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Tailoring Optical and Crystal Structural Properties of Bismuth Ferrite Based Nanomaterials via Ion Doping for Enhanced Photocatalytic Activity

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Bismuth ferrite based Gadolinium (Gd) modified nano crystallite powder was synthesized by the hydrothermal method. The effects of Gd additive on the phase formation, crystal structure, optical properties, and photocatalytic performance were investigated. Crystal structure, crystallite size and phase formation were used to determine by X-ray diffraction (XRD) technique. Additionally, the structural phase formation was also studied by Raman spectroscopy. Average crystallite size, phase and peak analysis were determined using the X' Pert High Score Plus program. According to the XRD peak pattern, it was determined that the structures of the synthesized sample was formed in the polycrystalline $Bi_{25}FeO_{40}$ (Sillenite) phase. The average crystallite sizes of 3 % Gd modified $Bi_{25}FeO_{40}$ sample was calculated as 50 nm. By using absorption edge data, the bandgap value was determined as 1.98 eV. Photocatalytic performance was evaluated in an environment where methylene blue was used as an organic pollutant, by UV-Vis spectrophotometer under a solar simulator. The photocatalytic efficiency was calculated as 70 %. Such a high efficiency was attributed to increased optical absorption, narrowing band gap, thereby, probably the efficient separation and migration of photogenerated charge carriers. It was concluded that although unintentionally formed Sillenite during synthesis of bismuth ferrite is useful for photocatalysis. Furthermore, it was pointed that the optical properties by means of crystal structure is able to be tailored by doping to increase the photocatalytic activity.

Keywords: *Photocatalytic performance, Optical properties, Crystal structural properties, Bismuth ferrite, Sillenite phase*

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1. Introduction

As the environmental and energy problems faced by humanity increase, the material properties needed to solve them also need to improve. Within this theme, the material that scientists adhere to the most are semiconductors [1].

Science and technology-based industry and industrial production have continuously advanced by utilizing both

surface and underground natural resources to meet the growing needs of humanity. However, this process has led