

## Investigation of Physical Properties of W-Doped CeO<sub>2</sub> and Mo-Doped CeO<sub>2</sub>: A Density Functional Theory Study

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**Abstract :** A systematic investigation on structural, electronic, and magnetic properties of Ce<sub>0.75</sub>A<sub>0.25</sub>O<sub>2</sub> (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 CeO<sub>2</sub> 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<sub>2</sub> compound which exists within the value of 5.314 Å and the value of 5.317 Å for Mo-doped CeO<sub>2</sub>. The present results show that Ce<sub>0.75</sub>A<sub>0.25</sub>O<sub>2</sub> (A=W, Mo) systems exhibit semiconducting behavior in both spin channels. Although undoped CeO<sub>2</sub> 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<sub>0.75</sub>W<sub>0.25</sub>O<sub>2</sub> and to be 2.002 μB for Ce<sub>0.75</sub>Mo<sub>0.25</sub>O<sub>2</sub> compounds. Calculated results indicate that the magneto-electronic properties of the Ce<sub>1-x</sub>A<sub>x</sub>O<sub>2</sub> (A= W, Mo) oxides supply a new way to the experimentalist for the potential applications in spintronics devices.

**Keywords :** FP-LAPW, DFT, CeO<sub>2</sub>, properties

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