Abstract

Conventionally synthesized TiO_2 particles are extensively used in paint, plastic, paper and cosmetic industries. In recent years, new synthesis techniques have been developed to control the size, shape, and structure of TiO_2 nanocrystals (NCs) to improve its performance in the emerging applications such as dye-sensitized solar cells, water splitting, supercapacitors, and photocatalysis. In the present work, hydrothermal synthesis technique is employed to control the size, shape, and exposed facets of TiO_2 NCs by varying the reaction parameters. A variety of shapes such as rod-like, capsule-like, cube-like, sheet-like, and ellipsoid-like TiO_2 NCs are synthesized for the first time using greener chemicals. The exposed facets of the NCs are thoroughly analyzed and the facets-dependent photocatalysis of TiO_2 NCs is studied. The photocatalysis is performed through the degradation of organic contaminants such as methylene blue and methyl orange dyes. It is found that the synergy of high-energy [{100} or {001}] and low-energy [{101}] exposed facets in the NCs plays important role for the enhanced photocatalysis. This can be attributed to the oxidizing and reducing nature of high-energy and low-energy facets, respectively, which lead to efficient charge separation under ultraviolet light irradiation. The reducing nature of low-energy {101} facets is further confirmed by selective deposition of noble metals (Au, Ag, and Pt) on the same facets of cuboid shaped NCs by photoreduction process. These noble metal nanoparticles (NPs) exhibit the surface plasmon resonance effect and found to assist in the visible light photocatalysis. Different combination of TiO_2 NCs, reduced graphene oxide (rGO), and Pt NPs composites are synthesized to study the hydrogen evolution reaction. The ternary Pt-TiO_2-rGO nanocomposite shows excellent electrocatalytic behavior with a maximum current density (126 $mA \cdot cm^{-2}$ at 300 mV overpotential), small Tafel slope (~30 $mV \cdot dec^{-1}$), high specific activity (3110 $mA \cdot mg_{Pt}^{-1}$), and high exchange current density (19 $mA \cdot cm^{-2}$). This is ascribed to the synergistic effect of TiO_2 NCs and rGO with former plays superior role than the later. The oxygen evolution reaction (OER) is studied with transition metal (Fe, Co, and Cu) doped TiO_2 NCs. The metal doping is confirmed using the X-ray diffraction, Raman spectroscopy, and Mott-Schottky analysis. A low overpotential for OER is attributed to d-orbital splitting of transition metal. Finally Au deposited TiO_2 NCs are synthesized for electrochemical hydrazine oxidation. The hydrazine oxidation is found to follow two steps suggesting two different mechanisms. In addition, the Au-TiO_2 NCs demonstrates 1.45 times mass activity than that of Au NPs only.

Key Words: Faceted TiO_2 nanocrystals, Hydrothermal synthesis, Photocatalysis, Electrocatalysis, Shape controlling agent, Doped-TiO_2, and TiO_2-based composites.