

Enhancing Antioxidant Properties of CeO₂ Nanoparticles with Nd³⁺

Doping: Structural, Biological, and Machine Learning Insights

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Table 1. Structural parameters of the prepared NPs.

Sample	d_{hkl} (nm)	$2(\theta)$	FWHM	D (nm)	a (nm)
CN0	0.310	28.67	0.300	27.33	0.5261
CN1	0.311	28.66	0.313	26.20	0.5263
CN5	0.312	28.62	0.343	23.90	0.5270
CN10	0.312	28.58	0.445	18.42	0.5277

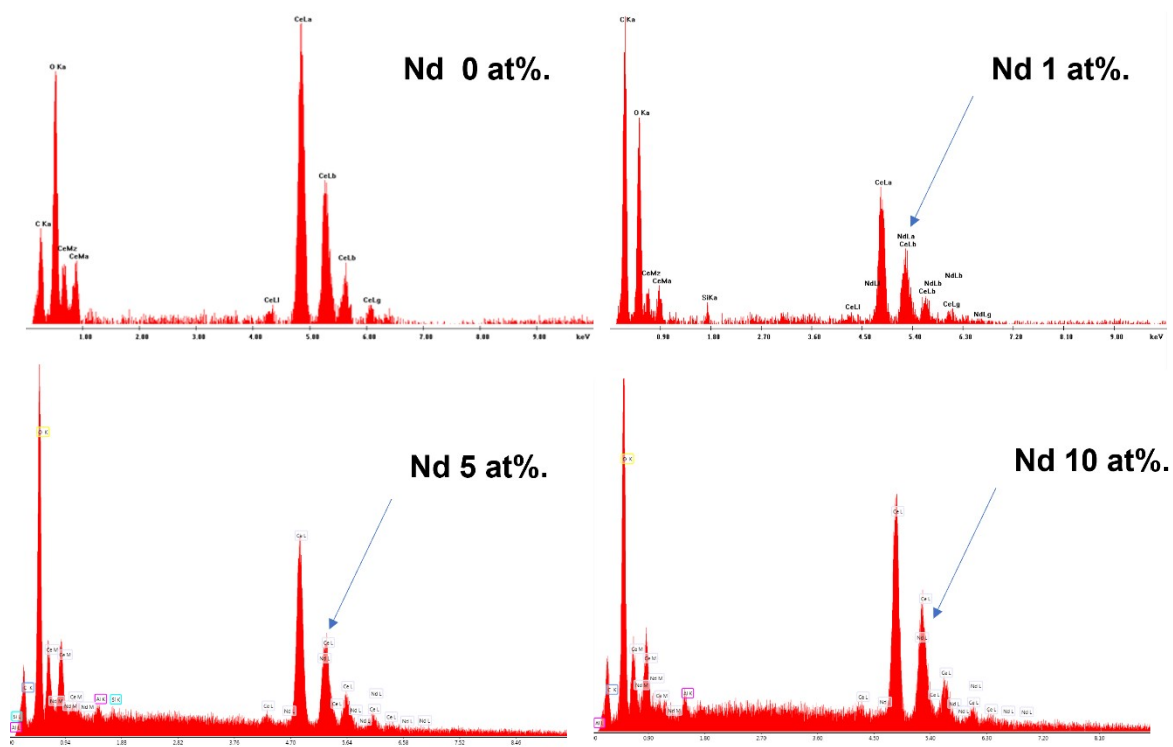


Figure S1. EDS spectrum of Nd-CeO₂ nanoparticles with different amounts of Nd.

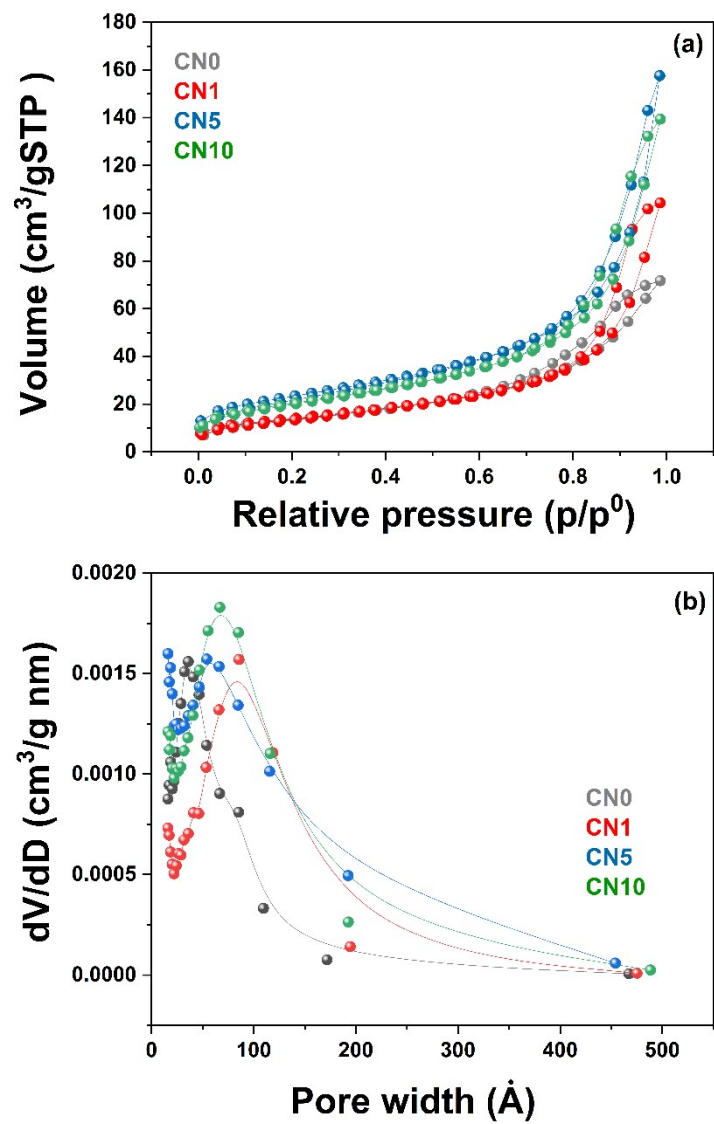


Figure S2. a) N₂-adsorption-desorption isotherm plots, b) pore size distribution of Nd-doped CeO₂ nanoparticles.

Table 2. S_{BET} , pore volume, and pore radius of prepared CeO₂-NPs.

Sample	S_{BET} (m ² /g)	Pore volume (cc/g)	Pore radius (Å)
CN0	49.240	0.106	35.824
CN1	50.004	0.157	85.610
CN5	83.815	0.233	16.057
CN10	73.258	0.208	66.815

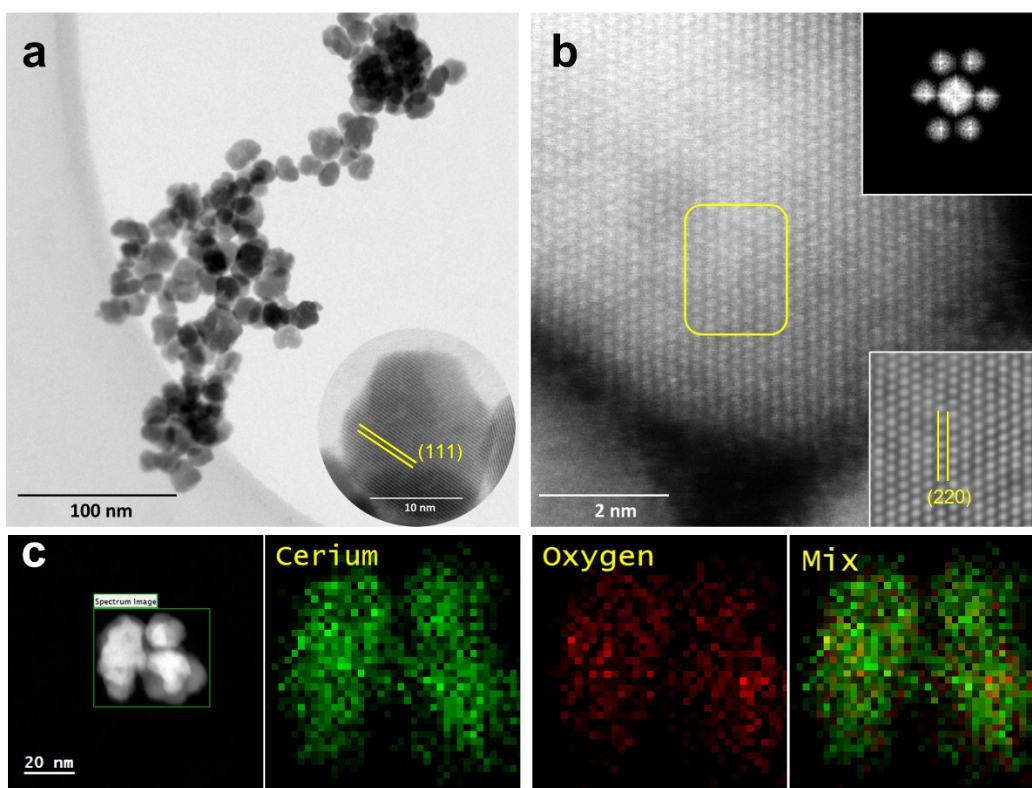


Figure S3. a) TEM/HRTEM image, b) STEM-HAADF image (inset is the inverse FFT), and c) EDS elemental mapping of CeO₂.

TEM/HRTEM image of CeO₂ (**Figure S3**) depicts that the nanoparticles are consistent with the observed morphology. 17.25 nm was determined to be the average particle size. The (fast-Fourier Transform) FFT and inverse FFT were utilized to analyze the interplanar distance (d_{hkl}) of 0.31 nm, leading to the identification of the (111) plane, as seen in the HRTEM inset. The surface's HRTEM picture in HAADF-STEM mode is shown in **Figure S3b**. In relation to the (220) plane, the d_{hkl} value is 0.19 nm. Cerium and oxygen are represented by a homogeneous distribution in **Figure S3c** spectrum picture and elemental mapping. It also displays a blend of elemental mapping.