

Name of Scholar: **Aaliyah Farooq**

Notification No: 576/2025

Name of Supervisor: **Dr. Sapan Kumar Jain**

Date of Award: 27-02-2025

Name of Department: **Chemistry**

Topic of Research: ***“Synthesis, Characterization and Application Studies of Conducting Polymer-based Copolymers”***

Findings

The thesis entitled “Synthesis, Characterization and Application Studies of Conducting polymer-based Copolymers” consisted of five chapters, each dealing with the design, synthesis, characterization, and application of conducting polymer-based copolymers as efficient photocatalysts for wastewater treatment and biophysical interactions. Chapter I provides a comprehensive overview of water pollution, elaborating on various categories of water pollutants. It also presents an in-depth study of photocatalytic degradation techniques employed in wastewater treatment. The chapter discusses the biophysical interactions of proteins such as Bovine Serum Albumin (BSA) and Human Serum Albumin (HSA) with conducting polymers (CPs) and CP-based copolymers. It further investigates the photocatalytic breakdown of hazardous pollutants using these materials under various irradiation sources (UV, visible, and microwave), highlighting the effectiveness of CPs and their copolymers as organic photocatalysts. Chapter II includes an extensive review of literature focusing on the role of conducting polymer-based copolymers in photocatalytic degradation processes and their interactions with serum proteins. The study reports, for the first time, the microwave-assisted degradation of Methyl Red (MR) dye using polythiophene (PTh), polyfuran (PFu), and their co-oligomers synthesized via ultra sonication in varying molar ratios (PFu/PTh: 80:20, 50:50, 20:80). Spectral and morphological properties of these materials were examined using FTIR, UV–visible, SEM, and elemental mapping techniques. These polymers and co-oligomers were employed as microwave-active catalysts for MR degradation, following a pseudo-first-order kinetic model. The PFu/PTh-50/50 catalyst achieved maximum degradation efficiency of 99%. Radical scavenging experiments confirmed the generation of active species responsible for the degradation, while LC-MS studies elucidated the degradation pathway and identified intermediate fragments. Chapter III focuses on the synthesis of water-dispersible polypyrrole

(WD-PPy) and polythiophene (WD-PTh) copolymers in different weight ratios. These materials were characterized both experimentally (^{13}C -NMR, FTIR, UV-visible) and theoretically using DFT/B3LYP functional and 6-31G(d) basis set via Gaussian 09 software. For the first time, detailed biophysical interaction studies of these polymers with BSA and HSA were conducted. The results revealed strong binding affinities, suggesting potential applications in biosensor development and inhibitor design. Chapter IV reports ultrasound-assisted synthesis of pyrrole-thiophene co-oligomers in different molar ratios (80:20, 50:50, 20:80), and their subsequent characterization using FTIR, UV-Vis, and SEM. The bandgap values ranged from 2.6 eV to 2.9 eV, indicating enhanced photocatalytic potential compared to the pristine polymers. The photocatalytic activity was evaluated for the degradation of Bisphenol A (BPA) under UV light, achieving a maximum degradation of 86% within 120 minutes using the PPy/PTh-80/20 catalyst. Radical scavenging studies and LC-MS analysis supported the proposed degradation mechanism and pathway. The results highlight the superior efficiency of organic photocatalysts over inorganic metal oxide-based systems for BPA degradation in shorter timeframes. Chapter V details the visible-light-induced degradation of 2,4,6-trichlorophenol (TCP) using polyfuran (PFu), polypyrrole (PPy), and their co-oligomers synthesized in varying weight ratios (20:80, 50:50, 80:20). The materials were extensively characterized using UV-visible, FTIR, XRD, EIS, and SEM-EDS techniques. The PFu/PPy-50/50 catalyst exhibited outstanding photocatalytic efficiency, achieving 96% degradation of 40 ppm TCP within just 30 minutes using only 30 mg of catalyst. LC-MS studies provided insights into the degradation mechanism. Additionally, photoluminescence spectra showed distinct emission behavior for furan, polyfuran, and their 1:1 composite (dual peaks at 430 nm and 550 nm), indicating potential optical sensing applications. The study demonstrates the potential of CP-based materials as eco-friendly, sustainable photocatalysts for efficient organic pollutant removal under visible light irradiation.