

## PÔSTER - RESUMO - MATERIAIS E BIOMATERIAIS

### CREATING ACTIVE OXYGEN VACANCIES ON CeO<sub>2</sub>:NiO SUPPORTED ON SBA-15 FOR ENVIRONMENTAL TECHNOLOGIES

*Danilo Waismann Losito (d.losito@unifesp.br)*

*Desconhecido 138 (fabio.bellot@int.gov.br)*

*Raimundo Crisostomo Rabelo Neto (rabelonetc@gmail.com)*

*Mauro Russélio David Jota (mauro.russelio@ime.eb.br)*

*Santiago José Alejandro Figueroa (santiago.figueroa74@gmail.com)*

*Tereza Da Silva Martins (tsmartins@unifesp.br)*

Cerium oxide-based nanocomposites are considered highly promising materials for environmental technologies due to their remarkable redox properties and unique structural, textural, and morphological features. In particular, ceria (CeO<sub>2</sub>) has attracted attention for its ability to undergo rapid Ce<sup>3+</sup>/Ce<sup>4+</sup> redox cycling, which is directly related to the presence of oxygen vacancies (OV). These vacancies act as active sites for gas adsorption and activation, making ceria-based systems excellent candidates for catalytic processes involving carbon dioxide (CO<sub>2</sub>). In this study, we investigated the incorporation of nickel oxide (NiO) into the ceria framework to produce SBA-15:CeNi nanocomposites with enhanced CO<sub>2</sub> interaction. The introduction of NiO into CeO<sub>2</sub> increases the concentration of OV, which are crucial for CO<sub>2</sub> physisorption and activation. These defects provide sites where CO<sub>2</sub> molecules can be retained and subsequently activated, facilitating their conversion in catalytic reactions. To

further improve the performance of the system, SBA-15 mesoporous silica was employed as a support. SBA-15 is well known for its ordered two-dimensional hexagonal mesostructure (p6mm space group), high surface area, and uniform pore distribution, which contribute to improved nanoparticle dispersion, reduced agglomeration, and stronger metal–support interactions. The nanocomposites were synthesized using nickel and cerium nitrate precursors via two different approaches: post-synthesis (PS) and direct synthesis (DS). Small-angle X-ray scattering (SAXS) confirmed that all samples preserved the 2D hexagonal mesostructure (p6mm space group) with narrow pore size distribution, characteristic of SBA-15. X-ray diffraction (XRD) revealed the presence of cubic fluorite-type CeO<sub>2</sub> and halite-type NiO, both crystallizing in the Fm-3m space group. Raman and X-ray photoelectron spectroscopy (XPS) analyses demonstrated successful Ni doping into the ceria lattice, generating structural defects such as OV and promoting the coexistence of Ce<sup>3+</sup>/Ce<sup>4+</sup> species. Scanning and transmission electron microscopy (SEM/TEM) highlighted morphological differences between the samples, with superior nanoparticle dispersion observed in the PS-derived material. CO<sub>2</sub> adsorption–desorption studies revealed that SBA-15:CeNi prepared by PS route exhibited enhanced CO<sub>2</sub> retention compared to DS sample and Ni-only SBA-15 composites. This improvement was attributed to smaller particle size, higher dispersion, and increased OV concentration. Importantly, catalytic tests demonstrated that SBA-15:CeNi-PS achieved 95.6% selectivity in CO<sub>2</sub> methanation, underscoring its potential as a highly efficient candidate for carbon capture and conversion technologies. Overall, the results highlight oxygen vacancies as an important factor in CO<sub>2</sub> interaction, which may be studied not only for catalytic methanation but also for other applications where OV play a central role, such as gas sensing and adsorption. This study therefore provides valuable insights into the design of advanced nanocomposites that combine structural stability, high dispersion, and defect engineering to address solutions for environmental challenges.

We acknowledge financial support from CAPES (88887.807767/2023-00), INCT/INEO, CNPq (408449/2024-1), and FAPESP (2025/27044-5). We thank M.C.A. Fantini, C.L.P. Oliveira, T.M. Germano, and A.C.F. da Silveira (USP) for SAXS support; F.F. Ferreira (UFABC) for XRD; Â. Albuquerque (LNNano-CNPEM) for XPS; CaPGPQ-UNIFESP Diadema for SEM and Raman; and N.S. Gonçalves for Raman assistance.

Palavras-chave: structural defects; ceria oxide; nickel oxide; post-synthesis; direct synthesis; carbon capture.