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Ferromagnetism in CdO*X* (*X* = Mn and N) with and without intrinsic point defects: A density functional theory

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ABSTRACT

The purpose of this study is to further understanding of the structural, electronic, magnetic properties of CdO doped with transition metal (Mn) and non metal element (N). The calculations are performed by the developed full-potential augmented plane wave plus local orbitals method within the spin density functional theory. As exchange–correlation potential we used the generalized gradient approximation (GGA) form. Moreover, the electronic structure study for our compounds was performed with and without oxygen deficiency. We treated the ferromagnetic and antiferromagnetic states and we found that all compounds are stable in the ferromagnetic structure, and all doped materials CdO:Mn and CdO:N adopt the half metallic character. In addition, we notice that the oxygen vacancy destroyed the ferromagnetism in N doped CdO, while Mn doped CdO becomes semiconductor.

1. Introduction

Spintronics devices, which utilize both the charge and the spin freedom of electrons to create new functionalities beyond conventional semiconductor devices, have attracted much attention recently [1]. The search for materials combining properties of the ferromagnet and the semiconductor has been challenging because of differences in crystal structure and chemical bonding [2]. Dilute magnetic semiconductors (DMSs), are thought to be ideal materials for this field, enabling versatility in doping and fabrication of various structures and simple integration with the dominant semiconductor technology. As a wide ranging band gap of 2.2–2.7 eV semiconductor with a direct gap, CdO draws the attention of scientists for its potential use in UV laser diodes and UV-blue light emitters [3]. Very recently, CdO has also been identified as a promising host material for the realization of DMSs due to the prediction of possible ferromagnetism in $Cd_{1-x}Mn_xO$ [4]. Computational methods based on density functional theory (DFT) also predict ferromagnetism in most 3d transition metal (TM) based CdO [5–7]. More recently, it has also been predicted that the ferromagnetism in class of oxides can be induced by native defects, bringing new challenges for understanding the origin of ferromagnetism in these oxide compounds. We could mention for example, Ca vacancy in CaO [8–12], Hf vacancy in HfO_2 [13–15], In_2O_3 [12,16,17], TiO_2 [13] and ZnO [6,18]. In this paper, we present our first principles studies of the structural, electronic and magnetic properties of Mn and N doped CdO. The aim of our study is to understand the role played by defects in the origin of ferromagnetism in such narrow band gap semiconductor. The paper is organized as follows: in Section 2, we present the method of calculation, Section 3 contains all results and discussions, and finally we finish with a summary and conclusion in Section 4.

2. Computational method

The calculations were performed by using the full potential linearized augmented plane wave plus local orbitals (FP-L/APW + lo) method based on the spin-polarized DFT and implemented in Wien2k [19] code. The exchange and correlations electronic energy were calculated with the generalized gradient approximation (GGA) [20]. Further, a muffin-tin model for the crystal potential is assumed and the unit cell is divided into two regions, within and outside the muffin-tin sphere. Inside the muffin-tin sphere, the spherical harmonic expansion is used and outside the sphere the plane wave basis set is chosen. The valence part is treated within a potential expanded into spherical harmonics up to $l = 4$. The valence wave functions, inside the spheres, are expanded up to $l = 10$. In order to achieve the energy convergence, we have

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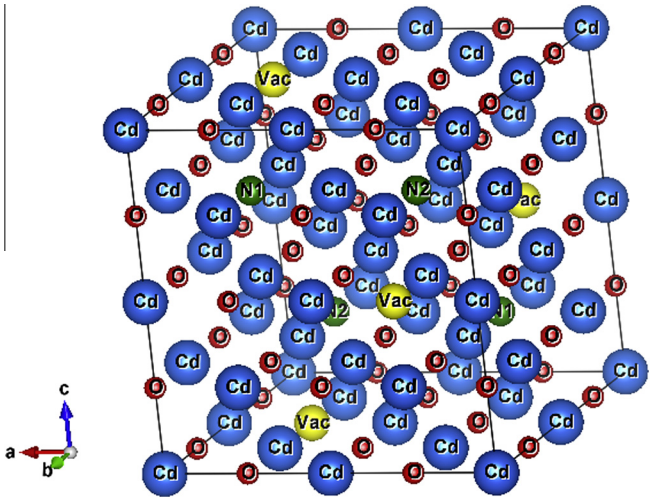

Fig. 1. Schematic structure diagram for 2 × 2 × 2 supercell of CdO, positions of the host atoms (Cd and O), dopant (N) and oxygen vacancy (vac) are labeled.

expanded the basis function up to $R_{MT*}K_{MAX} = 7$ (R_{MT} is the average radius of the spheres muffin-tin and K_{MAX} is the maximum value of the wave vector $K = k + G$). The charge density was expanded with $G_{max} = 14$. The relativistic effects are taken into account by using scalar relativistic. We have adopted the values of 2.3, 2.3, 1.45 and 1.9 a.u. for Cd, Mn, O and N atoms, respectively. Our calculations were performed in the rocksalt ferromagnetic phase, at the concentration $x = 0.125$, where two Cd are substituted by two Mn atoms and two O by two N atoms. We have considered the ferromagnetic FM and antiferromagnetic AFM phases. All calculations were performed using unit cell parameters optimized by minimizing the total energy as function of volumes. The self-consistent calculations are considered to be converged only when the calculated total energy of the crystal converged to less than 1 mRy. Ferromagnetic stability is determined by the total energy difference (ΔE) of the supercell between antiferromagnetic (AFM) state and ferromagnetic (FM) state. A representative structure diagrams corresponding to all studied systems are shown in Figs. 1 and 2. In Fig. 1, the positions of host atoms (Cd and O) and dopant (N) along

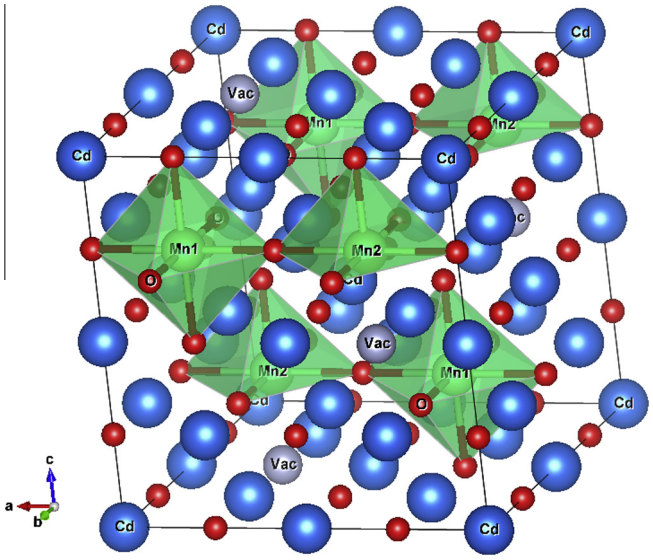

Fig. 2. Schematic structure diagram for 2 × 2 × 2 supercell of CdO, positions of the host atoms (Cd and O), dopant (Mn) and oxygen vacancy (vac) are labeled.

Table 1
Calculated values for the lattice parameter (in Å), bulk modulus (in Gpa) and ΔE (in mRy) for all configurations considered in the present study.

Systems	*a*	*B*	Δ*E*
$Cd_{16}N_2O_{14}$	9.4432	119.896	+2.05
$Cd_{16}N_2O_{13}$	9.3702	118.662	−8.51
$Cd_{14}Mn_2O_{16}$	9.4836	129.897	+0.73
$Cd_{14}Mn_2O_{15}$	9.4217	125.565	+150.8

with oxygen vacancy are labeled. While Fig. 2, represents, the positions of Cd, O and Mn with oxygen vacancy. The lattice parameter *a*, based on optimization of the energy of the perfect lattice, was calculated to be $a = 4.67$ Å and compared very well with the corresponding experimental value of 4.69232 Å [21]. The oxygen vacancy is simulated by using $Cd_{16}N_2O_{13}$ and $Cd_{14}Mn_2O_{15}$ super cells and the optimization of all atomic coordinates was carried out using the same procedure as discussed above.

3. Results and discussion

The structural properties are obtained by minimization of the total energy depending on the volumes of CdNO and CdMnO in FM and AFM phases with and without oxygen vacancy using GGA. We computed the lattice constants, bulk moduli by fitting the total energy versus volume according to Murnaghan's equation of state [22]. The obtained results are listed in Table 1. Up to now, no experimental or theoretical lattice constant of the compound has been reported. However, we can see that the introduction of

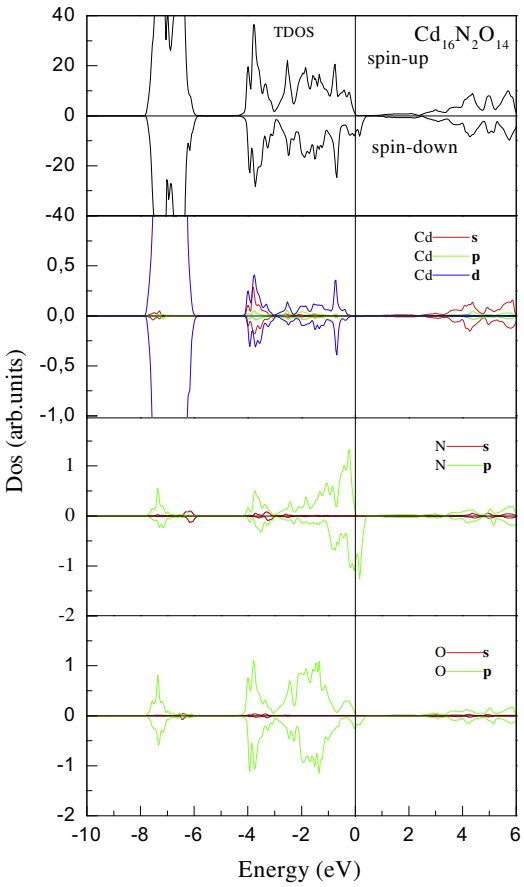

Fig. 3. Total DOS and partial PDOS of $Cd_{16}N_2O_{14}$ compound.