S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES
Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR
Chemical and Biological Sciences

23rd August, 2022 **4.00 PM** **FERMION/ ONLINE**

SPEAKER

Dr. Samrat Ghosh
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TITLE OF THE TALK

Why Charge Transport is Pivotal for the Photocatalytic Hydrogen Evolution in Two-dimensional Porous Organic Semiconductors?

ABSTRACT

Visible light driven hydrogen evolution from water is a promising strategy to convert and store solar energy as chemical energy.1 Covalent organic frameworks (COFs) are front runners among different classes 2D materials, owing to their tunable porosity, crystallinity, optical and electronic properties. Photocatalytic activity of COFs depends on numerous factors such as band gap, crystallinity, porosity, exciton migration, stability of transient species, charge separation and transport.2 However, it is challenging to fine tune all these factors simultaneously to enhance the photocatalytic activity. Here, we have established a correlation between charge transport and photocatalytic hydrogen evolution through structure–property–activity relationship combined with microwave spectroscopy and first–principles calculations. Careful molecular engineering allowed us to tune the light absorption (i.e. band gap), crystallinity, porosity, layer stacking and charge carrier generation and transport of a series of isoreticular COFs. We have assessed how these properties and the interplay between them impact photocatalytic activity of studied COFs. From the structure–property–activity relationship, we found that light absorption and charge carrier generation and transport are the prime factors, which influence the photocatalytic H2 production of COFs in much greater extent than other factors.3,4

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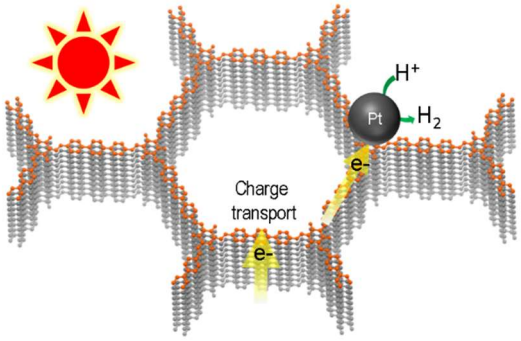

Figure 1. Schematic representation showing the transport of photoexcited charge carriers for the proton reduction.

References

1. T. Wang et al. Chem. Rev. 2018, 118, 5201–5241.
2. T. Banerjee et al. ACS Energy Lett. 2018, 3, 400–409.
3. S. Ghosh et al. J. Am. Chem. Soc. 2020, 142, 9752−9762.
4. S. Ghosh et al. Chem. Mater. 2022, 34, 736–745.

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