ANALYSIS OF GAP ENERGY AND ELECTRONIC STRUCTURE OF PEROVSKITE LAYER NaLnTiO4 (Ln = Y, La, Nd) WITH DENSITY FUNCTIONAL THEORY APPROACH AS CANDIDATE SOLAR CELL AND ANTI-BACTERIA

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ABSTRACT

Utilization of solar energy in the development of renewable energy and antibacterials faces several challenges, namely to increase efficiency and reduce production costs. On this basis, it is very important to develop materials related to the use of sunlight to be applied in solar cells and antibacterials. Based on the foregoing, this research analyzes the perovskite layer NaLnTiO4 material and its derivatives, namely $NaY_{(1-x)}La_xTiO_4$ and $NaLa_{(1-x)}Y_xTiO_4$ (x = 0.25 , 0.50 and 0.75) which is stated in the following objectives: (1). Knowing the effect of the initial calculation method, namely local density approximation (LDA) and generalized gradient approximation from Perdew-Burke-Ernzerhof (GGA+PBE) on the value of bandgap energy and density of states (DOS) in NaLn(1-x)LxTiO4. (Ln = Y, La and L = La, Y), and (2). Knowing the effect of variations in the concentration of Lanthanum (La) on the band gap energy and density of states (DOS) on $NaY_{(1-x)}La_xTiO_4$ and $NaLa_{(1-x)}Y_xTiO_4$ (x = 0, 0,25 , 0,5 , and 0.75). Implementation of calculation of band gap energy and electronic structure using CASTEP code. Data obtained through density functional theory (DFT) approach with local density approximation (LDA) and generalized gradient approximation from Perdew-Burke-Ernzerhof (GGA+PBE) as a change correlation function in the form of a graph plot of the band structure of NaLnTiO4 and its derivatives $NaLn_{(1-x)}L_xTiO_4$ (Ln = Y, La, Nd). The graph is further processed to obtain information about the band gap energy (Eg) and density of states (DOS) of the material. The results of the calculation of the band gap energy of NaYTiO4 and $NaY_{(1-x)}La_xTiO_4$ (x = 0.25 , 0.50 and 0.75) with variations in the concentration of Lanthanum and LDA as a function of the correlation of changes obtained respectively 3.447 eV, 3.384 eV, 3.356 eV, and 3,560 eV. Calculations using GGA+PBE as a correlation function of changes resulted in band gap energies of 3,250 eV, 3,039 eV, 2,963 eV, and 2,930 eV, respectively. The results of the calculation of DOS characters for all samples show that the valence band is dominated by O-2p atomic orbitals and the conduction band is dominated by Ti-3d atomic orbitals. Substitution of the La atom at the Y site atom cannot produce an intermediate band, but only widens or narrows the band gap at $NaLa_{(1-x)}Y_xTiO_4$ (x = 0.25 , 0.50 and 0.75). The results of this study indicate that NaLaTiO4 and its derivatives have an indirect band gap type. The DOS character in this study shows the main role of the O 2p and Ti 3d atomic orbitals. NaLaTiO4 has a band gap energy of 3,742 eV (LDA) and 3,630 (GGA+PBE). In the NaLaTiO4 derivative, band gap energy values ??are obtained in the range of 3,492 eV to 3,678 eV with LDA and GGA+PBE as a correlation function of change. The LDA calculation method has a higher band gap energy than GGA+PBE. $NaLaTiO_4$ and its derivatives can be applied as power plants, catalysts, and batteries, considering the properties of the products.

Kata Kunci: *NaYTiO4, NaLaTiO4 Initial Principle Calculation, DFT, Bandgap Energy, DOS*