First Calculation Study of the Electronic Structure of Semiconductor Titanium Dioxide (TiO2) Anatase Type doped by Metals and Non-Metals: Ti(1-x)MxO(2-y)Ly with (M = V, Cr and L = N, C) as Candidates Photocatalyst Material, Photohydrophilicity and Photovoltaic

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ABSTRACT

The use of solar energy in the development of renewable and antibacterial energy faces several challenges, namely to increase efficiency and reduce production costs. Based on this, it is very important to develop materials related to the utilization of sunlight for application as solar cell materials, antibacterial and superphotohydrophilicity. Based on this, this research was carried out to develop anatase type semiconductor material titanium dioxide (TiO2) and its derivatives: Ti(1-x)MxO(2-y)Ly (M = V, Cr and L = N, C with x = 0 .00; 0.25; 0.5 and y = 0.5; 0.25; 0.00). The research was planned for 1 year with the aim of knowing the bandgap energy and electronic structure or density of state (DOS) in the anatase type TiO2 semiconductor based on initial calculations (ab initio) because: (1). the influence of the type and percentage of metal exchanging atoms, namely V and Cr, (2). the effect of the type and percentage of non-metallic exchanging atoms, namely N and S, (3). the effect of the type and percentage of metal (V, Cr) and non-metal (N, C) exchanging atoms simultaneously.

The generalized gradient approximation from Perdew-Burke-Ernzerhof (GGA+PBE) is used to describe the exchange-correlation functional. A cutoff energy field wave of 500 eV and k-point: 10x10x 4 (these results were obtained from optimizing the cutoff energy and k-point of anatase TiO2 crystals). Electronic structure and DOS calculations were performed for unt cells: 1x1x1, and super cells: 2x1x1 and 2x2x1 respectively on TiO2 crystals of metal V, Cr and non-metallic N, C.

Based on the results of theoretical calculations using the density functional theory (DFT) approach and generalized gradient approximation from Perdew-Burke-Ernzerhof (GGA+PBE) it can be concluded (1). The Cr atom scavenger in TiO2-anatase has a bandgap energy that is always smaller than that of the V atomic cradle at various percent of similar concentrations. The addition of a 4.06% Cr atom fragment has resulted in a band gap energy in the visible region of 2.377 eV, while the addition of a 3.98% V atom gap has resulted in a bandgap energy in the visible region of 2.917 eV. The smallest band gap energy of 1.663 eV was produced from 32.55% of Cr atoms in TiO2-anatase, while the smallest band gap energy of 2.397 eV was produced from 31.89% of V atoms in TiO2-anatase; and (2). The N atom scavengers in TiO2-anatase have a band gap energy that is always smaller than the C atom scavengers at various percent of similar concentrations. The addition of a 0.94% C atomizer has produced a band gap energy in the visible region of 1.92 eV, while the addition of 1.095% of an N atom has resulted in a bandgap energy in the visible region of 1.85 eV. The smallest band gap energy of 1.54 eV is produced from 4.38% of N atoms in TiO2-anatase, while the smallest band gap energy of 1.74 eV is produced from 3.75% of V atoms in TiO2-anatase

Kata Kunci: *Anatase, Gap Energy, Electronic Structure*