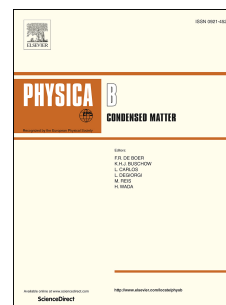


Accepted Manuscript

Conduction-and valence band offsets of $\text{Zn}_{1-x}\text{Mg}_x\text{Se}/\text{Zn}_{1-y}\text{Mg}_y\text{Se}$ heterointerfaces

O.A. Al-Hagan, N. Bouarissa, A. Gueddim, H. Algarni, T.F. Alhuwaymel, M.Ajmal Khan



PII: S0921-4526(18)30351-X

DOI: [10.1016/j.physb.2018.05.019](https://doi.org/10.1016/j.physb.2018.05.019)

Reference: PHYSB 310881

To appear in: *Physica B: Physics of Condensed Matter*

Received Date: 9 March 2018

Revised Date: 11 May 2018

Accepted Date: 12 May 2018

Please cite this article as: O.A. Al-Hagan, N. Bouarissa, A. Gueddim, H. Algarni, T.F. Alhuwaymel, M.A. Khan, Conduction-and valence band offsets of $\text{Zn}_{1-x}\text{Mg}_x\text{Se}/\text{Zn}_{1-y}\text{Mg}_y\text{Se}$ heterointerfaces, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.05.019.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Conduction-and valence band offsets of $\text{Zn}_{1-x}\text{Mg}_x\text{Se}/\text{Zn}_{1-y}\text{Mg}_y\text{Se}$ heterointerfaces

O. A. Al-Hagan¹, N. Bouarissa^{2,*}, A. Gueddim³, H. Algarni^{1,4}, T. F. Alhuwaymel⁵, M. Ajmal Khan¹

¹Department of Physics, Faculty of Science, King Khalid University, P. O. Box 9004, Abha 61413, Saudi Arabia

²Laboratory of Materials Physics and Its Applications, University of M'sila, 28000 M'sila, Algeria

³Materials Science and Informatics Laboratory, Faculty of Science, University of Djelfa, 17000 Djelfa, Algeria

⁴Research Center for Advanced Materials Science (RCAMS), King Khalid University, P. O. Box 9004, Abha 61413, Saudi Arabia

⁵National Centre for Nanotechnology, King Abdulaziz City for Science and Technology (KACST), P. O. Box 6086, Riyadh 11442, Saudi Arabia

Abstract

Based on the model-solid theory coupled with a pseudopotential approach within the virtual crystal approximation, the conduction and valence band offsets (CBO) and (VBO) of the unstrained and strained $\text{Zn}_{1-x}\text{Mg}_x\text{Se}/\text{Zn}_{1-y}\text{Mg}_y\text{Se}$ heterointerfaces have been investigated. The calculated elastic constants C_{11} and C_{12} for ZnSe and MgSe are found to agree to within 7% with experiment. Our findings showed that for electrons the CBO is negative whereas the Mg content of the overlayer (x) is lower than the Mg content of the substrate (y). Nevertheless, the reverse can be seen when $x > y$. As regards the light-and heavy holes the VBOs remain negative as far as the Mg concentration of the overlayer is lower than that of substrate layers and become positive in the opposite case. The alignment of the bands is found to be of type II (staggered) whatever is the Mg compositions of both the overlayer and the substrate layer. The relaxed and strained band-gap energies versus the composition y have been computed and the results are examined and discussed.

Download English Version:

<https://daneshyari.com/en/article/8160389>

Download Persian Version:

<https://daneshyari.com/article/8160389>

[Daneshyari.com](https://daneshyari.com)