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Structural, electronic, and magnetic properties of Mn-Doped InP nanowire

Pankaj Srivastava [a, *], Avaneesh Kumar [a], Neeraj K. Jaiswal [b]

[a] Nanomaterials Research Group, ABV– Indian Institute of Information Technology and Management (IIITM), Gwalior, 474015, India
[b] Discipline of Physics, Indian Institute of Information Technology, Design and Manufacturing, Jabalpur, M.P., 482005, India

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ABSTRACT

In the present work, we investigate structural stability, electronic and magnetic properties of InP nanowire (NW) oriented along (111) direction and doped with Mn using first-principles calculations. Structural analysis revealed that incorporation of Mn atom in NW geometry results in strong reconstructions of surface atoms relative to core atoms. For single Mn-doped NW, partially filled *d* orbital of Mn atom results in magnetic semiconducting behavior due to non-degenerate electronic band-gap (~0.1 eV). We have further considered the effect of Mn–Mn coupling on the electronic/magnetic properties of InP NW. Anti-ferromagnetic coupling state is observed as most favorable state based on total energy calculations. A half-metallic ferromagnetic coupling is also observed in case of Mn-pair doped at sub-surface of NW. The present results predict that the system doped with Mn pair between surface and core region are energetically more favorable than others.

1. Introduction

Owing to enormous potential applications of nanowires (NWs) significant achievement have been made to grow one dimensional (1-D) NWs with controlled diameter and crystallinity. It has been reported that NWs can be used in functional nano-scale devices, which also provide a path for fabricating optical devices and building block for photonic integrated circuit at nanoscale level [1–3]. The successful realization of both n- and p-type doped InP NWs became a promising nanostructure for next generation nanoscale devices [4]. There are many ways by which NWs can be successfully synthesized *viz.* chemical vapor deposition (CVD), thermal evaporation, intermittent laser-ablation catalytic growth, in-situ formation in liquid templates, vapour liquid solid (VLS) etc. [5–7]. Zhao et al. [8] successfully synthesized branched InP NWs with single crystalline and twinning structure using solvothermal synthesis method. They suggested that the synthesized sample can be indexed as sphalerite-structured, cubic phase InP with lattice constant of a = 5.858 Å. Martensson et al. [9] reported fabrication of InP NWs arrays along (111) phase, using metal–organic vapour phase epitaxy.

There are various reports available on electronic properties of semiconductor NWs, which is a function of shape, size, and crystallographic orientation of NW and can be alter through the process of doping [10–13]. Bukala et al. [12] reported that (111) oriented NW is more stable than (110) oriented NW in zinc-blende (ZB) configuration. Algre et al. [14] found that transition metal (TM) doped InP NWs synthesis using VLS process prefer to be ZB instead of wurzite structure and oriented

* Corresponding author.
E-mail address: pankajs@iiitm.ac.in (P. Srivastava).

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along most common (111) growth direction. Over last few decades, study of TM doped in nanostructures leads to generation

Table 1
Calculated lattice constant and energy band-gap of ZB InP bulk structure.

Parameters	Present calculation	Other theoretical calculations	Experimental
Lattice constant (Å)	5.86	5.65 [33], 5.85 [34], 6.01 [34], 5.99 [35]	5.85 [8], 5.86 [36,37]
Energy gap (eV)	0.83	0.56 [34], 0.26 [34], 0.84 [35]	1.42 [38], 1.46 [39]

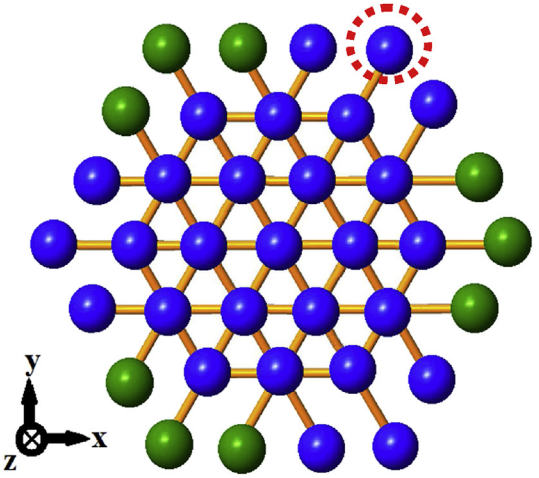

Fig. 1. Schematic top view of 7 Å radius InP NW oriented along (111) direction. Where green and blue balls represent P and In atoms respectively. The red circle represents doping site of Mn atom. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

of a novel class of nanomaterials called diluted magnetic semiconductors (DMS), which is potentially important towards spintronic applications [15–18]. Interaction of half-filled *d* orbital of transition metal with *p* orbital of host atom leads to interesting properties for magneto-optical application [19]. Khalid et al. [20,21] experimentally observed that incorporation of Mn ions leads to ferromagnetism in InMnP material. They also added that with different number of Mn ions in InMnP material results in different electrical and magnetic properties. Weert et al. [22] studied the effect of impurity doping on the optical properties of InP NWs. Arantes et al. [23] observed an induced magnetism in Ge NWs due to incorporation of Mn ions and can be a potential candidate for ferromagnetic quasi-1D system. Arantes et al. [23] also observed that NW exhibit lower formation energy when Mn ion is doped at center rather than on the surface. On contrary, Schmidt et al. [24] found that bulk-like position near the surface of nanowire is more favorable site for dopant Mn atom. Djedid et al. [25] investigated structural, elastic, electronic, and magnetic properties of GaMnP and InMnP material in cubic phase. Most of the work was focused on exploring the properties of InP NWs in its hexagonal phase [26–29]. On the other hand, scope is there to study the electronic, magnetic, and structural properties of ZB InP NWs. In another study, Schmidt [30] reported the effects of Mn doping on energetic and magnetic properties of very thin InP NWs. Commenting primarily on coupling of doped Mn pair in the InP NWs, their studies revealed that Mn pair prefers core of NW than on the surface. However, they have not explored the possibility of single Mn atom in InP NW. Hence, in the present study, we have systematically investigated the structural, electronic, and magnetic properties of ZB unpassivated Mn- (single atom and pair of atoms) doped InP NW using density functional theory (DFT) based first principle calculations.

2. Methodology

Present calculations were performed under the framework of DFT based supercell approach using Atomistix ToolKit Virtual NanoLab (ATK-VNL)[1]. Local spin density approximation (LSDA) exchange correlation functional with Perdew-Zunger parametrization [31] was used to account the exchange correlation effect for spin-polarzied calculation. We have used double-zeta polarized basis set for all the constituent atoms. The grid mesh cut-off for plane wave expansion is set to 75

[1] Quantumwise ATK-VNL version 14.1, www.quantumwise.com.