THESIS INFORMATION

Title: **DESIGNED SYNTHESIS OF NOVEL METAL–ORGANIC FRAMEWORKS FOR PHOTOCATALYST APPLICATION**

Major: Organic Chemical Technology

Major code: 62.52.75.05

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Scientific contribution

We contribute to the science the novel approach to synthesize MOFs material based Ti-oxo cluster which is rare in MOFs chemistry. The synthetic scheme was provided to prove the *in situ* formation of Ti-oxo cluster during the robust synthesis. The work was also contributed to MOFs chemistry the route which can overcome the challenges for the synthesis of MOFs based Ti-oxo cluster which normally occur as sol, gel, or amorphous solid. The development of new, crystalline, and extended structures, most notably based on Ti(IV), has been of great interest to the community of materials scientists owing to the difficulty in realizing such materials (a total of 5 Ti MOFs are known, compared to thousands of other metal ions). There remains an absence of a universal approach for achieving new Ti-MOFs.

In this work, we describe the designed synthesis and full characterization of a new two-dimensional titanium-based hybrid material. This material was achieved through an unprecedented synthetic protocol whereby the rich chemistry of titanium oxo clusters in combination with dynamic organic covalent bond formation was used. We further demonstrate the significantly high photocatalytic performance of MOF-901, -902 via the visible light mediated polymerization of methyl methacrylate. Specially, MOF-901, -902 outperformed the commercially available Degussa P-25 TiO_2 photocatalyst and other related MOFs. This report paves the way for future design of MOF materials based on combining the MOF and covalent organic framework (COF) approaches. Indeed, by incorporating the high conjugated imine linking unit, MOF-902 absorbs the visible light at red-shift region leading to low band gap energy (*ca*. 2.50 eV). The visible light responsive activity of MOF-902 was confirmed by the

photocatalytic properties enhancement. MOF-902 exhibited high performance in photocatalysis application of polymerization reaction with various monomers such as MMA, BMA, and St, resulting in high molecular weight (M_n) and low PDI of polymer products. Containing higher conjugation system of linking building unit in the framework, MOF-902 exhibited significantly better performance as a heterogeneous photocatalyst than MOF-901 in polymerization reactions. The photocatalysis property of MOF-902 also outperforms the commercial catalyst P25-TiO_2 as well as other MOFs possessing similar band gap energies.

In view of the growing importance of crystalline, microporous materials for clean energy and photocatalytic applications, we feel that this communication will be of broad interest to chemists, physicists, and engineers studying porous materials design and properties.

Moreover, we have successfully synthesized and characterized three novel MOFs including two Fe(III)-based MOFs and one Cu(II)-based MOFs namely MOF-903, -904, and VNU-18, respectively. The crystal structures of these MOFs have been analyzed to study the three dimensional crystalline structures and topologies. The structural characteristics of these MOFs including thermal stability, porosity, and crystallinity were investigated by thermogravimetric analysis (TGA), nitrogen adsorption isotherm at low pressure, and powder X-ray diffraction analysis (PXRD).

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