Polythiophene/Non-fullerene Donor-acceptor Covalent Conjugates and Their Hybrids for Light Energy Harvesting Technologies

Faseeh Akbar,[a] Sana Iqbal,[a] Arwa Sohail,[a] Sumbleen,[a] Shahryar Rasheed[a] and Basit Yameen*[a]

[a] Department of Chemistry and Chemical Engineering, Syed Babar Ali School of Science and Engineering, Lahore University of Management Sciences (LUMS), Lahore-54792, Pakistan

Presenter [Faseeh Akbar] : 22130024@lums.edu.pk *Corresponding Author: basit.yameen@lums.edu.pk

ABSTRACT

Artificial photosynthesis of hydrogen peroxide (H_2O_2) using organic photocatalysts offers a sustainable alternative to the energy intensive anthraquinone process. Herein, we report a donor-acceptor (D-A) double cable polymer (DCP) based on polythiophene (PTh) and perylene diimide (PDI) for the artificial photosynthesis of H_2O_2. Covalent integration of the electron donating PTh and electron accepting PDI within a single polymer architecture promotes efficient charge separation and interfacial charge transport which results in enhanced photocatalytic activity. The synthesized PTh-PDI-DCP exhibited superior photophysical, photoelectrochemical (PEC) and photocatalytic performance compared to the individual (D & A) components and their physical blend. To further enhance activity without altering the intrinsic polymer structure, functional hybrid systems were developed using plasmonic gold nanoparticles (AuNPs) and reduced graphene oxide (rGO). The optimized hybrid interfaces significantly improved electronic communication, suppressed charge recombination and accelerated charge transfer kinetics. Among all investigated systems, PTh-PDI-DCP/rGO and PTh-PDI-DCP/AuNPs demonstrated the highest H_2O_2 production under visible-light irradiation. Time-resolved photoluminescence and electrochemical analyses confirmed enhanced interfacial charge separation in the hybrid systems. Immobilization of the photocatalysts on porous, hydrophobic poly(vinylidene fluoride) (PVDF) membranes (photocatalyst@PVDF membrane) enabled facile recovery and stable operation over repeated photocatalytic cycles. Overall, this work highlights DCP-based hybrid photocatalysts as an effective strategy for efficient solar to chemical energy conversion and sustainable artificial photosynthesis of H_2O_2.

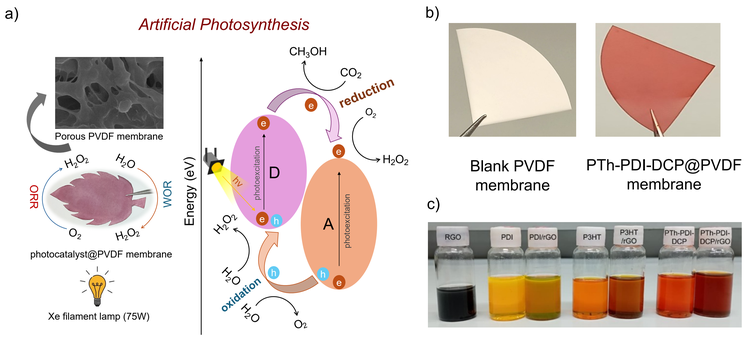

Figure 1. (a) Graphical depiction of the artificial photosynthesis of H_2O_2; (b) PVDF membrane before and after coating with the photocatalyst; (c) photocatalysts' solutions used for the artificial photosynthesis of H_2O_2.

Band-gap alignment, characterization and photophysical behaviour

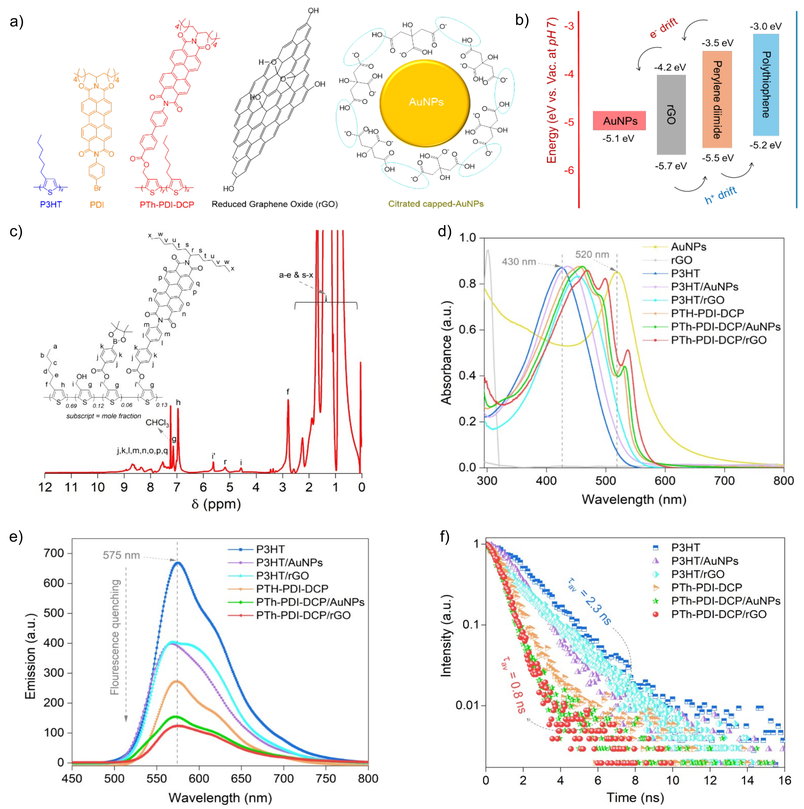

Figure 1. (a) Chemical structures of the materials employed in this study; (b) band-edge alignment of the materials; (c) ^{1}H NMR spectrum of PTh-PDI-DCP; (d) UV-Vis absorption spectra; (e) photoluminescence (PL) emission spectra recorded at an excitation wavelength (λ_{exc}) of 440 nm; and (f) time-resolved photoluminescence (TRPL) spectra recorded at excitation wavelengths (λ_{exc}) of 440 and detection wavelength (λ_{det}) 575 nm.

Photoelectrochemical and photocatalytic studies

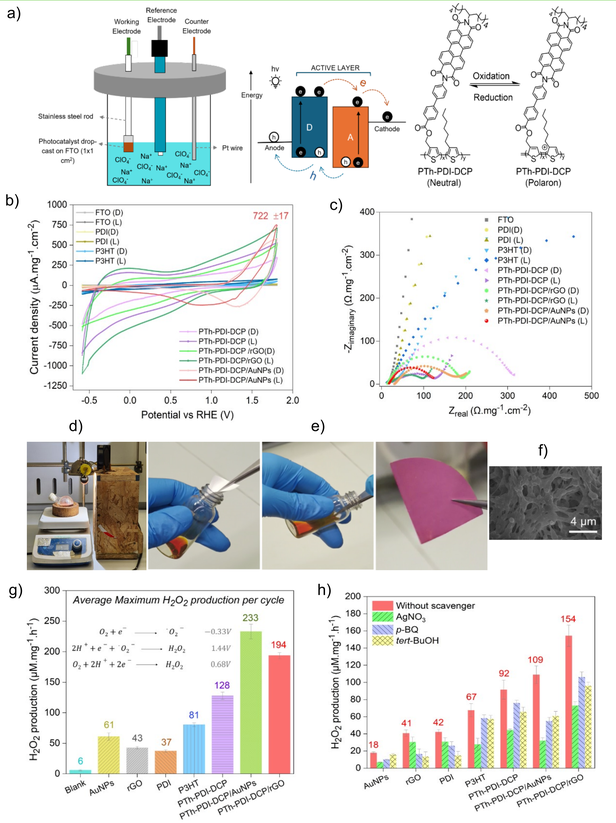

Figure 1. (a) Schematic illustration of the photoelectrochemical (PEC) process; (b) cyclic voltammograms; (c) electrochemical impedance spectroscopy (EIS) Nyquist plots; (d) digital photograph of the experimental setup used for the artificial photosynthesis of H_2O_2; (e) immobilization of the photocatalyst onto the PVDF membrane; (f) SEM micrograph of the photocatalyst-coated PVDF membrane; (g) maximum H_2O_2 concentration generated by each photocatalyst during artificial photosynthesis; and (h) mechanistic investigations elucidating the reaction pathway involved in the artificial photosynthesis of H_2O_2.

References: a) *ACS Appl. Mater. Interfaces 2025, 17, 19, 28609-28621*, b) *ACS Appl. Energy Mater. 2025, 8, 18, 13861-13876*; c) *Faseeh et al., Polymer Chemistry, 2026, Advance Article*; *d) J. Mater. Chem. C, 2023,11, 16037-16048*