Investigation on Some Metal Phthalocyanine Nanostructures and Their Composites for Multifunctional Applications

Synopsis submitted by

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Synopsis

In recent times, nanoscience and nanotechnology are widely considered as one of the most promising areas of scientific and technological development. They evolve as an important multidisciplinary research field combining various areas of physics, chemistry, biology and engineering. Interestingly, nano-sized materials exhibit significantly enhanced features with respect to their bulk counterparts as a result of their reduced dimension(s) lying in nanometer length scale. In general, nanostructured materials can be categorized as two-dimensional (2D), one-dimensional (1D) and zero-dimensional (0D) materials. In the present dissertation, synthesis and characterization of few 2D and 1D nanostructured materials, and their heterostructures are investigated. The morphological and dimensional modifications of nanomaterials are achieved by varying the synthesis routes. The suitability of synthesized materials in some environment and energy related fields is also examined.

Nanostructures of one class of organic semiconductors, namely metal phthalocyanine (MPc) in its pristine form and their heterostructures with various two dimensional (2D) layered materials *viz.* reduced graphene oxide (*RGO*) and molybdenum disulfide (MoS_2) are first investigated. The reason behind the choice of MPc is that MPcs possess advantages like ease of preparation, low temperature synthesis, low cost, mechanical flexibility, and many more. Thus, a simple room / low temperature chemical route for the synthesis of zinc phthalocyanine (*ZnPc*) and copper phthalocyanine (*CuPc*), and their hybrids is adopted here. The nanostructures of *ZnPc* (nanoflake) and those of *CuPc* (nanowire, nanotube, microrod) are synthesized, and subsequently characterized to find their structural, morphological and compositional descriptions.

As for application of the above synthesized materials in the environmental field, wastewater remediation offers one of the most important prospects. It aims at reduction in water pollution through the color contaminants removal from the industrial wastewater. Organic dyes present in textile wastewater, hamper aquatic animal life as well as human health. For the purpose of dye removal, conventional methods like ultraviolet (UV)/visible light assisted catalysis, ozonation, Fenton are employed using different catalytic materials. The special feature of pristine *CuPc* without any functional group (sulfo, nitro, etc.) is its high hydrophobicity, which makes it unsuitable for catalytic dye degradation through its tendency of lack of mixing in aqueous medium. Thus, performance of the heterostructure synthesized from *CuPc* with *RGO*, as a catalyst in dye removal is examined here. However, in recent years, dye degradation follows new kinds of efficient advanced oxidation processes (AOP) that use the powerful effect of ultrasonic irradiation. Among various AOPs, sonophotocatalysis and sonocatalysis of one textile dye namely, rhodamine B (*RB*) are investigated here respectively using *CuPc* nanowire and *RGO-CuPc*. The influences of different operational parameters *viz.* initial dye concentration, catalyst dosage, dissolved gas, pH, on these processes are also studied. Results establish the superiority of *RGO-CuPc* in the field of ultrasound based catalysis.

Energy has always played a promising role in human survival and civilization. Survey of worldwide energy resources and their consumption indicate that fossil fuels are the primary energy source and take the dominant role in the overall energy consumption. In last few decades, issues related to fossil fuel depletion and uneven distribution of energy resources are of prime environmental concerns. Such ever-increasing energy demand, all over the world, makes exploring alternative renewable natural energy resources like hydro, solar, air, etc. very much essential. Thus, energy conversion, storage and harvesting become the most attractive field of contemporary research. In this dissertation, study of electrochemical supercapacitors (SCs), fuel cells and solar cells based on MPc nanostructures and their hybrids are explored. In case of energy storage, electrochemical performances of some inorganic transition metal oxides as supercapacitor electrode have been well studied, as revealed from existing literature. Electrochemical activities of some substituted MPcs reported so far, have been studied in acidic electrolyte. The activity of unsubstituted MPcs as electrode material is not yet explored. In this dissertation, performances of pristine *CuPc* and *ZnPc* as supercapacitor electrode materials are investigated in alkaline medium. In the context of energy conversion, sluggish nature of oxygen reduction reaction (ORR) in fuel cells calls for the development of efficient electrocatalyst materials. Noble metals such as *Pt*, *Pd* are standard ORR catalysts, but poor stability, high cost and resource scarcity hinder their commercialization. As an alternative, *RGO* and MoS_2 based *CuPc* heterostructures are examined here as ORR electrocatalyst in alkaline medium. MoS_2-*CuPc* heterostructure emerges as more efficient catalyst compared to *RGO-CuPc* hybrid.

Solar cell is one of the important solar energy harvesting systems. Here, organic solar cells (OSCs) with two different absorber materials ($OC_1C_{10}PPV{:}PCBM$ and *P3HT:PCBM*) are simulated using ATLAS Device Simulator (SILVACO). Layers of appropriate materials, termed as transport layers, added to the basic solar cell structure facilitate effective segregation of photo-generated electrons and holes, and improve the cell performance. Thus, role of various transport layer materials, including *CuPc*, and that of carrier mobility in the absorber materials in controlling the cell performance are investigated here. Employing *CuPc* as the hole transport material along with another electron transport layer yields a photo conversion efficiency (PCE) as high as 3 times of that of the basic solar cell. Perovskite based solar cells (PSCs) have already been established as much more efficient compared to OSCs. From some *Pb*-based PSCs, record efficiency of ~ 23% has been reported. But their performance degrades over time under the atmospheric exposure and prevents their commercialization. More importantly, the environmental issues associated with the hazardous effects raised from *Pb*-based materials urge for exploring new *Pb*-free perovskite material as absorber. Thus, simulation of solar cell of cesium based double-perovskite (Cs_2TiBr_6) with various inorganic / organic transport materials are carried out for the first time and presented here. In this case, the PCE of the basic cell gets doubled with the use of *CuPc* as HTL along with another ETL material. The obtained PCE is still low as compared to *Pb*-based PSCs, but much higher than polymer based OSCs. Most importantly, highly hydrophobic nature of *CuPc* makes it popular for the design of moisture stable solar cells, which in turn, enhances the life of solar devices. In addition, the environment friendly nature of such *Pb*-free PSCs is expected to turn them as emerging absorber materials for next generation solar cell.

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