

## Graphical abstract

Two series of MTV-MOFs, MTV-UiO-66(COOH)<sub>2</sub> and MTV-UiO-66(OH)<sub>2</sub> are synthesized in a modulated synthesis approach yielding highly defected MTV-MOFs structures. Active sites are provided in the structure through the functionalized linkers, and the defected clusters. These active sites serve as the drive for the catalytic activity of the MTV-UiO-66 structures in the esterification reaction of butyric acid with butanol for butyl butyrate production.

