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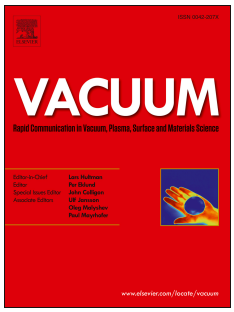

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Mudar Ahmed Abdulsattar, Mohammed T. Hussein, Tasneem H. Mahmood

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Stability, electronic and vibrational properties of GaAlN wurtzoid molecules and nanocrystals: A DFT study

Mudar Ahmed Abdulsattar[1*], Mohammed T. Hussein[2], Tasneem H. Mahmood[3]

[1]Ministry of Science and Technology, Baghdad, Iraq
[2]Department of Physics, College of Science, University of Baghdad, Baghdad, Iraq
[3]Department of Physics, College of Science for women, University of Baghdad, Baghdad, Iraq
*Corresponding author Tel.: +964 7901335231, E-mail: mudarahmed3@yahoo.com

Abstract

Electronic structure and vibrational characteristics of GaAlN wurtzoids at the molecular-nanoscale limit are investigated. The investigated properties include energy gap, vibrational properties, and phase stability against transition to GaAlN diamondoids. At the molecular-nanoscale limit, wurtzite GaAlN nanocrystals are represented by wurtzoids. The properties of GaAlN molecules and nanocrystals as a function of Ga and Al contents are shown. The results show that the energy gap depends on size, shape and surface conditions. Molecules with hydrogen passivated surface have wide energy gap while bare molecules have smaller energy gaps. On the other hand, vibrational longitudinal optical mode of bare molecules experiences a redshift after surface hydrogen passivation with smaller vibrational reduced masses and force constant at a given frequency. Differences between GaAlN two limits (GaN and AlN) are explained by the existence of d orbitals in Ga atoms. Calculated Gibbs free energy of atomization show the stability of wurtzoids against transition to the diamondoids at the molecular-nanoscale limit for both bare and hydrogen passivated cases.

Keywords: AlGaN; nanocrystals; wurtzite; zincblende.

Introduction

Gallium aluminum nitride or aluminum gallium nitride (GaAlN or AlGaN) is recently under focus due to its use in producing semiconductors of 3.4 to 6.2 eV direct energy gap depending on its alloy composition [1]. As a result of its wide gap, this alloy is used in blue to ultraviolet light emitting diodes (LEDs) [2]. For the same reason, GaAlN can also be used as an ultraviolet light detector [3]. GaAlN heterostructures can be made in combination with other semiconductors such as GaN, AlN or InN [2]. Vibrational spectroscopy (such as IR and Raman) is one of the frequently used methods to explore materials specifications. Longitudinal optical (LO) mode is normally the highest intensity mode in its vibration frequency region. The value of the experimental LO mode for GaAlN varies between 748-831 cm^{-1} corresponding to the two limits of GaN and AlN respectively [4,5].

A new trend in modeling bulk solids and crystals is to use molecules at the molecular-nanoscale limit to represent solids or crystals. These molecules have structural and surface properties or specifications that are very close to the original bulk solid and its surface. Examples of these molecules include wurtzoids, diamondoids, cuboids, nanotubes and other molecular cages [4, 6-8]. This method was applied successfully to simulate reactions, energy gaps and vibrational properties of solids [6-8]. The results of