High efficient photoluminescence of SiO_2 and Ce-SiO_2 microfibres and microspheres

Juan M. Ruso [a], *A. Noel Gravina* [b#], *Noelia L. D´Elía* [b#], *Paula V. Messina* [b]*

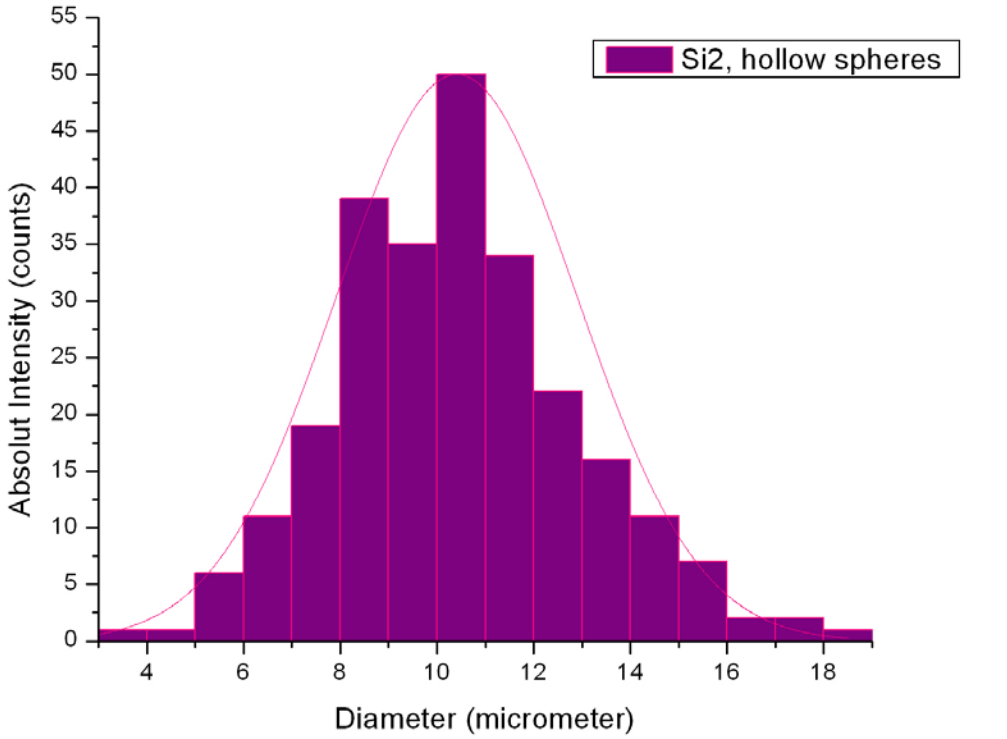
(a) Soft Matter and Molecular Biophysics Group, Department of Applied Physics, University of Santiago de Compostela, Santiago de Compostela, 15782, Spain. (b) Department of Chemistry, Universidad Nacional del Sur, (8000) Bahía Blanca, Argentina. INQUISUR-CONICET

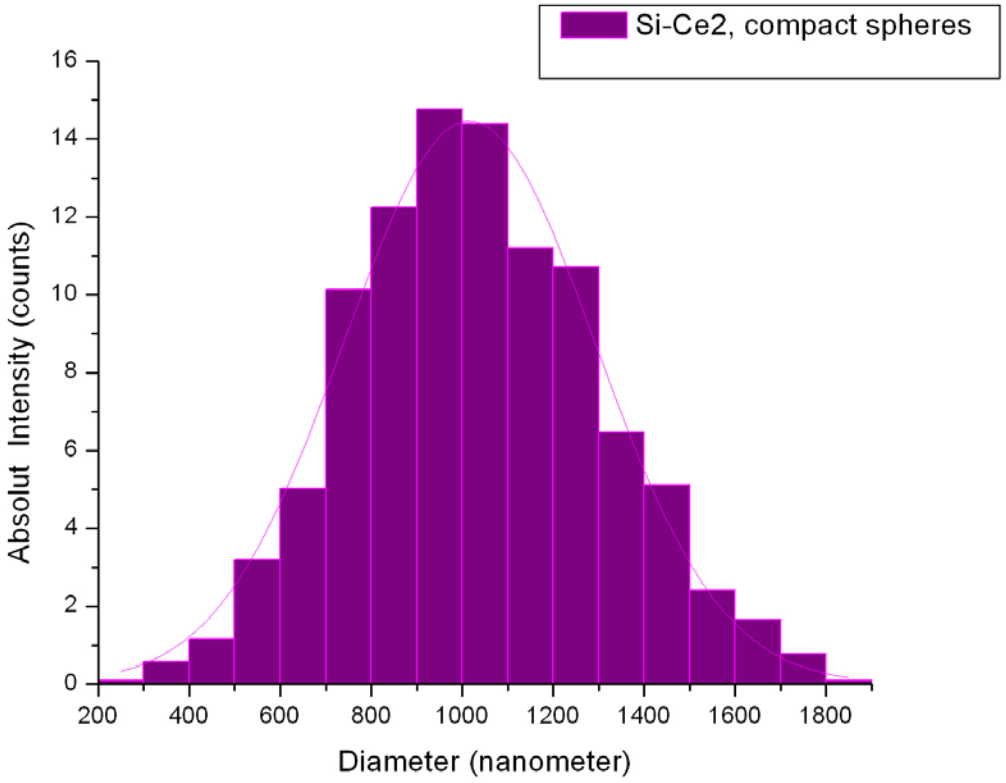
* Author to whom correspondence should be addressed. Tel: +54 291 4595159. Fax: +54 291 4595160. Electronic mail: pmessina@uns.edu.ar.

[#] Have the same participation in this work.

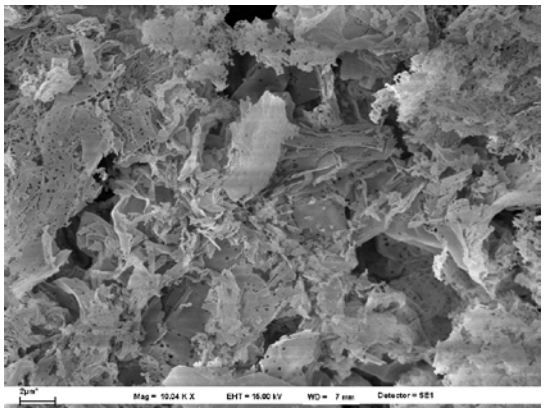
Electronic Supplementary Information (ESI),

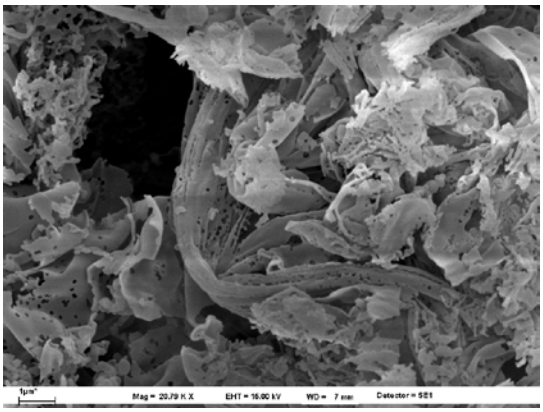
Representative size distribution histograms of hollow crystaline silica spheres (Si2) and Ce-doped crystalline compact silica spheres (Si-Ce2), similar results are obtained for all materials.



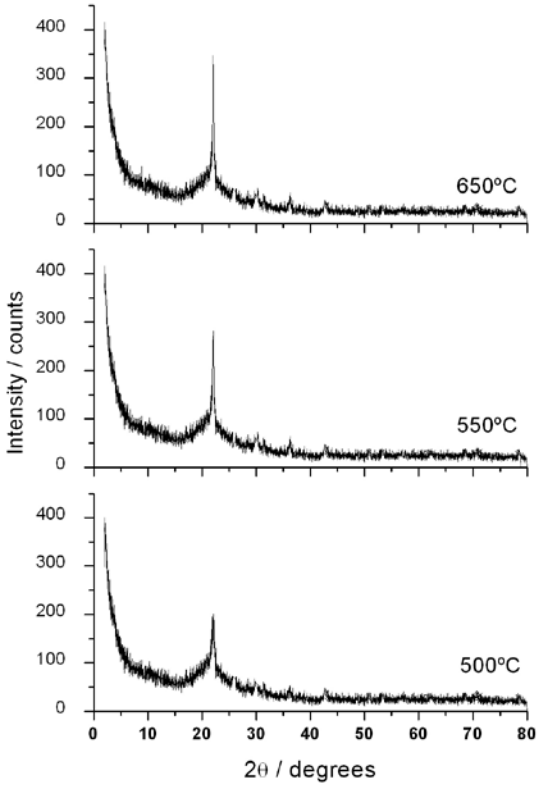


SEM Characterization of the material templated with water/CTAB-ButOH/ iso-octane microemulsion. Nano-sheet structures can be appreciated. Such structures are probably created by the micro-droplet interaction and fusion during the material synthesis.

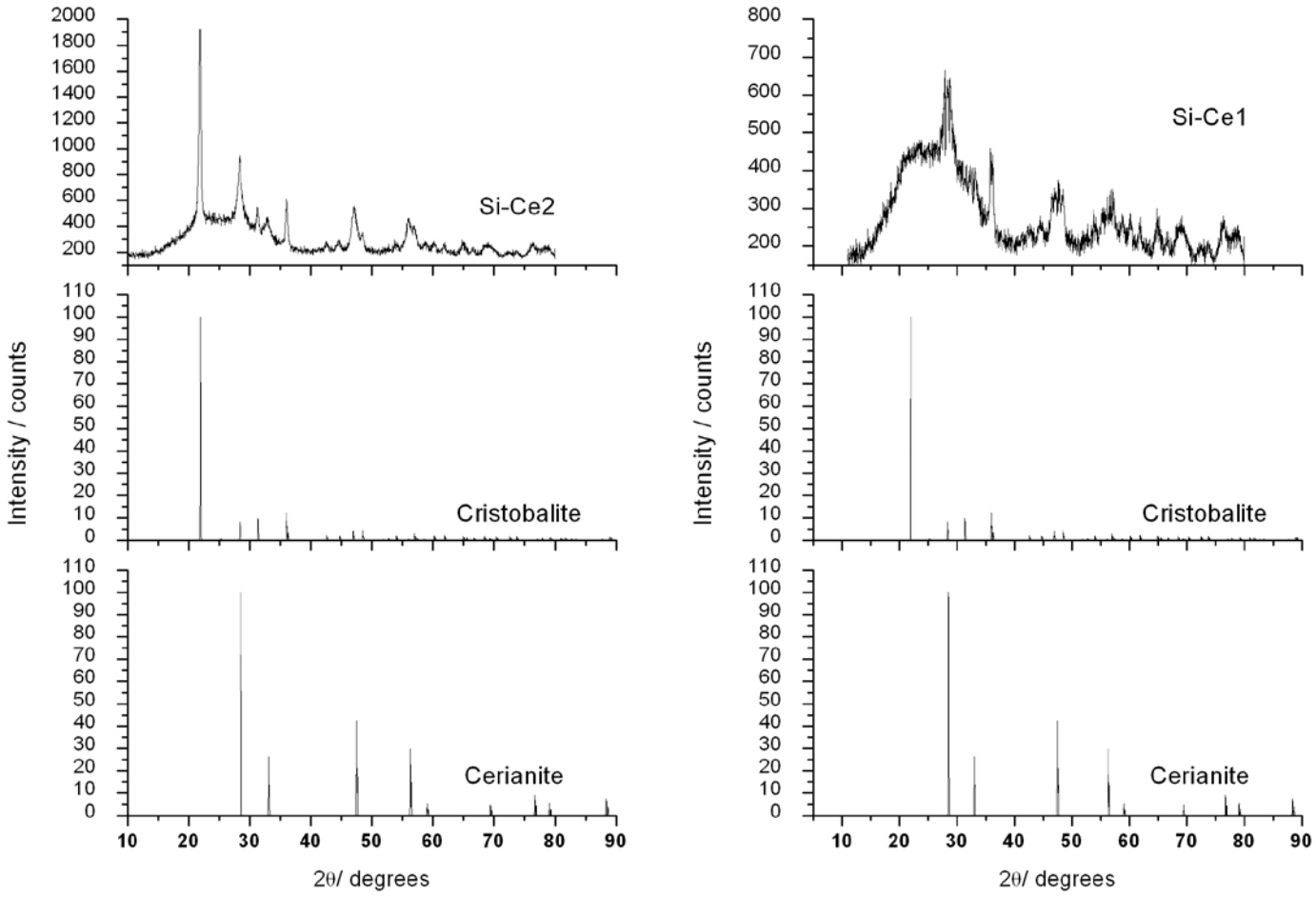




X-ray diffraction patterns (XRD) of crystalline Si2 material calcined at 500, 550, 650ºC.

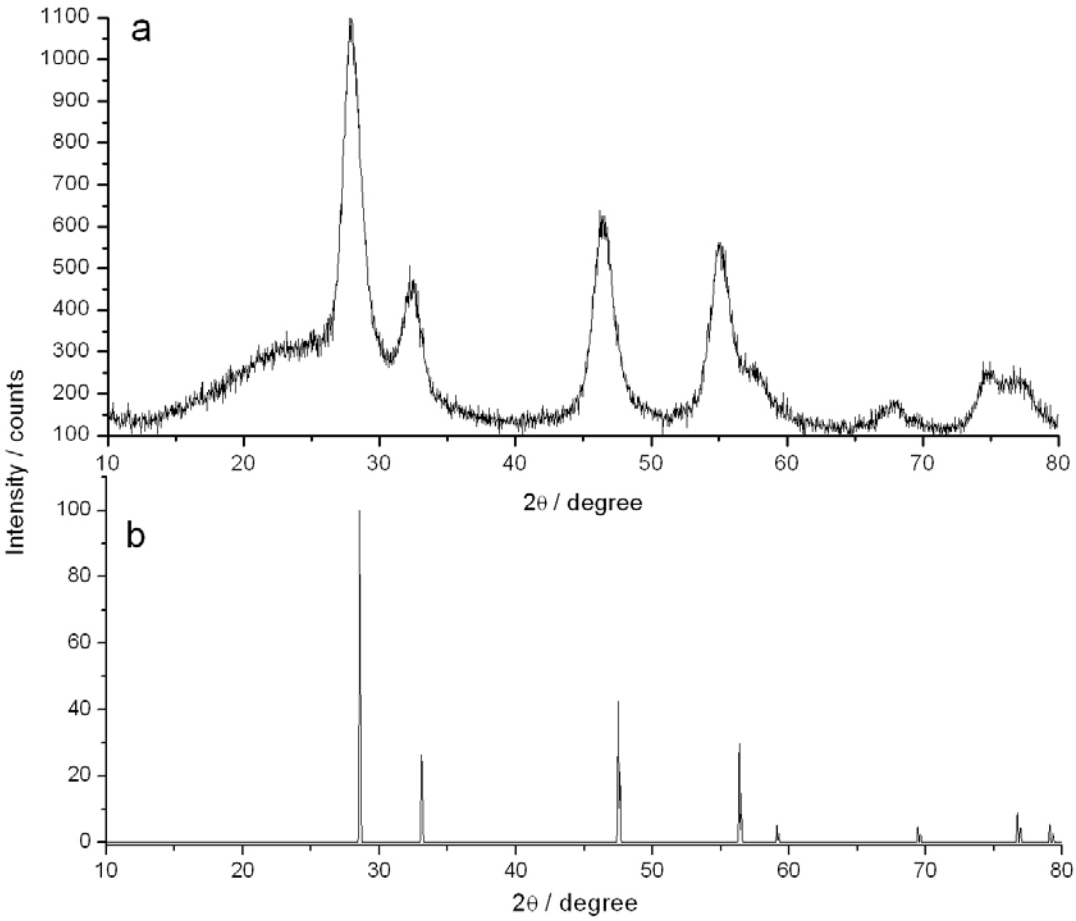


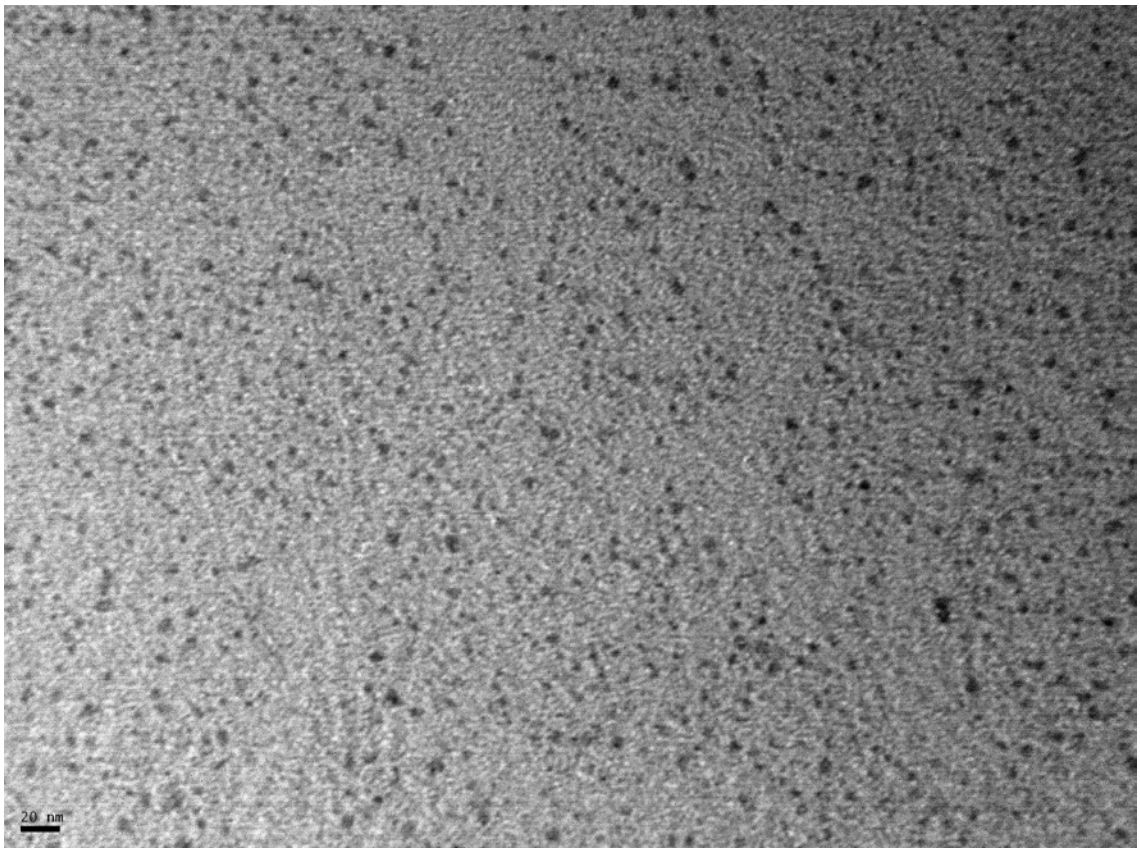
XRD patters of Ce-doped materials Si-Ce1 and Si-Ce2

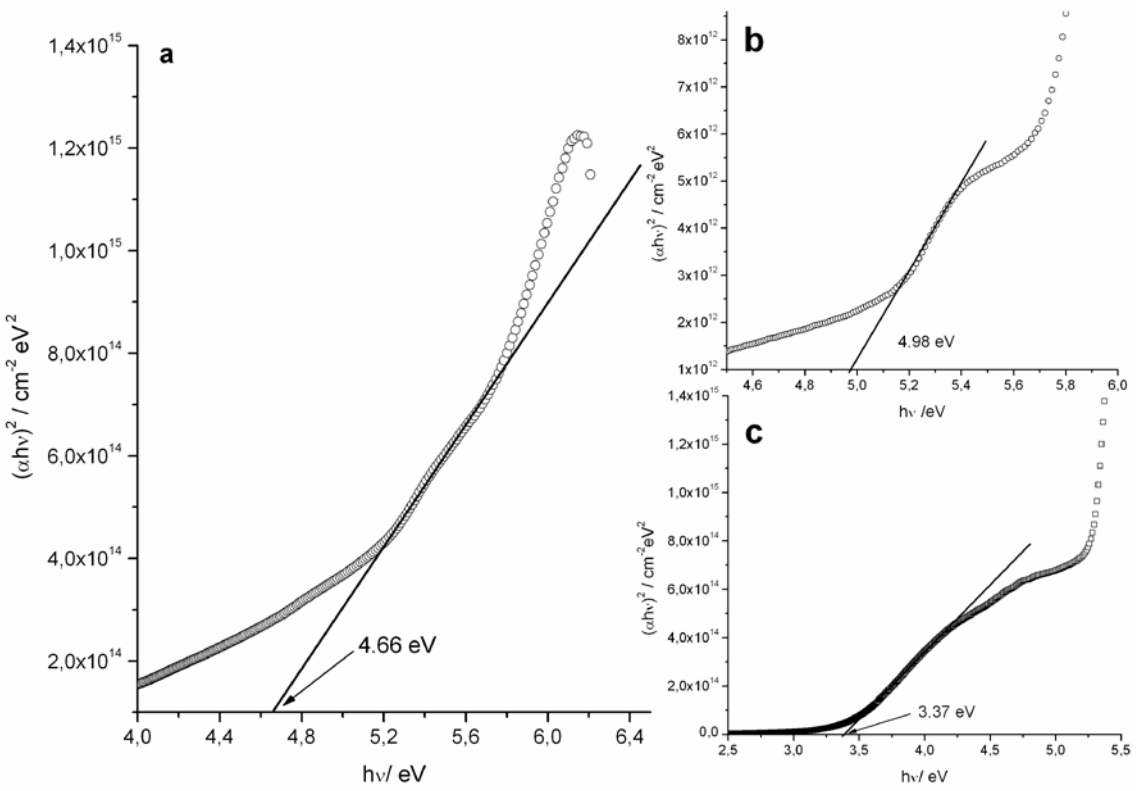


Characterization by TEM of CeO_2 nanoparticles prepared using a water/CTAB-ButOH-$Ce(Val)_3$/ oil microemulsions systems. No differences can be appreciated by changing the oil microemulsion phase. X-ray diffraction pattern of CeO_2 nanoparticles. The diffraction peaks observed show a good match with those of bulk cerium oxide (cerianite, R050379-9 from RUFF database[1]). There is a considerable broadening of the peaks, suggesting that these particles are very small in dimensions. The observation of material microstructure by TEM, revealed the presence of small particles of CeO_2 of d ~ 5 nm in agreement of the results obtained by DRX.

[1] http://rruff.info/







Band gap energy estimation of (a) Si-Ce2, (b) Si2 and (c) CeO_2 nanomaterials by plotting $(\alpha h\nu)^m$ of the microcrystalline materials against the photon energy ($h\nu$).

The band gap energy was estimated by plotting $(\alpha h\nu)^m$ of the microcrystalline materials against the photon energy ($h\nu$). Where α is the absorption coefficient, $h\nu$ is the photon energy, E_g is the band gap energy. If we assume that the transition of electrons through the forbidden zone occurs between states corresponding to the maximum of the gap and the valence band minimum conductance; taking into account only direct transitions $m = 2$. The adsorption (A) is converted to the absorption coefficient using the following relationship[2] $\alpha = (2.303 \times 10^3 / lc) A\rho$, where A is the adsorption of the sample; ρ is the density of crystobalite (2.33 g cm^{-3}) for SiO_2 materials and of cerianite (7.132 g cm^{-3}) for CeO_2 nanoparticles[3], l is the cuvette length (1 cm), and c is the concentration of the sample (c = 0.001g cm^{-3}). The band gap energy was determined by extrapolating the adsorption coefficient (α) to zero. The computed band gap values for siliceous and Ce-doped silica materials ($E_{g,\ Si2=}$ 4.98 eV and $E_{g,\ Si\text{-}Ce2=}$ 4.66eV) are highly inferior to the

[2] Serpone N, Lawless D, Khairutdinov R. J. Phys. Chem. 1995, 99, 16646
[3] S. Sathyamurthy, K. J. Leonard, R. T. Dabestani, M.P. Paranthaman. Reverse micellar synthesis of cerium oxide nanoparticles. Nanotechnology 16 (2005) 1960-1964.

experimental band gap values obtained for SiO_2 polymorphs (8.9 eV for α-quartz and superior values for β-quartz, α-cristobalite, β-cristobalite and tridymite[4 48]) and similar to those obtained for silicon based metal-oxide-semiconductors (MOS)[56 49, 50]. The computed band gap values ($E_{g, CeO2}$ = 3.37 eV) for ceria nanoparticles is similar to those observed in literature[3, 7]

N_2 adsorption-desorption information data of the materials templated with water/CTAB-ButOH/ ciclohexane and water/CTAB-ButOH/ n-hexane microemulsions. Adsorption parameters were obtained from N_2 adsorption-desorption isotherms measured at 77.6 K with a Micrometrics Model Accelerated Surface Area and Porosimetry System (ASAP) 2020 instrument. Each sample was degassed at 373K for 720 min at a pressure of 10^{-4} Pa.

Microemulsion System	**S_{BET} m^2/g**	**S_{tmp} m^2/g**	**S_{text} m^2/g**	**V cm^3/g**	**D_{aap} nm**
Water/CTAB-ButOH/ciclohexane	65.72	1.23	64.49	8.70×10^{-6}	9.61
Water/CTAB-ButOH/n-hexane	13.66	1.09	12.57	3.72×10^{-4}	8.93
Water/CTAB-ButOH/n-heptane	11.08	0.32	10.76	1.50×10^{-5}	7.49
Water/CTAB-ButOH/isooctane	20.37	0.29	20.08	9.00×10^{-6}	11.25

S_{BET}, BET surface area; S_{tmp}, t-plot micropore area; S_{text}, t-plot external surface; V, t-Plot micropore volume; D_{aap}, adsorption average pore diameter by BET.

[4] Gnani E, Reggiani S, Colle R, Rudan, M. VLSI DESIGN 2001, 13 (1-4), 311
[5] Yamasaki T, Kaneta C, Uchiyama T, Uda T, Terakura K. Physical Review B 2001, 63, 1153141
[6] Städale M, Tuttle B, Fischer B, Hess K. Journal of Comp. Electronics. 2002, 1, 153.
[7] M.G. Sujana, K.K. Chattopadyay, S Anand. Characterization and optical properties of nano-ceria synthesized by surfactant-mediated precipitation technique in mixed solvent system. App. Surf. Sci. 254 (2008) 7405-7409.