Thesis title: Development of Bismuth Oxyhalide Nanostructures for Photocatalytic and Energy Harvesting Applications

Abstract

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One of the major aims of nanotechnology related research is to use the improved properties of tailored materials for mitigating some of the prominent problems the world is facing currently. Production and utilisation of clean energy and environmental issues are the major concerns for sustainable development. However, for exploiting the huge potential of the nanomaterials for the application in above areas, the utmost need is to synthesise predesigned nanostructures with controlled morphology, structure, phase crystallinity etc. This research was directed to design and develop some controlled route for the synthesis of bismuth oxyhalide nanostructures for fruitful utilisation in the mentioned fields. To address the associated complexities of the synthesis process, property evaluation extensive analyses of the obtained data have to be performed and this was done.

Recent years have seen many advances in research and a variety of approaches aimed at developing efficient, pollution-free technologies to cope with highly polluted and toxic water contaminants and turn them into non-toxic waste removal products. The photocatalysis technology is one of many technologies that has been found to be efficient and environmental friendly because it uses sunlight as a source of artificial light to demineralize pollutants in a sustainable and cost-effective manner. In addition to removing organic pollutants such as organic textile dyes, this pocess can also be used to treat pesticides, herbicides, phenolic compounds, heavy metals, and pathogens like bacteria and fungus. The photocatalysis can also greatly accelerate the biodegradation of organic pollutants. It is also capable of being used in solar harvesting methods.

A new group of material called bismuth oxyhalides has captivated many researchers to its impressive photocatalytic properties. It is a wide band gap (3.2 ~ 3.6 eV) material with layeard tetragonal matlocatic structure. In addition, it has many other lucrative properties including high stability, low cost, and magnetic separation. This group of material has been tested for efficiency, affordability, water spliting and photocatalytic activity in the visible as well as UV spectrum.

As described in this thesis, bismuth oxyhalides and bismuth based materials were synthesised for use in photocatalysis and energy harvesting. The thesis begins with an introduction to the field of nanoscience and nanotechnology (chapter 1), semiconductors, bismuth oxyhalides, catalysis, as well as a quick overview of the synthesis and processing of materials and their various physical properties as well as various applications in catalysis and energy harvesting. In chapter 2, literature is reviewed on the photocatalytic and energy-harvesting applications and synthesis methods of bismuth oxyhalides. An overview of the basic working principles and the essential tools used in all courses of study are discussed in chapter 3.

Contaminated water by various sources such as by textile wastewater can't be used for drinking. In addition to being highly carcinogenic, sewage-polluted water poses a serious threat to human health. There is an urgent need for the degradation and transformation of these harmful pollutants into harmless ones. The purification of wastewater has been accomplished by a variety of strategies. Photocatalysis has been widely accepted among them due to its high efficiency, non-selectivity, and low cost. High recombination rates of photogenerated carriers limit the photocatalytic activity of wide band gap semiconductors. The development of new hybrids with semiconductor coupling, from the perspective of a moderate application perspective, is one of the strategies used to improve the catalytic performance. Chapter 4 describes a simple hydrothermal synthesis strategy to develop sheet like nanocomposite semiconductors composed of bismuth oxychloride and graphene oxide (BOC-GO) that can have spatial separation and absorb light, with efficient photocatalytic degradation about 99.59 % at 60 minutes under visible light irradiations. In chapter 5, bismuth oxychloride (BiOCl) was synthesised by hydrothermal method by variation of citric acid percentage in the precursor which resulted different morphologies. These materials were evaluated for hydrogen evolution reactions with high overpotential about 72 mV/dec (w.r.t. Platinum) and photocatalytic activity about 97.64 % at 10 minutes illumination under visible light for the best material. The chapter 6 presented synthesis of time and temperature varied pure bismuth oxychloride (BiOCl) by heating method (oil bath) with 3D hollow microspheres like structure for highly efficient dye-sensitisation catalytic performance about 98.92 % degradation for only 6 minutes irradiation for the best sample under visible light. The (110) crystal facetes were predominantly exposed and the corresponding lattice planes are the most water absorber, which is calculated from the density functional theory (DFT). In chapter 7, results of photocatalytic dye degradation under UV light illuminations by the pure bismuth oxychloride (BiOCl) nanomaterial synthesised for different times are presented. An impressive performance of about 99.21 % degradation in only 15 minutes was achieved.
Chapter 8 presents a grand summary of the major findings of the thesis and scope of future research work.

Keywords: Bismuth Oxychloride, Graphene Oxide, Nano-composite, Citric Acid, Textile Dye, Hydrogen Evolution, DFT Calculation, Visible-light, UV-light, Photocatalysis, Dye Sensitization, Water Remediation.

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