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A first principles study of Nd doped cubic $LaAlO_3$ perovskite: mBJ+U study

Sandeep [a,*], D.P. Rai [b], A. Shankar [c], M.P. Ghimire [d], R. Khenata [e], R.K. Thapa [a]

[a] Dept. of Physics, Mizoram University, Aizawl 796004, India
[b] Dept. of Physics, Pachhunga University College, Aizawl, Mizoram 796001, India
[c] Department of Physics, University of North Bengal, Darjeeling 734013, India
[d] Condensed Matter Physics Research Center, Butwal-13, Rupandehi, Lumbini, Nepal
[e] Laboratoire de Physique Quantique et de Modlisation Mathmatique (LPQ3M), Dpartement de Technologie, Universit de Mascara, 29000 Mascara, Algerie

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ABSTRACT

The structural, electronic and magnetic properties of Nd-doped Rare earth aluminate, $La_{1-x}Nd_xAlO_3$ (x=0–100%) are studied using the full potential linearized augmented plane-wave (FP-LAPW) method within the density functional theory. The effects of Nd substitution in $LaAlO_3$ are studied using super-cell calculations. The electronic structures were computed using modified Beck Johnson (mBJ) potential based approximation with the inclusion of Coulomb energy (U) for Nd-4f state electrons. The $La_{1-x}Nd_xAlO_3$ may possess half metallic behavior on Nd doping with finite density of states at E_F. The direct and indirect band gaps were studied as a function of Nd concentration in $LaAlO_3$. The calculated magnetic moments in $La_{1-x}Nd_xAlO_3$ were found to arise mainly from the Nd-4f state electrons. A probable half-metallic nature is suggested for these systems with supportive integral magnetic moments and high spin polarized electronic structures in these doped cases at E_F. The controlled decrease in band gap with increase in concentration of Nd doping is a suitable technique for harnessing useful spintronic and magnetic devices.

1. Introduction

Perovskite compounds ABX_3 have been studied a lot in recent years due to their important applications [1,2] ranging from ferroelectric, piezoelectric [3], high electronic and ionic conductivity, diverse magnetism, colossal magnetoresistive effects [4], paraelectricity, superconductivity and aslo as topological insulators [5]. Single crystalline substrates of $RAlO_3$ such as $LaAlO_3$, and $YAlO_3$ are commonly used for the epitaxy of thin films of high temperature super conductor (HTSC), magneto resistive materials, and GaN films [6]. The structural, electronic, transport, magnetic and specific heat in 4d- perovskites were studied with doping [7]. Yb-2p and V-4p as dopants in $YAlO_3$ were suggested for tunable solid-state lasers [8,9]. Dielectric resonators and substrates for microwave components having high quality factors were also studied through dielectric permittivity studies [10–12]. The perovskite compounds in the field of electronics [13], optics [14] and energy conversion applications [15] have remained popular studies among all technologically important compounds. Due to its preferable dielectric nature and suitable thermal properties $LaAlO_3$ has been suggested for replacing silicon dioxide (SiO_2) as superconductive substrate, superconducting microwave devices and the high k gate oxide [16]. At room temperature $LaAlO_3$ was reported to be in rhombohedral structure with $R3c$ space group [17]. Nakatsuka *et al.* have reported ideal $Pm3m$ cubic perovskite structure at room temperature [18]. The multiferroic applications of $LaAlO_3$ on doping with transition metals along with its use as host material makes it important to be explored extensively [14]. Limited numbers of studies were observed till date on the ferromagnetic and optical properties of transition metal doped $LaAlO_3$ [19–21]. Change in band gaps in β-SiC with doping of N-atom for C were studied by Hong-Sheng *et al.* to report substantial modification in band gaps [22]. Additional absorption peaks in $KMgF_3$ were explained using doping studies by Fang *et al.* [23]. The weakening of magnetic moment and magnetic stabilized energy in defective graphene with hydrogen chemisorbed single-atom vacancy (H-GSV) were analyzed by Shu-Lai *et al.* [24]. The decrease in conductivity of ZnO was predicted and compared with experimental results by Hou Qing-Yu *et al.* [25] using pseudopotential method. Optical properties of TiO doped with two atoms were studied with by Qing *et al.* [26]. A thermodynamic formalism based on *ab initio* electronic structure calculations were applied to $Ba_cSr_{(1-c)}TiO_3$ perovskite solid solutions to predict that the spinodal decomposition could serve as the universal mechanism of

* Corresponding author.
E-mail address: sndp.chettri@gmail.com (Sandeep).

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the nanocluster formation [27]. Further, Shi-Bin *et al.* studied the effect of polarization doping of AlGaN and predicted it as more efficient doping technique [28]. Zylberberg and Zuo-Guang [29] have studied the dielectric properties of Bismuth-doped $LaAlO_3$ to correlate the higher dielectic properties using high polarizability of Bi^{3+} ion with alone electron pair. Namjoo *et al.* [30] have studied the structural electronic and optical properties of InAs, InSb, and their ternary alloys $InAs_xSb_{1-x}$ ($x=0.25$, 0.5, 0.75) within density functional theory using the modifed Becke-Johnson exchange-correlation functional (mBJ-LDA) [31], to report the

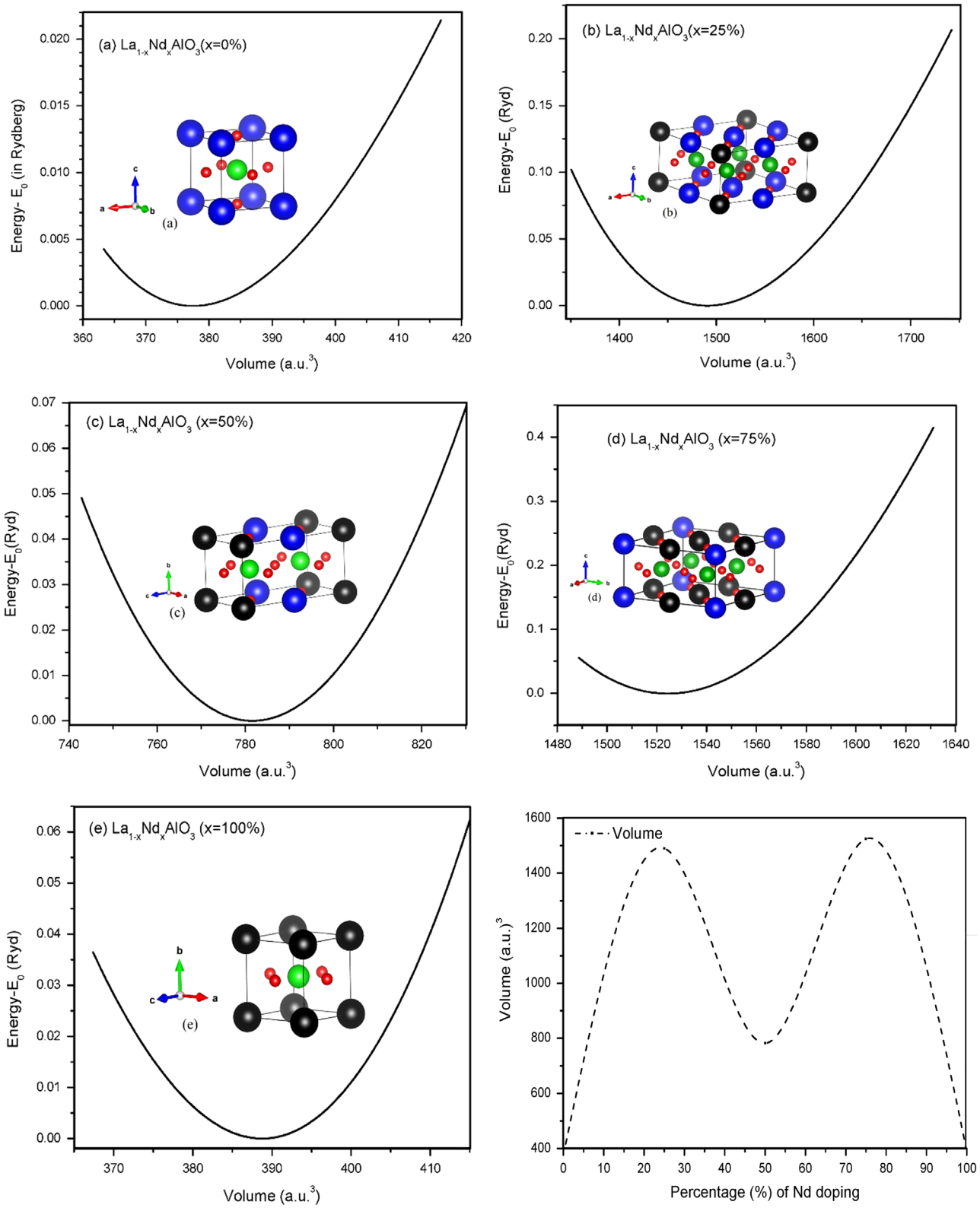

Fig. 1. Crystal structure and Energy vs Volume curve for (a) $La_{1-x}Nd_xAlO_3$ (where $x=0\%$ or (0/8) (b) $La_{1-x}Nd_xAlO_3$ (where $x=25\%$ or (2/8), (c) $La_{1-x}Nd_xAlO_3$ (where $x=50\%$ or (4/8)50%, (d) $La_{1-x}Nd_xAlO_3$ (where $x=75\%$ or (6/8) and (e) $La_{1-x}Nd_xAlO_3$ (where $x=100\%$ or (8/8) and (f) Plot of percentage of Nd doping vs volume for $La_{1-x}Nd_xAlO_3$ Blue=La, Black=Nd, Green=Al and Red=O. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)