

1116 - Modulating active sites in MOFs for improved Lewis acid or base catalysis

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We will discuss ways to modify robust MOFs to maximize their catalytic activity. For Zr-MOFs like UiO-66, electron-withdrawing substituents on the terephthalates strongly enhance catalytic activity in Lewis-acid reactions such as the 'ene' reaction. A linear free energy relationship has been uncovered between rate constants and Hammett's σ substituent constant. Additionally we are able to increase the number of acid defect sites in these MOFs, while keeping the structure fully intact, using CF_3COOH as a synthesis modulator, and HCl as a crystallizing agent. As many clusters contain more than one coordinatively unsaturated site, bimolecular reactions like hydride exchange (e.g. in Oppenauer oxidations) are strongly accelerated. Finally, we discuss the basic activity of CPO-27 type MOFs, which is related to the proton affinity of the structural phenolates. The experimental and theoretically verified activity order is $\text{Ni} > \text{Cu} \sim \text{Co} > \text{Mg} > \text{Zn}$.

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