

Title: Tuning the potentials of aluminum phosphide nanotube photocatalyst for wastewater treatment through band gap engineering: a DFT study

Author Names: Yahaya Saadu Itas, Razif Razali, Mayeen Uddin Khandaker and Imed Boukhris

Abstract: The photocatalytic properties of semiconductor materials, which are controllable through the design of the bandgap structure, make them a promising catalyst for wastewater treatment. This work investigated the photocatalytic properties of single-walled aluminum phosphide nanotube (SWAIPNT) doped with different concentrations of boron (B) atoms for wastewater treatment. Analysis of the structural, electronic and optical properties of the SWAIPNT photocatalyst was performed using the density functional theory approach in terms of plane wave basis set and pseudopotential. SWAIPNT was found to be stable to B doping with 3.6% and 7.1% concentrations. The obtained formation energy values of 12.33 eV, 12.00 eV and 11.98 eV and also cohesive energies of -0.82 eV, -0.75 eV and 0.79 eV for pristine, 3.6% and 7.1% B-doped SWAIPNTs, revealed the systems' well mechanical and thermodynamic stabilities. Results also revealed that cohesive energy decreases with an increase in concentration of B dopant, which significantly enhances efficient thermal stability. Electronic band gap calculations revealed that pristine SWAIPNT demonstrated a direct band gap value of 0.2 eV. Due to B doping, an indirect band gap value of 1.4 eV was obtained with 3.6% B-doped SWAIPNT, which agreed well with band gaps of other photocatalysts used for wastewater purification. Analysis using optical absorption spectra revealed that 3.6% B-doped system absorbs visible light while 7.1% doped system absorbs both visible and ultraviolet light. This study found both 3.6% and 7.1% B-doped SWAIPNT as suitable photocatalysts for wastewater treatment under solar irradiation, with the 3.6% B-doped system demonstrating relatively better performance for wastewater treatment.

Keywords: Single-Walled Aluminum Phosphide Nanotube (SWAIPNT) Boron Doping Density Functional Theory (DFT) Electronic Band Gap Engineering Optical Properties

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