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Electronic, magnetic and optical properties of transition metal doped Nd_2O_3: A DFT insight

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ABSTRACT

The structural, electronic, magnetic, and optical properties of transition metal doped rare earth neodymium sesquioxide (Nd_2XO_3, where X = Co, Cr, Mn, Ni, and Zn) were investigated here by first-principles simulations considering the density functional theory (DFT) framework. Comparing the energy band structures, density of states, and the overall charge density distribution, we have seen that the transition metal doping improves the application of the Nd_2O_3 (NDO) in many technological aspects. Spin-polarized calculations were quite satisfactorily described, and from this theoretical interpretation using DFT we've fruitfully explained the mechanism behind the magnetic behavior of all doped samples. The electronic and optical properties of doped NDO samples were well-tuned by transition metal atoms. Finally, we have observed that the values of total magnetization of transition metal substituted NDO samples were substantially enhanced compared to that of pure NDO, which would be very attractive in diverse applications.

1. Introduction

Rare-earth (RE) oxides and sesquioxides are nowadays an interesting area of research for their significant applications in numerous electronic industries. Within the field of nanoscience and nanotechnology, these sesquioxides materials are very attractive for their peculiar physical properties. From the beginning of RE technology, RE systems research have focused on by different experts to discover many fascinating characteristics. There are so many important applications of RE oxides and sesquioxides as catalysis and are enormously important materials in the field of RE [1]. Even though voluntarily oxidized RE elements, they appeared through their fluctuating strength [2]. Depending on appropriate conditions, the RE oxides from neodymium (Nd) onward (except terbium, Tb) arise naturally as RE sesquioxides RE_2O_3, and RE atoms are found in the trivalent (RE^{3+}) configuration in their ground state [3]. Recently, L. Petit et al. [1] have investigated the First-principles study of rare-earth oxides. Singh et al. [4] have studied the calculations of the electronic structure, reflectivity, and optical conductivity of La_2O_3, Pr_2O_3, and Nd_2O_3(NDO). Mohammad et al. [5] have reported the electronic structure of NDO. Another group of researchers Fumitaka Arai et al. [6] have studied resonant photoemission study of electronic structure of RE sesquioxides, (R_2O_3; R = La, Pr, Nd, Sm, Eu, Gd, Er, Tm, Yb and Lu). First-principles electronic structure calculations of cerium oxide (CeO_2 and Ce_2O_3) were discussed by N. V. Skorodumova et al. [7] Rare-earth sesquioxides R_2O_3 and oxysulfides R_2O_2S (R = La, Ce, and Pr) have been theoretically investigated by first-principle by M. Mikami et al. [8]. R. Haensel et al. [9] have described the optical absorption of the REs (Ce, Pr, Nd and Sm). The optical properties based on the optical phonon structure of rare-earth sesquioxides (RES) have found in several literatures [10–14]. The analytical escalation and elemental properties such as density of states, and band structures are the main focused areas for theoretical and computational investigations on RES [15–17]. Presently, density functional theory (DFT) based calculations in electronic structure have been considered a very fruitful way of explaining the electronic properties of traveling valence electrons in solid-state structures. In the field of condensed-matter physics, first-principles calculations of *f*-electron systems are of great challenge for the presence of localized as well as current theoretical methods based on itinerant states, particularly in the local-density or generalized gradient approximation [18]. Recently, due to its extensive range of applications, NDO has drawn more attention from several researchers in this modern era. Considering the electronic properties, neodymium sesquioxide, Nd_2O_3 (NDO) is very convenient for both scientists and technologists. NDO has concerned plenty of research in numerous fields from photonics to

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