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Characterization of Metal-Organic Frameworks with Synchrotron and Neutron Sources for Catalytic Applications

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The chemical-flexibility, tunable pore size and chemical and structural stability of MOFs can be used to design active sites at the molecular level and to produce heterogeneous catalysts, which can be characterized with atomic precision.[1] In this contribution, we show how advanced characterization at synchrotron sources can be used to reveal the mechanism of formation of UiO-66 under microwave irradiation conditions. The synthesis of UiO-66 was monitored with in-situ X-ray diffraction at the material science beamline at the Swiss Light Source revealing the influence of modulators and aging in the yield and crystallite size of the material [2].
In addition, we present how X-ray and neutron sources can help identify active sites in catalysis and the structure of adsorbed species. We developed a catalytic methodology that uses such metal complexes to catalyze Suzuki-Miyaura cross coupling reactions in unprecedented mild conditions, at a low temperature of 40 ℃ and with a mild organic base such as triethylamine and characterized the relation between active site and selectivity [3]. The use of a MOF-immobilized catalysts results in a ten-fold reduction of the metal and ligand contamination in the reaction products. We also show how MOFs with MOF-74 and UMCM-1 topologies push Co-catalyzed hydroformylation into kinetic regimes not available under standard conditions. The micropores of MOFs increase the olefins density beyond neat conditions and partially prevent the adsorption of syngas allowing branched selectivity up to 90% using olefins with no directing groups, which is not achievable with existing Co catalysts.[4] Neutron diffraction revealed the structure of the adsorbed alkenes.

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