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Name of the Supervisor: Prof. Tokeer Ahmad

Name of the Department/Centre: Chemistry

Topic of Research: Synthesis, Characterization and Applications of Metal Doped Titanium Dioxide Nanoparticles

Findings

The work of my Ph.D thesis has been on designing nanostructured multifunctional heterogeneous catalysts for photo-, electro, photoelectro-catalytic hydrogen evolution applications, in a broader sense, focusing mainly on synthesis and applications of metal doped titanium dioxide nanoparticles for sustainable energy and environment. The synthesized nanoparticles were characterized to examine their structural and elemental purity, size, shape, specific surface area and optoelectronic properties by using different sophisticated techniques like X-ray diffraction (XRD), Transmission electron microscopy (TEM), scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX), Raman, photoluminescence (PL) spectroscopy, UV-Vis diffused reflectance spectroscopy (UV-Vis DRS) and Brunauer-Emmette-Teller (BET) surface area studies. The complete work of my doctoral thesis is divided into six chapters in which Chapter 1 is introduction which gives the brief overview of the catalysis and properties of nanostructures materials as catalysts. Also, the importance of metal-oxide based nanomaterials in catalysis. The remaining five chapters were experimental ones focusing on different metal doped titanium dioxide. Chapter 2 deals with the synthesis of pristine and Sr doped TiO₂ nanostructures. In this chapter, Pristine TiO₂ and Sr-doped TiO₂ (1%, 2.5% and 5%) nanoparticles were synthesized at low temperatures via an eco-friendly hydrothermal route for water-splitting applications. Chapter 3 deals with the

synthesis of Mg-doped TiO₂ nanostructures via a low-temperature solution route for water splitting application. Experimental investigations deduced that the incorporation of Mg²⁺ ions in the TiO₂ resulted in the increase of hydrogen generation catalytic activity of titanium dioxide owing to the synergistic effect provided by the remarkable surface area and the presence of defects introduced by doping. Chapter 4 deals with the synthesis, characterization and water splitting applications of pristine TiO₂ and 1 to 5% Cu-doped TiO₂ nanoparticles. Here in this chapter, highly efficient nanocatalysts with a high specific surface area were successfully synthesized by the cost-effective environmental friendly hydrothermal method. It was thus revealed that the band gap tuning with the desired dopant concentration ways for enhanced photo/electrocatalytic sustainable energy applications. Chapter 5 discusses the synthesis and structural characterization of pure, 1%, 2.5% and 5% Zn-doped TiO₂ nanostructures for the photocatalytic and electrocatalytic water splitting applications. The synergistic impact of pure TiO₂ and Zn-doped TiO₂ nanocatalysts is responsible for the increased kinetics of H₂ evolution, as it increases the separation and transfer of photo-charged (e^{-}/h^{+} pair) carriers and decreases overpotential values. Chapter 6 deals with the hydrothermal synthesis, structural characterization, photocatalytic and photo-electrocatalytic applications of Ag-doped TiO₂ nanoparticles for overall water splitting activity. Here in this chapter, experiments indicated that the incorporation of Ag ions in TiO₂ boosted the hydrogen generation catalytic activity of TiO₂ due to the extraordinary surface area and the presence of oxygen vacancies/defects.