

# Structural and photocatalytic behavior of thermally stable SiO<sub>2</sub>@TiO<sub>2</sub> core-shell particles

Ubirajara Pereira Rodrigues Filho<sup>1\*</sup>, Elias Paiva Ferreira Neto<sup>1</sup>, Vitor Pires Martinez<sup>1</sup> Jean Minar Santa Cruz Yabarrena<sup>1</sup>, Sajjad Ullah<sup>2</sup>

<sup>1</sup>*Instituto de Química de São Carlos, Universidade de São Paulo, São Carlos, Brazil,*

<sup>2</sup>*Institute of Chemical Sciences, University of Peshawar, Peshawar, Pakistan*

\*e-mail: [uprf@iqsc.usp.br](mailto:uprf@iqsc.usp.br)

TiO<sub>2</sub> photocatalytic activity closely depends on physical properties such as surface area, crystallinity, morphology, particle size and crystalline phase of titania, with anatase being the most active photocatalytic polymorph of TiO<sub>2</sub><sup>1</sup>. In order to make possible the use of TiO<sub>2</sub> photocatalysts in different applications it is important to develop synthetic strategies that allow control over such physical properties, especially in the case of nanometric TiO<sub>2</sub>, which suffers from drawbacks such as tendency to agglomeration, phase transformation and decrease in surface area upon thermal treatment<sup>2</sup>. Furthermore, stabilization of TiO<sub>2</sub> in anatase form at high temperatures (T > 800°C) avoiding anatase-to-rutile transformation is required in applications that involves high temperature processing (e.g. self-cleaning coatings and photocatalytic ceramics). Aiming to address these issues, in this study we report preparation of thermally stable SiO<sub>2</sub>@TiO<sub>2</sub> core-shell nanocomposites<sup>3</sup>. Such nanocomposites can be prepared by the grafting and controlled hydrolysis of titanium alkoxides on the surface of silica particles dispersed in ethanol/isopropanol mixtures. Electron microscopy analysis evidences uniform coating of SiO<sub>2</sub> spheres (mean size 200 nm) with a TiO<sub>2</sub> shell constituted of 5-7 nm titania nanocrystals. The SiO<sub>2</sub>@TiO<sub>2</sub> particles thermal stability was studied by *in-situ* synchrotron powder X-Ray diffraction with temperature range spanning from room temperature to 1000°C and *ex-situ* X-ray diffraction from room-temperature to 1200°C. Both measurements prove the phase stability of the anatase up to 1200°C, and slight size increase of the crystallite size at 1000°C. Improvement of the photocatalytic activity of SiO<sub>2</sub>@TiO<sub>2</sub> is observed upon calcination between 800 and 1000°C, while a drastic decrease in photoactivity is observed for calcined unsupported titania caused by almost complete conversion of anatase into rutile and significant loss of specific surface area. Moreover, photoactivity decrease was also observed for heat-treated SiO<sub>2</sub>@TiO<sub>2</sub> samples with high TiO<sub>2</sub> loading (>30%) and which formation of unsupported titania particles occurred due to homogenous nucleation during sol-gel deposition, further confirming the importance of core-shell morphology for enhanced thermal stability and photocatalytic activity.

1. Schneider, J.; Matsuoka, M.; Takeuchi, M.; Zhang, J.; Horiuchi, Y.; Anpo, M.; Bahnemann, D. W. ;*Chem. Rev.* **2014**, *114*, 9919.
2. Porter, J. F.; Li, Y.-G.; Chan, C. K. ;*J. Mater. Sci.* **34**, 1523.
3. Ullah, S.; Ferreira-Neto, E. P.; Pasa, A. A.; Alcântara, C. C. J.; Acuña, J. J. S.; Bilmes, S. A.; Martínez Ricci, M. L.; Landers, R.; Fermino, T. Z.; Rodrigues-Filho, U. P. ;*Appl. Catal. B Environ.* **2015**, *179*, 333.

The authors would like to thank São Paulo Research Foundation (FAPESP) for financial support (grant#2013/24948-3 and grant #2011/08120-0)