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DFT study of Mn-doped CeO_2: The structural and electronic properties

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***Abstract*—The structural and electronic characteristics of manganese doped cerium oxide are investigated by means of the density functional theory with Habbard parameter approach. Experimental evidence and other theoretical findings corroborate the computed electronic characteristics, bulk modulus, cell volume, and equilibrium lattice parameter for ceria. By replacing the Ce atom with Mn, the bond length, bulk modulus, cell volume, and lattice parameter are all reduced. In the meantime, we see a narrowing of the band-gap. Interestingly, it is seen that the strength of the oxygen occupied states to cerium empty states transition and the covalent nature of the cerium oxygen bond are both reduced when manganese is doped into ceria. The heavy manganese doped ceria system may be used for applications involving the spin dependent current and light absorption, since it exhibits steeper absorption peaks spanning from 3.0 to 3.44 eV of spin down and spin upper, respectively.**

***Keywords*—ceria, manganese doping, Hubbard parameter, electronic properties.**

I. INTRODUCTION

This Ceria (CeO_2) has several uses in current catalytic technology, including three-way catalysts (TWCs), solid oxide fuel cells (SOFCs), and high oxygen storage capacity (OSCs) [1,2]. Various technological applications may be attributed to CeO_2's oxygen vacancy creation and transit capabilities. In addition to its long history of use as an oxygen storage material, cerium oxide (CeO_2) has recently attracted attention as a material with optical component and laser hosting potential. Optical coatings, whether single or multilayered, have long made use of CeO_2 as a film material due to its high refractive index. It can effectively absorb ultraviolet radiation and is also used to safeguard light-sensitive items by adding it to glass (2−4% CeO_2). There have been reports suggesting cubic CeO_2 as a possible alternative to rutile SnO_2 [3] and TiO_2[4]. According to Veszelei et al.,[4] CeO_2 outperformed TiO_2 under the influence of light of $\lambda < 400$ nm due to its significant absorption. In contrast to TiO_2-rutile, Miyauchi et al [5] .hypothesized that cerium dioxide's considerably smaller photocatalytic behavior reduced the deterioration of the compound containing ultraviolet absorber species by limiting the generation of reactive oxygen species.

According to Goubin et al. [6], ceria has a refractive index of 2.35, a strong UV absorption rate, and a band gap of 3.2 eV. The fact that transition metals are characterized by a short ionic radius and a strong valence is intriguing. The electrical structure of transition metals is comparable to that of noble metals. To boost the performance of mental oxide, the current catalytic industry commonly uses transition metals, which are excellent modified elements. To illustrate the significant impact on electrical and magnetic characteristics, Park et. al [7]. investigated the effects of atomically-substitution doping of 3d transition metals in titanium dioxide. They determined that reducing the band gap by doping TiO_2 with Fe (or Co, Ni) was the result; ground states of Ni-doped TiO_2 are paramagnetic, whereas ground states of Co-doped TiO_2 are antiferromagnetic. In contrast, systems that include iron do have ground states with magnetic properties that include orbital components of magnetism. The structural and optical characteristics of ZnO were studied by Anghel et al.[8], who evaluated the impact of doping by various transition metal ions on these properties. They discovered that doping with chromium, manganese, iron, cobalt, or nickel had a substantial influence on both the electrical and optical aspects of the material. According to the calculations done by Kim and Bishop et. al [9]. on ceria that has been doped with transition metal praseodymium (Pr) and its optical absorption spectrum, the appearance of the Pr doping electronic states inside the band gap of CeO_2 caused a wide response of light in the visible spectrum from 2.0-3.3 eV, giving the material a reddish-orange hue. The optoelectronic characteristics of pure and metal doped CeO_2 have piqued the interest of scientists, and there are tests demonstrating that the material's properties are modified or enhanced when transition metals like iron, cobalt, or nickel are doped into the material. As an example, in an experiment, Li and Wang et. al [10]. utilized the co-precipitation method to create a variety of $Ce_{1-x}Fe_xO_2$ (x=0, 0.2, 0.4, 0.6, 0.8, and 1) complex oxide catalysts. Among these, they discovered that $Ce_{1-x}Fe_xO_2$ exhibited a high capacity for oxygen storage, excellent redox firmness, and intensive interaction between both cerium and iron species. Through experimental investigation of the optical characteristics of cobalt-doped

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