Self-assembly of Organic Molecules

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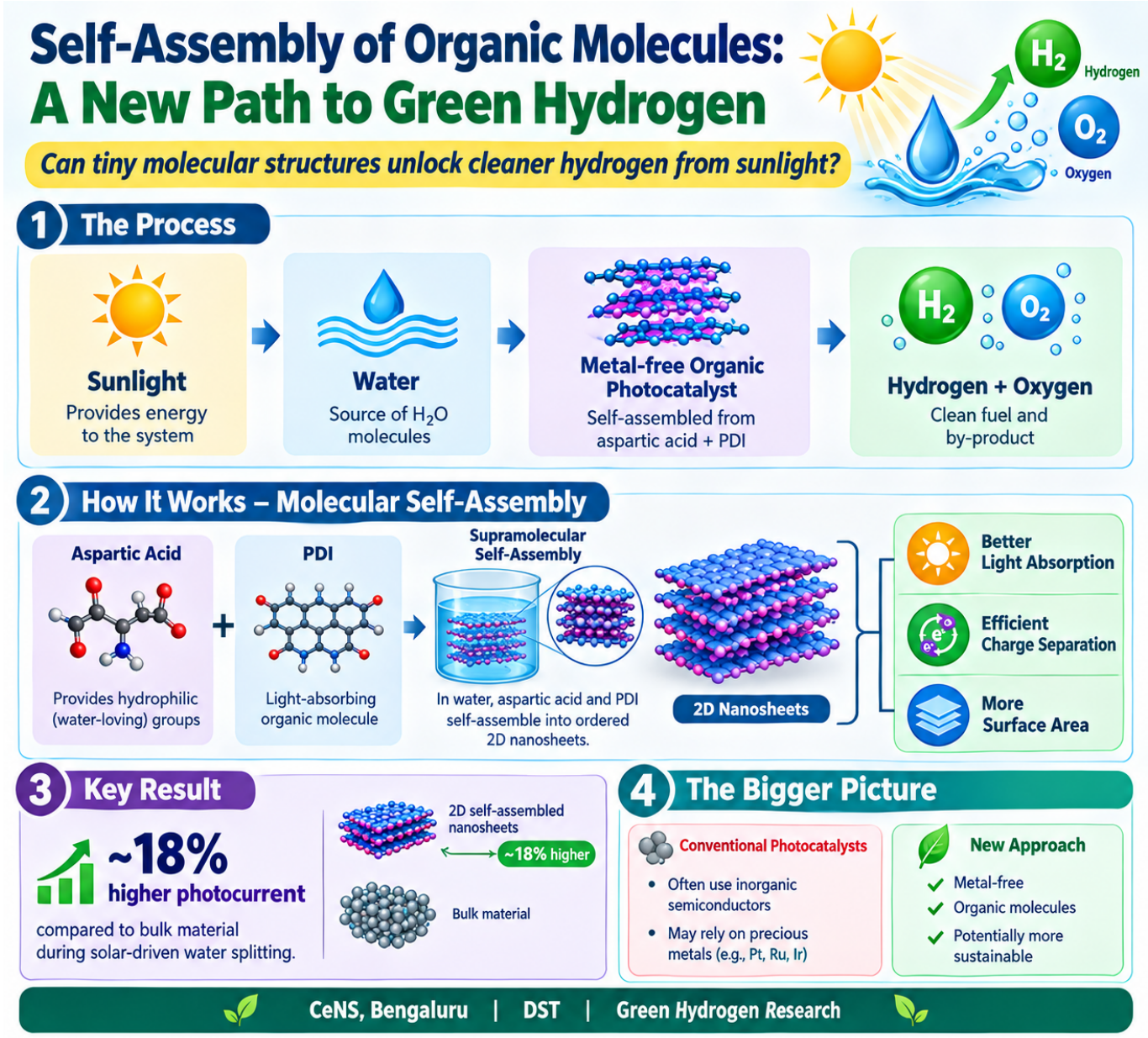
Why in News?

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.



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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