Charge-transfer regulated visible light driven photocatalytic H_2 production and CO_2 reduction in tetrathiafulvalene based coordination polymer gel

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Short Description of presentation (Abstract)

The much-needed renewable alternatives to fossil fuel can be achieved efficiently and sustainably by converting solar energy to fuels via hydrogen generation from water or CO_2 reduction. Herein, a soft processable metal-organic hybrid material is developed and studied for photocatalytic activity towards H_2 production and CO_2 reduction to CO and CH_4 under visible light as well as direct sunlight irradiation. A tetrapodal low molecular weight gelator (LMWG) is synthesized by integrating tetrathiafulvalene (TTF) and terpyridine (TPY) derivatives through amide linkages and results in TPY-TTF LMWG. The TPY-TTF LMWG acts as a linker, and self-assembly of this gelator molecules with Zn^{II} ions results in a coordination polymer gel (CPG); Zn-TPY-TTF. The Zn-TPY-TTF CPG shows high photocatalytic activity towards H_2 production (530 µmol $g^{-1}h^{-1}$) and CO_2 reduction to CO (438 µmol $g^{-1}h^{-1}$, selectivity >99%) regulated by charge-transfer interactions. Furthermore, in situ stabilization of Pt nanoparticles on CPG (Pt@Zn-TPY-TTF) enhances H_2 evolution (14727 µmol $g^{-1}h^{-1}$). Importantly, Pt@Zn-TPY-TTF CPG

produces CH_4 (292 µmol $g^{-1}h^{-1}$, selectivity >97%) as CO_2 reduction product instead of CO. The real-time CO_2 reduction reaction is monitored by in situ DRIFT study, and the plausible mechanism is derived computationally.
Paper published based on this study: ***Nat. Commun. 2021, 12, 7313.***

What will the audience take away from your presentation?

- The audience will be able to understand how Gel-based soft processable material (i.e., Coordination Polymer Gel) can be utilized for photocatalytic application.
- A novel approach for the development of photocatalyst material with earth-abundant metal ions. This approach can be further extended by designing new gelators molecules. The efficiency of CPG based material towards practical application is more promising compared to traditional solid-state catalysts in many aspects however it is still underexplored.
- The main advantages of using gel-based material for photocatalysis will be explained in detail during this talk, such as, the 3D interconnect network morphology in hydrated self-assembly that enhances the diffusion of reactant towards the catalytic centers during the photocatalytic process.

Biography of presenting author

Dr. Parul Verma studied Chemistry at the Banaras Hindu University, INDIA and graduated as M.Sc. in 2014. She then joined the research group of Prof. Tapas K. Maji at the (Molecular Material Lab) JNCASR, Bangalore, INDIA for Ph. D. degree. She has finished her Ph. D. in Aug 2021 and currently working as a post-doctoral researcher at the same institute.

Research interests

Organic and Metal-Organic Hybrid 'Soft' Materials towards **Hydrogen Production, Carbon dioxide Reduction** and Optoelectronic Applications.

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