# Effect of the core thickness on the physical properties of $ZnO/TiO_2$ core/shell nanostructures: First-principles study

Slimane HAFFAD

*Département de Technologie, Faculté de Technologie, Université de Bejaia, Algerie*

In this work, we employed density functional theory [1] to study the effect of ZnO thickness on the physical properties of $ZnO/TiO_2$ core/shell nanostructures and their impacts when these structures are used in photocatalytic or photovoltaic systems [2]. We varied the thickness of the core from 4 to 16 A°. The effect of the thickness on the electronic and mechanical properties was analyzed at GGA and GGA+U levels. The results show a non-uniform variation in the energy gap of the core/shell nanostructure suggesting a compensating mechanism due to the electronic defect states [3]. A larger energy gradient between the conduction band of ZnO and the conduction band of $TiO_2$ was observed which favors the transfer of the excited electrons from ZnO to $TiO_2$, in agreement with experiments [4]. However, the heterostructure shows a good resistivity even for a very fine core thickness. With such thin core/shell structures, the ratio of surface/volume can be increased and a longer exciton lifetime is expected when they are used in dye sensitized solar cells (DSSCs)[2].

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[3] S. Haffad, G. Cicero, and M. Samah, arXiv:1702.02545v1 [physics.comp-ph].

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