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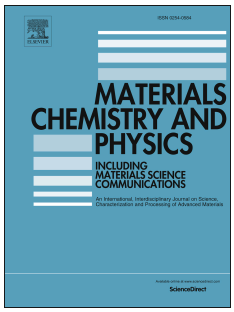

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Electronic structure of wurtzite $Tl_xIn_{1-x}N$ alloys

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Abstract

The structural and electronic properties of wurtzite $Tl_xIn_{1-x}N$ materials have been investigated from first principles within the density functional theory (DFT). Band structures were obtained with the modified Becke-Johnson (MBJLDA) approach. A narrow band gap of 63 meV, induced by a strong spin-orbit coupling, is predicted in the hypothetical thallium nitride. The band gap inversion in TlN suggests that this compound is a promising candidate for a topological insulator. The lattice parameters of $Tl_xIn_{1-x}N$ alloys exhibit a linear behavior as a function of a Tl content x. An incorporation of Tl atoms in these systems leads also to a linear decrease of a band gap. For $x > 0.3$ a very narrow energy gap, analogous to that of the pure TlN, is revealed. The band gap reduction of 26 meV/%Tl is comparable in value to those reported in the literature for dilute Bi-doped GaSb and InSb. The Tl-doped InN systems are promising materials for infrared optoelectronic devices.

Keywords: semiconductor alloys, nitrides, electronic structure, crystal structure, ab-initio calculation

1. Introduction

The investigations of Bi-doped III-V semiconductors have shown that such materials exhibit a rapid reduction of a band gap as a function of a Bi content [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. The presence of Bi atoms in these systems leads also to a strong enhancement of spin-orbit coupling (SOC), which enlarges a separation between the heavy hole and the split-off

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