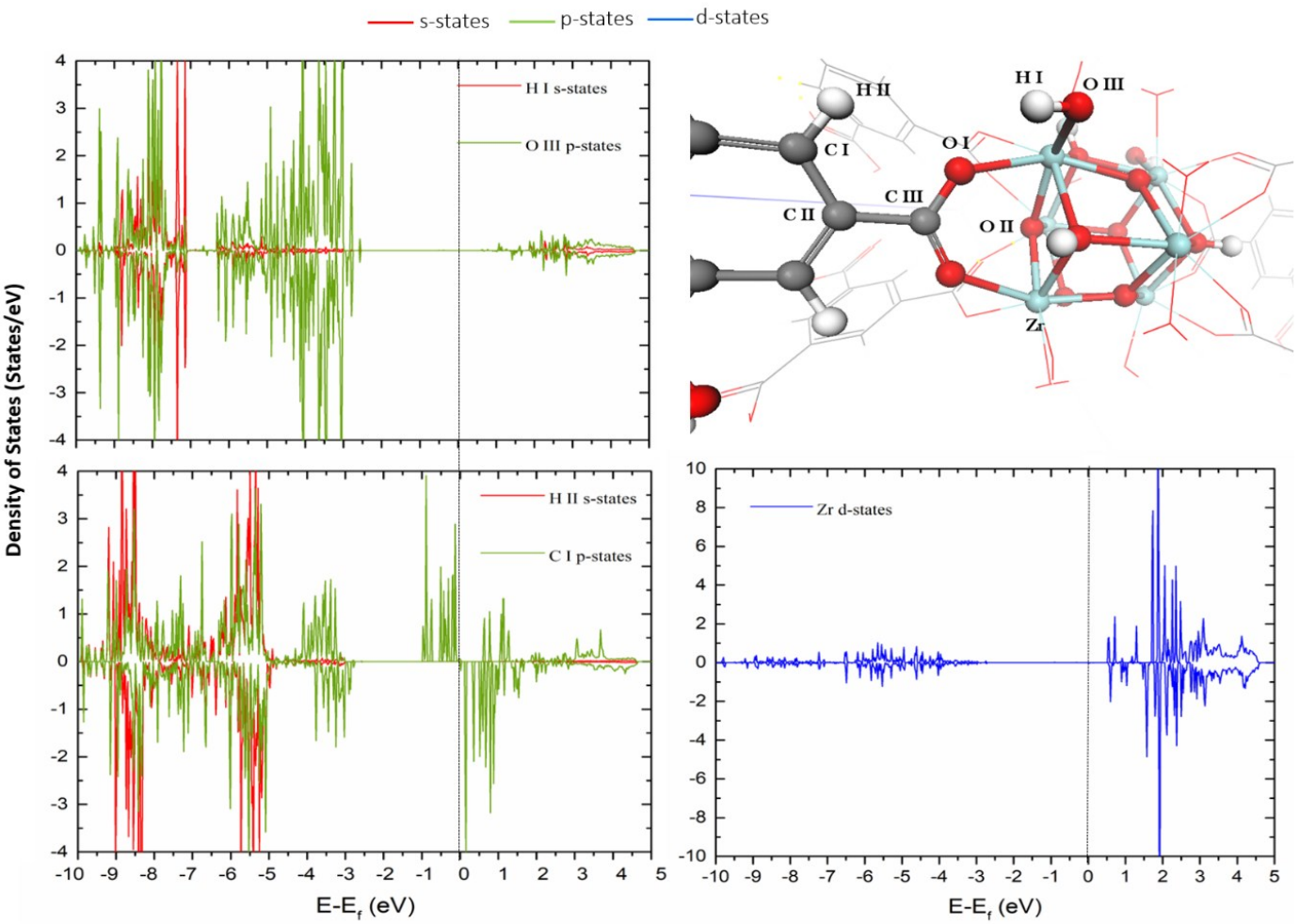

Figure S4. Nomenclature used for the studied carbon, oxygen and hydrogen atoms. States overlapping supporting covalent bonding and d-states of zirconium atoms.

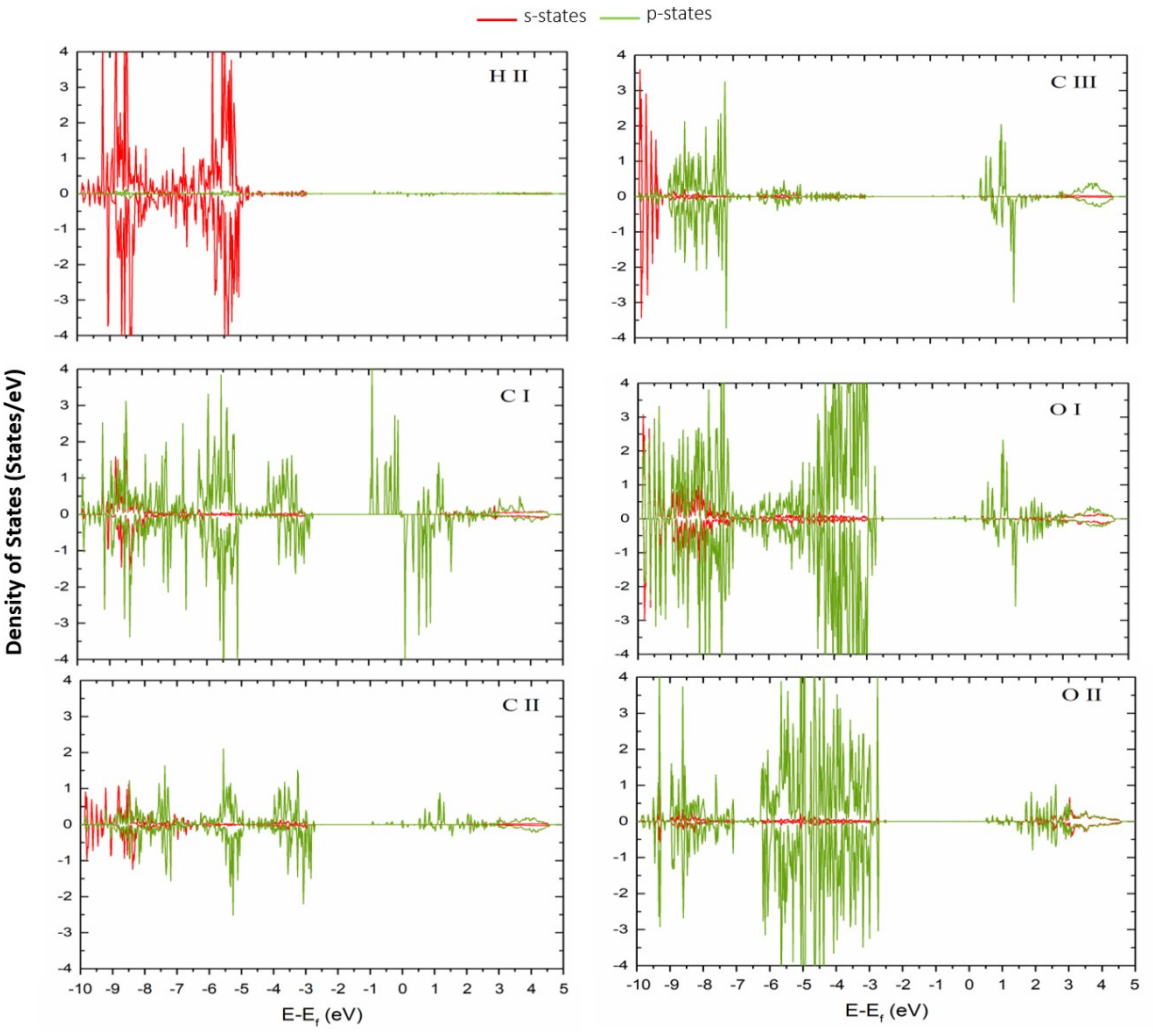

Figure S5. Partial density of states of the defect-free structure after activation process.