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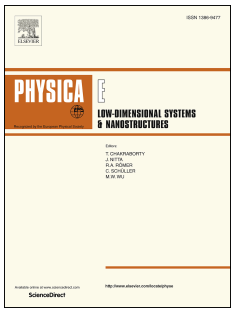

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Asad Ali, Gul Rahman, Tahir Ali, M. Nadeem, S.K. Hasanain, M. Sultan

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Enhanced band edge luminescence of ZnO nanorods after surface passivation with ZnS

Asad Ali[a,b*], Gul Rahman[c], Tahir Ali[d], M. Nadeem[d], S.K.Hasanain[e], M.Sultan[*b]

(a) *Preston Institute of Nanoscience and Technology, Preston University, Islamabad, Pakistan*
(b) *Nanoscience and Technology Department, National Centre for Physics, Quaid-I-Azam University Campus, Islamabad, Pakistan*
(c) *Department of Physics, Quaid-i-Azam university, Islamabad* 45320, *Pakistan*
(d) *Physics Division, PINSTECH, Nilore, Islamabad, Pakistan*
(e) *COMSTECH Secretariat, 33 Constitution Avenue, G-5/2, Islamabad*

Correspondence: asadqau88@gmail.com sultan@ncp.edu.pk

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Abstract

We report on the passivation of surface defects of ZnO nanorods by surface layer deposition. ZnO nanorods and ZnS-ZnO hybrid nanostructures are grown on FTO coated glass substrate by chemical bath deposition method. XRD spectrum of ZnO nanorods shows the preferential growth along the *c*-axis. SEM analysis confirms the nearly aligned growth of the ZnO nanorods with a hexagonal shape. XPS measurements were performed to confirm the deposition of the surface layer and surface stoichiometry. Room temperature photoluminescence of ZnO nanorods showed two emission bands, viz. the band edge emission and the blue-green emission, with the latter being associated with the defect states arising from the surface of ZnO nanorods. The band edge emission is significantly increased as compared to blue-green emission after ZnS surface layer deposition on ZnO nanorods. The quenching of blue-green emission is explained in terms of reduced surface defects after ZnS deposition. Density functional theory (DFT) calculations are used to understand the mechanisms of defect passivation in ZnS-ZnO nanostructures and we show that the S atoms prefer the O site as compared with the Zn and interstitial sites.

1. Introduction

ZnO nanostructures have attracted considerable attention due to their excellent electrical and optical properties. These properties make ZnO one of the suitable materials for use in next-generation optoelectronic devices [1]. ZnO is a nontoxic material and can be synthesized using cost-effective solution process such as Chemical Bath Deposition (CBD) method. ZnO based nanostructures have wide range of applications in a device technology. They have been used in photovoltaics in different device architectures such as in planar and rod like geometries. ZnO nanostructures are also been used in gas and bio sensors, transistors, optically pumped lasers,