Design, synthesis and characterization of novel covalent organic framework-based hybrid photocatalysts

Nowadays, energy crisis and environmental pollution have become worldwide concerns. Photocatalysis, as a green and sustainable technology that uses solar energy for either hydrogen production via water splitting or environmental degradation of pollutants, is considered to be a promising strategy to overcome these issues. Since the first report of TiO_2 as a photocatalyst, many inorganic semiconductors have been explored for water splitting and pollutants degradation both in liquid and gaseous phases. However, the efficiency of these photocatalysts, especially under visible light irradiation is far below the requirement of commercialization. Therefore, searching for high efficient, low cost, stable, visible-light responsible photocatalysts is still a challenge in photocatalysis field.

Recently, inspired by natural photosynthesis, organic materials such covalent organic frameworks (COFs) have emerged as new promising photocatalysts because of their tunability, stability and highly porous structure. Covalent organic are molecular “Legos” and the vast structural diversity of COFs implies a great prospect for tuning the desirable physicochemical properties for photocatalytic applications However, development of new modification method (including pore engineering and proper functionalization) of COFs to obtain visible-light active photocatalytic system is still a challenge. Significantly, the homogeneous pores within COFs can be used as a vessel to introduce functional particles, in this regard the integration of various quantum dots in a semiconducting COF backbone in order to enhance light absorption, charge separation and transfer is proposed for the first time.

The aims of this project are: (1) to develop a new class of covalent organic frameworks (COFs)-based photocatalysts by combining COFs with quantum dots (heavy metal free QDs) into hybrid system exhibiting enhanced photocatalytic activity in hydrogen generation and pollutants degradation reactions; (2) to investigate the influence of QDs attachment method to the surface of COF materials (including COF, COF/bulk semiconductor and COF/MOF core/shell structures) on the optical, surface and photocatalytic properties; and (3) to explain excitation and photocatalytic mechanism of covalent organic frameworks-based hybrids in photocatalytic reactions under UV-Vis and Vis light irradiation.

All obtained nanostructures will be characterized to estimate: crystal structure, crystallite size and lattice parameters using XRD technique, surface composition of COF-based photocatalysts using XPS, morphology (SEM, EDX and TEM microscopy), optical properties (DRS UV-Vis and PL spectroscopy), surface area and porosity (BET method). Furthermore, better understanding of photocatalytic mechanism in the presence of COF-based materials and development of quantitative structure-properties relationship model to correlate COF-based hybrids properties with their photocatalytic efficiency can be significant point for further design of new highly active photocatalysts.