# UNIVERSITI TEKNOLOGI MARA

# CHARACTERISATION AND INFLUENCE OF CERIUM AND CHROMIUM ON THE PHOTOCATALYTIC ACTIVITY OF SOL-GEL DERIVED TITANIUM DIOXIDE UNDER SUNLIGHT RADIATION

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#### ABSTRACT

Semiconductor titanium dioxide is a promising photocatalyst however due its wide band gap only ultraviolet region can be utilized for waste water treatment application. Therefore, in this thesis focuses on the preparation and characterization of pure titanium dioxide, cerium doped titanium dioxide and chromium doped titanium dioxide at doping levels ranging from 0.1 to 1.0 wt%. The primary objective of this study is to narrow the  $TiO_2$  band gap energies in order to enhance the photocatalytic efficiency under visible light. Samples was synthesized via sol-gel method and characterized by X-Ray diffraction method (XRD), Field Emission Scanning Electron Microscope (FESEM) and also UV-Vis diffused reflectance spectroscopy (DRS). The photocatalytic activity under visible sunlight illumination was demonstrated by photocatalvtic decomposition of methylene blue in water using UV/Vis spectrophotometer. XRD pattern of samples heated at 500°C for 4 hours revealed that pure titanium dioxide consists of both polymorphs anatase and rutile. Cerium doping appeared to have inhibited the anatase-rutile phase transformation while Chromium doping resulted in a lower anatase to rutile phase transformation (A-R transformation) at highest Chromium doping. The morphology on doped samples showed conjugated spherical particles. The diffuse reflectance analysis demonstrated that the absorption edge cerium and chromium dopants helped to reduce the band gap energy by shifting towards the visible region. The photocatalytic activity of doped titanium dioxide with lower band gap energy presented higher percentage of methylene blue degradation compared to pure titanium dioxide. However, cerium doping gave better photocatalytic performance compared to chromium doping with energy band gap is 2.79 eV and 89% of degradation methylene blue. Meanwhile, the simple models of cerium and chromium doped titanium dioxide were built to study the influence of both dopants on TiO<sub>2</sub> and the corresponding electronic structures were calculated and consistent with theoretical results by the Density Functional Theory (DFT) method. It can be concluded Ce-doped  $TiO_2$  is a suitable photocatalyst under visible light.

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## CHAPTER ONE INTRODUCTION

#### **1.1 BACKGROUND**

Various organic compounds that are widely used in industrial, agricultural, and domestic fields cause contamination of the environment and must be removed to an acceptable level (Alem & Sarpoolaky, 2010). Generally, there are quite a number of technologies that can be applied to solve such contamination problems such as photocatalysis, fenton and photo-fenton, which have received considerable attention due to their compliance with Green Chemistry concept in promoting innovative technologies that reduce or eliminate the use or generation of hazardous substances (Saepurahman, Abdullah, & Chong, 2010).

Kommineni et al. and Saritha et al. had investigated extensively the fenton process. The fenton process occurred by the production of OH radicals where Fenton reagent synthesized by means of addition of  $H_2O_2$  to  $Fe^{2+}$  salts. Iron was considered as the real catalyst. However, it could lead to complete mineralization of organic compounds and also need very low pH to keep iron in solution. This pH adjustment led to increase in operation and maintenance costs. Photo-fenton technique on the other hand is an extension from fenton process. This process used UV–vis light irradiation at wavelengths higher than 300 nm. The photolysis of  $Fe^{3+}$  complexes allows  $Fe^{2+}$  regeneration and the occurrence of fenton reactions due to the presence of  $H_2O_2$ . Unfortunately, large amounts of chemicals and manpower were required, before treatment, to obtain pH close to 3 in order to prevent ferric oxy-hydroxide precipitation (González-Bahamón, Mazille, Benítez, & Pulgarín, 2011).

Consequently, a lot of research has been published on the use of photocatalysis to remove impurities. This process was said to be capable of converting organic pollutants into harmless chemicals, and ideally, into the final products such as carbon dioxide and water (Alem & Sarpoolaky, 2010). In the past decades, photocatalysis technology has been shown to be another promising method to solve the environmental and energy crisis (J. Xie et al., 2010).