

Accepted Manuscript

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PII: S2352-2143(18)30206-5

DOI: [10.1016/j.cocom.2018.e00337](https://doi.org/10.1016/j.cocom.2018.e00337)

Article Number: e00337

Reference: COCOM 337

To appear in: *Computational Condensed Matter*

Received Date: 4 July 2018

Revised Date: 25 August 2018

Accepted Date: 24 September 2018

Please cite this article as: B.-e.N. Brahmi, T. Ouahrani, R.M. Boufatah, R. Boudefla, S. Bekhechi, Abdelkrim.Elhasanaï. Merad, Results of physical bowing parameters of $\text{ZnSe}_x\text{Te}_{1-x}$ ternary semiconductor from ab initio study, *Computational Condensed Matter* (2018), doi: <https://doi.org/10.1016/j.cocom.2018.e00337>.

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Results of physical bowing parameters of $\text{ZnSe}_x\text{Te}_{1-x}$ ternary semiconductor from ab initio study

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Abstract

Based on ab initio calculation, the structural, electronic and optical properties of $\text{ZnSe}_x\text{Te}_{1-x}$ ternary alloys have been studied using (FP-LAPW) approach. The calculations yielded a lattice parameter and bulk modulus that commonly agree well with experience when they are estimated within the Wu and Cohen-generalized gradient (WC-GGA) scheme. Besides, noticeable improvements in the prediction of electronic and optical properties were found by using the (WC-GGA) plus the modified Becke-Johnson potential parameterization. Strong nonlinear behavior characterizes the evolution of the band gap as a function of the Selenium atomic-composition increment. The positive optical bowing parameter is found in good agreement with the experience. Additionally, the topological analysis of the electronic localization domain indicates a delocalization of charges when the x -concentration to the Se atom is raised. We find that this delocalization is more related to optical properties evolution than to the widening of the energy gap.

Keywords: Bowing parameter, Opto-electronic properties, Structural properties, ternary semiconductor alloys.

2010 MSC: 00-01, 99-00

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