7th International Conference on
Smart Materials and Sustainable Technologies
April 08-09, 2019 | Toronto, Canada

VIDEO PRESENTATION | **DAY 2** *JOURNAL OF MATERIAL SCIENCES & ENGINEERING 2019, VOLUME 8 | DOI: 10.4172/2169-0022-C3-131*

Ab initio study of polytypism in ZnS, ZnSe and ZnTe

Akinola Samson Olayinka[1], Wilson Nwankwo[2] and Kingsley Eghonghon Ukhurebor[1]

[1]Department of Physics, Edo University Iyamho

[2]Department of Computer Science, Edo University Iyamho.

Ab-initio study of polytypism in ZnS, ZnSe and ZnTe was carried out within the popular density functional theory (DFT). The structural, electronic and optical properties of cubic zinc blende (ZB) and hexagonal wurtzite (W) polytypes of II-VI compounds: ZnS, ZnSe and ZnTe were obtained. Calculated properties were discovered to be influenced by the bonding structure of the polytypes. Electronics structure provides insight into the optical properties of the polytype. The results obtained for the optimized lattice parameters and round state energy as well as the band energies are comparable with available experimental results.

Biography

A.S. Olayinka is a Senior lecture in the Department of Physics, Edo University Iyamho, Nigeria. He has Ph.D in Physics. His research focus is the application of modern theoretical concepts of materials based on the quantum theory of solids and powerful computational methods to realistic situations. He uses various theoretical and computational tools to address societal needs, such as the development of novel materials for efficient solar application, materials for better energy storage, materials for thermoelectric applications and biomaterials.He has over 25 publications to his credit and has been serving as a reviewer to many journals.

akinola.olayinka@edouniversity.edu.ng