The Catalytic Ability of Vanadium based Metal Organic Frameworks for the Chemical Fixation of CO_2 with Epoxides

Kuruppathparambil Roshan Roshith, Gyu Young Hwang, Hye Min Jeong, 박대원†
부산대학교
(dwpark@pusan.ac.kr†)

Vanadium is one of the less explored elements for its catalytic activity towards the cycloaddition of CO_2 with epoxides to yield five membered cyclic carbonates. Considering the wide range of clusters and complexes that can be formed with vanadium nodes, a large number of metal organic frameworks with potential catalytic abilities could be synthesized. In this work, we examined the catalytic potential of two series of Vanadium based MIL metal organic frameworks; the ones with a) V-O-V infinite chains (V-MIL-47, V-MIL-48, V-MIL-68) and b) oxido centered V trimers (V-MIL-100, V-MIL101) along with tertiary butyl ammonium bromide co-catalysts. Among these, the highly porous V-MIL-47 was found most efficient which catalyzed the cycloaddition reaction of propylene oxide with CO_2 to propylene carbonate with high selectivity (>99%) and in high yields (>85%) at temperatures as low as 40 °C in 12-24 h reaction time. Density functional theory (DFT) was applied to find out the reaction pathways behind the catalysis.