Investigation on the role of oxygen vacancies in the Cd hyperfine properties in (Co, Mn)-doped CeO_2

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Ceria is known to have intrinsic oxygen vacancies that affect specific properties for semiconductor applications. Recently, incorporation of impurities to ceria for vacancy formation control as well as the role of dopants in the physical and chemical ceria properties have gained much attention, especially when doped with transition metals. Local disorder originated from oxygen vacancies and doping is the aim of several studies in which hyperfine interactions techniques have showed a great tool to investigate it. In particular, perturbed angular correlation spectroscopy (PAC) measurements with ^{111}Cd for pure and TM (Co, Mn)-doped CeO_2 have exhibited a range of quadrupole frequencies [1, 2]. In order to elucidate the several electric field gradients (*efg*) in these systems, we have carried out band structure calculations by means of density functional theory (DFT) in the ceria doped with Cd and TM (Co, Mn) to study the local disorder from the hyperfine interactions point of view. We performed spin-polarized calculation using the full-potential augmented plane-waves plus local-orbitals (FP-LAPW) method and Perdew–Burke–Ernzerhof generalized gradient approximation embodied into WIEN2k code [3]. We simulated several charge states in pure and TM-doped CeO_2 supercells with oxygen vacancies focusing on electronic distribution in the vicinity of Cd. Our *efg* results showed a good agreement with ^{111}Cd quadrupole frequency range obtained from PAC experiments. Thus, we improved the understanding about the role of Cd and TM in the ceria oxygen vacancy formation.

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