THE UNIVERSITY OF HONG KONG

DEPARTMENT OF CIVIL ENGINEERING

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Organic Semiconductor Photocatalysts for Water Splitting, Pollutant Degradation and Tumor Elimination under Visible Irradiation

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Date: December 4, 2023 (Monday)
Time: 3:00 p.m. – 4:00 p.m.
Venue: CPD-3.16, Run Run Shaw Tower, Centennial Campus, HKU

ABSTRACT

Organic supramolecular photocatalysts with full visible-light spectrum response have been successfully developed. Their photocatalytic redox and anti-cancer properties can be optimized by adjusting thermodynamic and kinetic conditions as well as photoelectric physicochemical properties. These properties depend on crystal structure, molecular chemistry structure, and morphological structure, with photocatalytic activity arising from molecular dipoles, ordered stacking, and nanostructure.

The degree of crystallinity of organic supramolecular crystals affects charge transfer behavior during the photocatalytic process. Self-assembled PDINH supramolecules exhibit strong oxidative capability under visible-light irradiation, applicable for photodegradation of pollutants and oxygen evolution. Strong π-π stacking between PDINH molecules promotes the effective long-range delocalization of electrons, enhancing photogenerated charge migration and separation, leading to significant photocatalytic activity. Highly crystalline PDINH supramolecular photocatalysts obtained by a high-temperature imidazole solvent method benefit from long-range ordered structure stacking, promoting charge transfer behavior and enhancing photocatalytic oxygen evolution by 1353 times (40.6 mmol g^{-1} h^{-1}). High crystallinity can also be achieved through urea-linked PDINH polymer structures.

Crystal internal electric fields controlled by molecular chemical structure can regulate the driving force for photogenerated charge separation. Carboxylic-modified PDINH molecules generate strong molecular dipoles, and the ordered stacking structure further produces an internal electric field, effectively promoting the separation of photogenerated carriers, serving as an effective photocatalyst for organic pollutant degradation and water oxidation. By replacing the anhydride functional group of PTCDA with a carboxylic group, PTA supramolecular crystal is obtained, with enhanced molecular dipoles and hydrogen bond polarization strengthening the built-in electric field, promoting photogenerated electrons to participate in hydrogen production reaction.

Ordered stacked porphyrin supramolecular photocatalyst SA-TCPP exhibits oxidative capabilities effective in eliminating solid tumors. A bio-safe dose of SA-TCCP is targeted injected into tumors, and under deep penetrating red light (600-700 nm) irradiation, tumors are eliminated completely within 10 minutes. Photogenerated holes, the most significant species in the photocatalytic therapy process, are abundant on the surface of photocatalysts in the cytoplasm. Solid tumors are completely

removed via photocatalyst injection and red-light irradiation.

The morphological structure of organic crystals impacts the migration behavior of photogenerated charges. Hydrogen-bonded organic framework tetracarboxylic perylene supramolecules with one-dimensional pore structure shorten exciton migration distance to sub-nanometers, thereby enhancing the utilization of photogenerated charges, enabling the photocatalyst to produce 1 mol of H_2 under daily outdoor sunlight. Highly selective conversion of CO_2 to ethylene is achieved using Cu_2-MOF organic semiconductor photocatalyst with high metal density.

ABOUT THE SPEAKER

Professor Zhu Yongfa is a professor and doctoral supervisor at Tsinghua University's Department of Chemistry and the Executive Deputy Director of the National Electron Spectroscopy Center. Prof. Zhu's research focuses on energy and environmental photocatalysis, as well as photocatalytic health.

Prof. Zhu received the Ministry of Education's Trans-century Outstanding Talent and the NSFC Outstanding Youth Fund. He has published 483 SCI papers, with over 43,900 citations and an H-index of 119. He has been recognized as an Elsevier Highly Cited Scholar (Chemistry) since 2014, a Clarivate Analytics Highly Cited Researcher (Chemistry) since 2018, and ranked 851st among the top 100,000 global scientists in 2021.

Prof. Zhu serves in various academic positions, including Founding Editor-in-Chief of *Science for Energy and Environment* (*SEE*), Associate Editor of *Applied Catalysis B*, and leadership roles in several professional societies and committees in the fields of chemistry, photocatalysis, and environmental purification.

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