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Investigation of structural and optical properties of pure and chromium doped TiO_2 nanoparticles prepared by solvothermal method

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ABSTRACT

This paper reports the synthesis of pure and Cr-doped TiO_2 nanoparticles with different doping concentrations by using a cost-effective solvothermal method. The as-synthesized nanoparticles were characterized by using X-ray diffraction, transmission electron microscopy and UV–Vis spectroscopy to study their structural and optical properties. The XRD pattern showed the prepared material is pure anatase of the crystalline phase. Using TEM measurement, the average particles size is found to be about 11–13 nm while selective area electron diffraction (SAED) patterns have confirmed the polycrystalline nature of the nanoparticles. The size of the crystallite is observed to be decreased with an increase in dopant (Cr) concentration. UV–Vis absorption spectra showed enhanced absorption in the visible range in accordance with the doping concentration of Cr with a red shift in the absorption edge. The band gap energy of doped nanoparticles decreases in accordance with an increase in dopant concentration due to the reduced particles size. This presented work would be useful to tune the optical properties of doped and undoped metal oxide TiO_2 for its optoelectronic applications.

Introduction

Presently, titanium dioxide (TiO_2) nanoparticles have got great importance due to its outstanding performance in a wide range of applications. TiO_2 nanoparticles have been widely investigated for its photovoltaics and photocatalysis applications. This material is a large band gap semiconductor oxide with high refractive index and chemically inert, non-toxic, photostable and inexpensive [1–4]. TiO_2 is a versatile material and has been demanded in dye-sensitized solar cells (DSSCs), hybrid organic-inorganic solar cells, polymer solar cells, heterojunctions based solar cells and photocatalysis applications. Dye-sensitized solar cells are one of the promising areas of research in the fields of material science and nanotechnology owing to the easy fabrication, low-cost and good photo-conversion efficiency [5,6]. The photoanode of the dye-sensitized solar cell is made of transparent conducting oxide substrate coated with a wide band gap semiconductor material sensitized with a dye. The promising semiconductor material of choice is TiO_2 because of its optical properties and photostability. However, alternative semiconductor materials such as ZnO, Nb_2O_5 etc. have also been investigated and showed good performance of the DSSCs [7,8]. Several approaches have been developed to modify the structure of photo-anode material for the optimum gain of DSSCs like doping of a metal ion into TiO_2 lattice. Acceptor dopants like chromium, vanadium, iron, copper, zinc etc. doped with TiO_2 have been used to fabricate the photo-anode of DSSCs [9–13].

When the size of the particles is reduced to several nanometer scale it results in a large surface-to-volume ratio with inimitable optical properties. TiO_2 has a tendency to absorb ultraviolet (UV) due to its wide band-gap i.e. 3.0–3.2 eV and therefore, a small portion of the solar spectrum gets absorbed by this material. Further, amazing properties of the TiO_2 can be attained by the metal doping which improves the lifetime of electron-hole and hence, prevents the recombination of photoexcited charge carriers. The purpose of metal-ions doping is to narrowing the band gap with a shift up the valence band or shift down the conduction band of the host material (TiO_2). Metal doping in TiO_2 facilitates the intrinsic properties with enhanced photoresponse in the visible wavelength. As a result, a shift of absorption band from UV to visible region i.e. red shift which has been regarded to the charge-transfer transition between the d electrons of the dopant and TiO_2 conduction band. For the doping, several dopants have been investigated among which metal-ion doping in TiO_2 is widely preferred with the transition metals like Cu, Co, Ni, Cr, Mn, Nb, V, Fe etc. [14–21]. Among these transition metal-ions, Cr is one of the demanded dopants

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