Exploring Surface Modification Engineering of Metal-Organic Frameworks for Adsorption and Catalysis

Young Kyu Hwang\*1,2

1,Korea Research Institute of Chemical Technology (KRICT)

2Korea National University of Science and Technology (KNUST)

Abstract

Metal-organic frameworks (MOFs) are porous crystalline solids with high surface area and tunable porosity having a multitude of applications in the realm of gas storage, adsorption, separation, and heterogeneous catalysis. For the applications, post-synthetic immobilization or incorporation of secondary functional objectives on ligand or metal sites paves the way for imparting adsorption and catalytic functionalities onto the MOF scaffold and has been researched extensively during the last decade. Here, the catalytic results of biomass conversion, CO2 hydrogenation, and simultaneous transformation of biomass and CO2 over a various kind of MOFs with different functionalities will be presented. First, a series of Zr-based metal organic frameworks (Zr-MOFs) containing various types of metal node to ligand coordination were synthesized and tested for catalytic transfer hydrogenation (CTH) reaction of furfural (FUR) to furfuryl alcohol (FOL). It was found that metal node, coordination plays a more important role than porosity in Zr-MOFs. Second, the facile methods for preparing single atom catalysts (SACs) by incorporating an Ir-complex into a zeolitic imidazolate framework (so called ZIF) support will be discussed. The organometallic Ir-complex was introduced at different stages of the porous coordination polymer synthesis, resulting in different immobilization efficiencies, particle shapes, and catalytic activities. Third, for base-free hydrogenation of CO2 the Mo132 cluster was immobilized in porous MIL-101(Fe) by in situ encapsulation method to be used as a heterogeneous catalyst. The resulting Mo132@MIL-100(Fe) not only maintained its structural integrity and activity during three consecutive recycling reactions but also exhibited increased TON compared to Mo132 cluster at the same reaction condition. This study provides the first instance of incorporation Mo132 cluster as a CO2 hydration catalyst to enhance the yield of formic acid (FA), and the similar strategy can be applicable to various aqueous-phase CO2 conversion. Finally, I will briefly touch the synthesis and application of mesoporous metal-organic frameworks for the capture and removal of toxic gases.

References

1. *Oh and Hwang et al., Chem. Mater. 34 (****2022****), 8153*
2. *Oh and Hwang et al., ACS Sustain. Chem. Eng. 9 (****2021****) 14051*
3. *Valekar and Hwang et al., ACS Catal. 10 (****2020****) 3720*
4. *Park and Hwang et al., Chem. Eng. J. 463 (****2023****) 142410*
5. *Oh and Hwang et al., ACS Appl. Mater. Inter. 15 (****2023****) 9296*
6. *Cha and Hwang et al., Chem. Eng. J. 439 (****2022****) 135612*