First principles study electronic properties of (110) surface GaAs/GaN nanowires

Y. Chaib[1] *, S. Benmokhtar[1], M. Moutaabbid[1], P.E. Hoggan [2], C. Robert-Goumet[2]

[1]*University of Casablanca, Laboratory of Chemistry and Physics of Materials LCPM, Faculty of Sciences, Department of Chemistry, Casablanca, Morocco*
[2] *Institute Pascal, UMR 6602 CNRS, University Blaise Pascal, 4 avenue Blaise Pascal, TSA 60026, CS 60026, Aubiere Cedex, France*

*e-mail : younesschaib@gmail,com

Abstract:

GaAs one of III-V compound semiconductor nanowires that exhibit direct band gap has attracted much attention of researchers due its potential application in the field of optoelectronic and microelectronic devices like photovoltaic cells, photo detectors, modulators, filters, integrated circuits and light emitting diodes [1,2], it has been widely studied both experimentally and theoretically, a fundamental understanding of its physical properties is still in demand of this novel material. During the manufacture of its nanowires, their surfaces present anomalies which bound to Ga-free broken bonds which are easily interacted with the environment and they oxidize for remedy this problem. We passivated these surfaces by the nitrogen for saturating their surfaces.

Motivated by the available literature on GaAs according to the crystalline plane (110), we carried out calculations for structural and electronic properties of GaAs in its stable zinc-blende phase using full potential linearized augmented plane wave method (FP-LPAW) designed within DFT. After that, we will passivate these nanowires by the nitrogen; we study the nutrient effect on their physical properties (GaAs / GaN) by keeping the same theoretical model used previously from a similar study that has been carried out on plane surfaces of GaAs showed that nitridation phenomena leads to the deposition of a thin layer of GaN and confers passivated to the solid [3].

[1] Y. Li, F. Qian, J. Xiang, C. M. Lieber, "Nanowire electronic and optoelectronic devices," Mater.
Today, vol. 9, pp. 18-27, Oct 2006.

[2] F. Patolsky, C. M. Lieber, "Nanowire nanosensors," Mater. Today, vol. pp. 20-28, April 2005.

[3] H. Mehdi, G. Monier, P.E. Hoggan, L. Bideux, C. Robert-Goumet , V.G. Dubrovskii, "Combined angle-resolved X-ray photoelectron spectroscopy, density functional theory and

kinetic study of nitridation of gallium arsenide," Applied Surface Sciences ,vol, 427, pp, 662-669, January 2018