World Academy of Science, Engineering and Technology
International Journal of Mathematical and Computational Sciences
Vol:14, No:12, 2020

Investigation of Physical Properties of W-Doped CeO_2 and Mo-Doped CeO_2: A Density Functional Theory Study

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Abstract : A systematic investigation on structural, electronic, and magnetic properties of $Ce_{0.75}A_{0.25}O_2$ (A = W, Mo) is performed using first-principles calculations within the framework Full-Potential Linear Augmented Plane Wave (FP-LAPW) method based on the Density Functional Theory (DFT). The exchange-correlation potential has been treated using the generalized gradient approximation (WC-GGA) developed by Wu-Cohen. The host compound CeO2 was doped with transition metal atoms W and Mo in the doping concentration of 25% to replace the Ce atom. In structural properties, the equilibrium lattice constant is observed for the W-doped CeO_2 compound which exists within the value of 5.314 A° and the value of 5.317 A° for Mo-doped CeO2. The present results show that $Ce_{0.75}A_{0.25}O_2$ (A=W, Mo) systems exhibit semiconducting behavior in both spin channels. Although undoped CeO_2 is a non-magnetic semiconductor. The band structure of these doped compounds was plotted and they exhibit direct band gap at the Fermi level (EF) in the majority and minority spin channels. In the magnetic properties, the doped atoms W and Mo play a vital role in increasing the magnetic moments of the supercell and the values of the total magnetic moment are found to be 1.998 μB for $Ce_{0.75}W_{0.25}O_2$ and to be 2.002 μB for $Ce_{0.75}Mo_{0.25}O_2$ compounds. Calculated results indicate that the magneto-electronic properties of the $Ce_{1-x}A_xO_2$(A= W, Mo) oxides supply a new way to the experimentalist for the potential applications in spintronics devices.

Keywords : FP-LAPW, DFT, CeO_2, properties
Conference Title : ICSRD 2020 : International Conference on Scientific Research and Development
Conference Location : Chicago, United States
Conference Dates : December 12-13, 2020