Analysis of the Structural, Electronic, and Optical Properties of Pure, Mono- and Co-Doped Anatase Type Titanium Dioxide (TiO2) (Co, Ni, N, and S) as a Photocatalytic Material Active in Visible Light

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ABSTRACT

Several aspects of the development of titanium dioxide (TiO2), namely: (a). dye-based photovoltaics (Grätzel cells) and quantum dot-based photovoltaics, (b). photocatalyst which plays a role in purifying the water and air environment, (c). photohydrophilicity (superhydrophilicity), namely the development of surface active hydrophiles by sunlight and ultra violet (UV) and (d). anti-bacterial. To improve the performance of TiO2, by shifting the light performance, namely from ultra violet light to visible light. This performance shift is carried out through doping TiO2 with metal atoms (Co, Ni) and non-metal atoms (N, S). Based on this, this research aims to determine the effect of mono- and co-doped metal atoms (Co and Ni), non-metal atoms (N and S) contained in anatas type titanium dioxide (TiO2) on the structure (lattice parameters), electronic properties (band gap energy values and density of state (DOS), and optical properties. Implementation of energy calculations or analysis of structural, electronic and optical properties using the CASTEP code. Data obtained through the density functional theory (DFT) approach with generalized gradient approximation from Perdew-Burke-Ernzerhof for solide (GGA+PBESol) as a change correlation function in the form of a graphic plot of the band structure of pure, mono- and co-doped TiO2 (Co, Ni, N, S). The graph is further processed further to obtain information about the magnitude of the band gap energy (Eg) and density of states (DOS) of the material

Kata Kunci: *Anatase, Gap Energy, Valence band, Conduction Band*