

Self-assembly of Organic Molecules

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Why in News?

Researchers at the Centre for Nano and Soft Matter Sciences (CeNS), Bengaluru have developed a novel metal-free organic photocatalyst for solar-driven green hydrogen production by utilizing the self-assembly of organic molecules.

- **Molecular Synthesis** - The team functionalized a light-absorbing organic dye molecule, **perylene diimide (PDI)** with a naturally occurring amino acid, **aspartic acid**.
- **Spontaneous Supramolecular Self-Assembly** - In water, these modified molecules spontaneously organized into highly ordered, *two-dimensional (2D) nanosheets* without altering their fundamental chemical composition.
- **Synergistic Molecular Drivers**
 - **Aspartic acid moiety**- Promotes strong, extended hydrogen bonding and increases the molecular dipole moment.
 - **PDI chromophore** - Drives strong π - π stacking and efficient light harvesting.

Key Technical Advantages

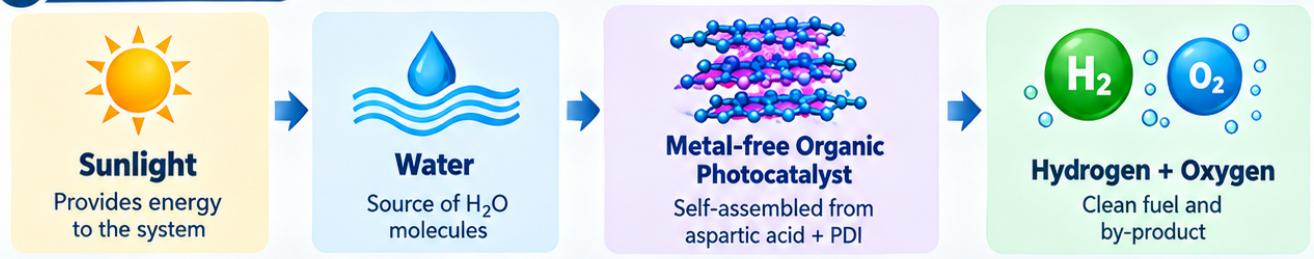
- **Enhanced Photocurrent**- The self-assembled 2D nanosheets generated nearly **18% higher photocurrent** during solar-driven water splitting compared to their bulk counterpart.
- **Broadened Light Absorption** - Supramolecular reorganization broadened the solar absorption spectrum and increased the accessible surface area available for catalytic reactions.
- **Improved Charge Transport**- Density Functional Theory (DFT) calculations revealed that the structural alignment
 - Enhances charge transport,
 - Reduces recombination losses, and
 - Effectively separates photo-generated charges to drive the hydrogen evolution reaction.

Self-Assembly of Organic Molecules: A New Path to Green Hydrogen

Can tiny molecular structures unlock cleaner hydrogen from sunlight?



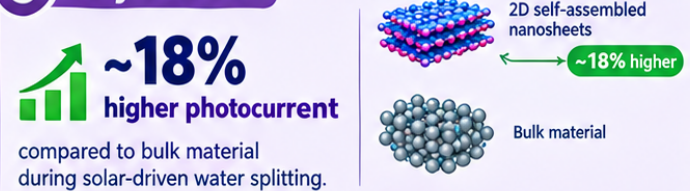
1 The Process



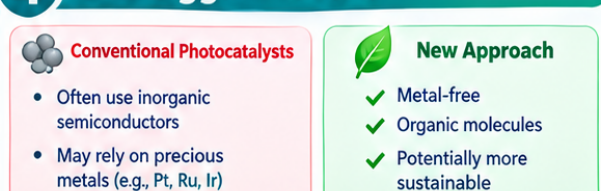
2 How It Works – Molecular Self-Assembly



3 Key Result



4 The Bigger Picture



CeNS, Bengaluru

| DST

| Green Hydrogen Research



Significance

- **Eliminating Precious Metals** - Most existing photocatalysts for water splitting rely on expensive inorganic semiconductors or scarce noble metals (e.g., Platinum, Ruthenium).
- This design provides a sustainable, cost-effective, and fully metal-free alternative.
- **Green Hydrogen Mission Alignment**- Supports India's National Green Hydrogen Mission by advancing indigenous research in solar fuel generation, artificial photosynthesis, and next-generation renewable energy materials.

Reference

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