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Defects and oxygen vacancies tailored structural and optical properties in CeO_2 nanoparticles doped with Sm^{3+} cation

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Abstract

In this study, the correlation between the concentration of dopant ions and oxygen vacancy defect of Sm-doped CeO_2 Nano-particles (NPs) were investigated systematically by X-ray diffraction (XRD), Ultraviolet-visible-Near Infrared spectroscopy (UV-Vis-NIR) and Surface-enhanced Raman spectroscopy (SERS). The nano-crystalline $Ce_{1-x}Sm_xO_2$ (x = 0.00, 0.02, 0.04, 0.06, 0.08 and 0.10) samples were synthesized using co-precipitation chemical route. The XRD measurements revealed that Sm^{3+} ions are successfully incorporated at the Ce^{4+} ion sites in the face centered cubic (*fcc*) lattice of CeO_2 NPs. The high-resolution transmission electron microscopy (HRTEM) and Selected area electron diffraction (SEAD) patterns were analyzed to study the surface morphology, crystallinity, atomic structure of the samples. The average particle size calculated with TEM images was obtained in the range of 5-8 nm for $Ce_{1-x}Sm_xO_2$ samples for all the doping concentrations. The UV-Vis-NIR spectroscopy and Surface-enhanced Raman Spectroscopy were analyzed to investigate the optical properties and defect structure in these NPs. The UV-Vis-NIR spectroscopy measurements revealed that due to aggregation of particles the optical band gap energy was varied with fluencies of Sm^{3+} ions as well as due to particle size variations of NPs. Peak asymmetry and broadening of Raman active mode further ascribed the presence of oxygen vacancy (whether extrinsic or intrinsic), which were varied with the fluencies of Sm^{3+} ions in CeO_2 NPs. This paper presented a systematic study on the fluencies of Sm doping in CeO_2 nano-particle lattice to understand the role of vacancies, intrinsic and extrinsic oxygen vacancies and their effect on tailoring the structural and optical properties of doped CeO_2 nano-particles for various applications like luminescent materials, oxygen transportation, catalysts, ultraviolet fuel cells, corrosion prevention etc.