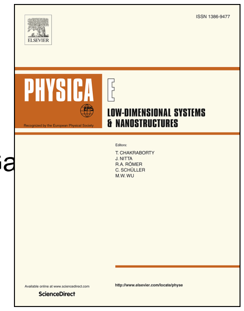
Accepted Manuscript



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PII: S1386-9477(17)31263-8

DOI: 10.1016/j.physe.2018.05.015

Reference: PHYSE 13146

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received Date: 18 August 2017

Revised Date: 23 March 2018

Accepted Date: 18 May 2018

Please cite this article as: N. Nik-Akhtar, A. Vaez, Topological phase and optical properties of bulks and nanolayers of ScNiX (X = Ga and In) half-Heusler compounds, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.05.015.

Topological phase and optical properties of bulks and nanolayers of ScNiX (X= Ga and In) half-Heusler compounds

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Abstract

In this paper, topological phase and optical properties of bulks and nanolayers (NLs) of the ScNiX (X= Ga and In) half-Heusler compounds have been studied. The calculations have been done based on the density functional theory in the framework of the Wien2k package. The generalized gradient approximation was used for the exchange-correlation functional. Electronic structures and density of states of the bulks and NLs of the compounds show that, they are non-magnetic and metal. It is found that, the bulks of compounds don't have topological phase, but the NLs of compounds have topological phase. Thus, the NLs of both compounds are topological metals. Important optical properties of these compounds were acquired. The results show that, there is optical anisotropy in the NLs, between the in-plane (x) and out-of-plane (z) directions. The absorptions of the bulks and NLs of the compounds are high in the UV range.

Keywords:

Half-Heusler compounds; Nanolayers; Density functional theory; Topological phase; Optical properties

1. Introduction

The ScNiX (X= Ga and In) compounds are half-Heusler compounds. Heusler compounds discovered in 1903, when Fritz Heusler, German engineer and chemist, discovered Cu_2MnAl alloy that was ferromagnetic, even though any of its constituent elements don't have magnetic properties [1]. Generally, chemical formulas of full-Heusler and half-Heusler compounds are A_2BC and ABC, respectively. The A and B atoms are from the rare earth or transition metals, and the C atoms are from the main group elements, that are non-magnetic [2]. The Heusler compounds crystallized in the face centered cubic (Fcc) structure. They are widely used in many fields such as: spintronics [3], construction of tunable band gap semiconductors [4, 5] and topological matters [6-9] with a high Curie temperature. Topological matters are new quantum materials which have protected boundary states. These matters are insulating (topological insulator), semiconducting (topological semiconductor) and metal (topological metal) in their bulks, but they are nearly perfect metal in their boundaries. Topological matters have widespread application in magnetic memory, logic devices, low-energy dissipation electronics, spintronics, thermoelectric, magnetoelectric and quantum computing mainly due to spin-orbit coupling and time reversal symmetry protected boundary states [10-15]. Due to the lack of high quality samples and the problems that exist in producing topological materials [16], many of these properties were expected in theory, but only few of them were realized by experiment.