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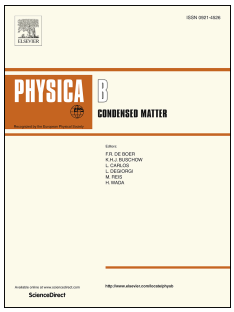

Fabrication, characterization and simulation of Zn-doped PbS nanopowder

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PII: S0921-4526(18)30427-7

DOI: 10.1016/j.physb.2018.06.026

Reference: PHYSB 310934

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

Received Date: 21 May 2018

Revised Date: 20 June 2018

Accepted Date: 21 June 2018

Please cite this article as: M. Liu, W. Li, Y. Wang, Q. He, Fabrication, characterization and simulation of Zn-doped PbS nanopowder, *Physica B: Physics of Condensed Matter* (2018), doi: 10.1016/j.physb.2018.06.026.

Fabrication, characterization and simulation of Zn-doped PbS nanopowder

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Abstract

The Zn-doped PbS nanopowder (NP) is fabricated by the surface growth in the solution phase and cation substitution method. The structure and morphology of NP are characterized by XRD, TEM and EDX. Electronic structure of Zn-doped PbS is investigated using first-principles calculations based on the density functional theory. It is found that Zn-doping in PbS will reduce the band gap, increase the valence bands degeneracy, and lead to the transition from direct band gap to indirect band gap. The interaction among Zn(4s), S(3p) and Pb(6p) orbitals plays a crucial role in the band modulation of Zn-doped PbS. The interesting band structure change due to the impurity can have a significant effect on the physical properties of PbS based material, such as optical and thermoelectric properties.

Keywords: Zn-doped PbS nanopowder; band structure; direct-indirect band gap transition; fabrication

1. Introduction

The lead sulfide (PbS) is an important narrow direct band gap semiconductor with many excellent physical and chemical properties [1-4]. It is widely concerned

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