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New trends in the electronic and optical properties of single walled carbon-boron nitride nanotubes (swcbnnt)/mos2 hetero-junctions for optoelectronics

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The design and construction of novel materials for optoelectronics and high computing resources has been proved possible through the creation of new band gap for example by doping a zero band gap material with a wide band gap material. However, the creation process through experimental means consumes time, expensive and tedious. It can also lead to failure due to limited materials. In order to curve this problem, scientists adopt theoretical modelling by appropriately applying computing tools to help narrow down the choices of materials so that the probability of success in experimental work can be achieved. The DFT in terms of quantum ESPRESSO and TDDFT in terms YAMBO approach in this research will be used to calculate the actual electronic and optical properties of the nano-sized SWCBNNT/MoS2 hybrid structures. The use of DFT in the calculation of material properties such as electrical, optical, mechanical and structural properties has been the most effective way by researchers of Nano science and technology. It helps predict potential novel candidate for specific applications. The computational methods employed in solving the electronic Schrödinger equation is the Ab-initio quantum methods coupled with Hartric Fork and GW-BSE. This method will help predict the electron density, absorption energy of the system and other optimized structural properties. Through the studies of literature, we have been able to find consistent variations of data between the experimental and the theoretical/computational results on the structural, optical, electronic, mechanical and thermal properties of one dimensional materials. For example, the studies of the optoelectronic properties of SWCNT and SWBNNTs were carried out only in the parallel directions to the nanotubes. The effect of eefects of diameter on the electrical band gaps were only studied on the individual SWCNTs and SWBNNTs not on the hetero combinations of SWCBNNT, the electrical and optical behaviors of new system of (5, 5) CBNNT have not been reported yet. In order to amend the gap between SWCBNNT semiconductivity and MoS2, we try to fabricate a hybrid system of SWBNNT and MoS2 interface called carbon-boron nitride nanotubes (CBNNTs)/MoS2 by computational coupling of SWCBNNT and MoS2 so that we create a small band gap smart material. With the successful hybridization of the SWCBNNT/MoS2 hetero-system, we will be able to produce smart materials for optoelectronics that resist high temperature such as high temperature batteries, sensors, high temperature transistors and ICs and also durable LED lights.

Biography

Yahaya Saadu Itas is a Ph.D Research Fellow in Federal University, Dutse-Nigeria. He is currently undergoing a visiting schoalar progrm at the Universiti Teknologi Malaysia (UTM), he has completed his Master Degree at the Liaoning University of technology China. He is currently a director research on computational conensed matter physics at the department of physics, Bauci State University, Gadau. Yahaya Saadu Itas specializes on fabricating new ideas especially in quantum computational nano science and technology so that new generaations of nano matrials can be intoduced to the next generations optoelecronics