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Entitled

*SYNTHESIS AND STRUCTURE-PROPERTY RELATIONSHIPS OF SUSTAINABLE NANOSTRUCTURED MATERIALS  
TOWARDS ENERGY AND ENVIRONMENT APPLICATIONS*

by

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Abstract

This doctoral research aims to advance clean energy technologies by developing specialized nanostructured materials. The study covers significant research themes, each forming separate sections in the thesis, explaining the important role of nanostructures in enhancing the efficiency and sustainability of energy devices and photocatalytic technologies.

The enduring effort toward stabilizing and improving the efficiency of dye-sensitized solar cells (DSSCs) has stirred the solar research community to follow innovative approaches. The primary objective of the research is centered on electrode materials design, which improves photoanodes' light-harvesting efficiency (LHE). To improve the Photoanode of DSSCs, a Metal-Organic Framework (MOF) derived porous photoanodes were developed which can effectively absorb dye molecules and improve LHE, resulting in high power conversion efficiency (PCE). Doping is a prospective methodology to tune the bandgap and broaden spectral absorption. Hence, a novel and cost-effective synthesis of high surface area transition metal (TM) doped TiO<sub>2</sub> nanocrystals (NCs) via the MOF route for DSSCs is explored. The TM dopants (i.e., Co, Mn, Fe, Ni), in TiO<sub>2</sub> lead to enhanced light absorption in the visible region. Among the TM dopants, a remarkable PCE of 7.03% was obtained for nickel-doped samples with increased J<sub>sc</sub> (14.66 mA/cm<sup>2</sup>) due to the bandgap narrowing and porous morphology of TiO<sub>2</sub>. As a second objective, platinum nanoparticles (Pt NPs) incorporated into multiwalled carbon nanotubes (MWCNT) composites with lower Pt content were developed as an efficient bifacial counter electrode (CE) material for DSSC applications. Pt NPs were homogeneously decorated over the MWCNT surfaces using a simple polyol method at relatively low temperatures. CEs fabricated using Pt/MWCNT composites exhibited excellent transparency and power conversion efficiencies (PCE) of 6.92 % and 6.09% for front and rear illumination. These results emphasize the significance of tailored nanostructures in optimizing the performance of optoelectronic devices and are expected to bring significant advances in DSSCs.

Furthermore, as a third objective, the developed Iron (Fe) doped MOF derived materials were applied for their performance studies for supercapacitor applications. The pseudo capacitors were fabricated using both TiO<sub>2</sub>/Fe-TiO<sub>2</sub> material as electrodes with KOH electrolyte at 0.6 V and studied the super capacitive performance using CV, GCD, and EIS analysis. A remarkable cycling life of 78% up to 25000 cycles and a superior capacitance of 925 F/g were obtained using the synthesized material. The fabricated asymmetric supercapacitor exhibits supercapacitive performance, favorable rate capability, and exceptional flexibility. The obtained properties demonstrate that nanostructured Fe-doped TiO<sub>2</sub> is an attractive active electrode material for high-performance supercapacitor applications.

As a fourth objective, an efficient composite material based on Ag NPs, MOF-derived Cobalt-doped TiO<sub>2</sub> NPs, and MXene is developed for clean water production via photocatalysis. A simple one-pot solvothermal method fabricated Ti<sub>3</sub>C<sub>2</sub> MXene decorated with MOF-derived Cobalt-doped TiO<sub>2</sub> and Ag nanoparticles (Ag NPs). The composite material combines the unique antibacterial properties of Ag NPs, high absorptive properties of metal-organic framework (MOF)-derived cobalt-doped titanium dioxide (TiO<sub>2</sub>), and catalytic properties of MXene. The resulting composite materials were characterized thoroughly to examine their effectiveness in the photocatalytic degradation of industrial dyes (methylene blue and methyl orange). The results show that 0.025 mg and 0.05 mg of the composite can degrade the MO and MB dyes respectively under the action of sunlight in 60 min.

**Keywords:** Metal organic framework, Dye sensitized solar cell, Electrode material, Doping, Super capacitor, Photocatalysis.