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Band-gap engineering and morphological control of TiO_2 nanoparticles by a semi-solvothermal route

TiO_2 has become a material of great interest for photocatalytic H_2 production, environmental purification and solar energy conversion.[1] It is generally accepted that anatase is the most active photocatalyst of the three possible polymorphs of TiO_2. The properties influencing the photoactivity of anatase particles have been reported to include surface area, crystallinity, crystallite size, crystal structure;[2,3] and the morphology of the particles. Among the key parameters boosting the photocatalytic efficiency of anatase nanoparticles, an increased light absorption to extend the optical response to the visible, together with an improved charge separation of the electrons and holes generated upon photoexcitation, shall be enumerated. Conventional TiO_2 anatase nanoparticles have a bandgap of 3.20 eV which only allows the excitation of carriers by light with wavelengths smaller than 387 nm (UV region); if visible light harvesting is to be enabled, this gap should be narrowed. In this work, pure anatase nanoparticles have been obtained using a solvothermal process with reduced band-gap and/or reactive faces. Trifluoroacetic acid is used as morphological control and doping agent, and urea is employed as a reduction agent.[4,5] Through the careful choice and control of the working conditions, it is possible to control the final properties of the produced nanoparticles, e.i. morphology, size, crystallinity, crystal phase, network defects and band gap. The obtained results point out that in order to improve the photocatalytic performance, a well-designed intrinsic defective TiO_2 system for visible light driven photocatalysis should meet all three requirements simultaneously: (i) reduced band gap for visible light absorption, (ii) appropriate energy level to initiate photocatalytic reaction, and (iii) proper defect species or highly active surfaces to separate photo-generated charge-carriers (electrons and holes) for reaching high catalytic performance.

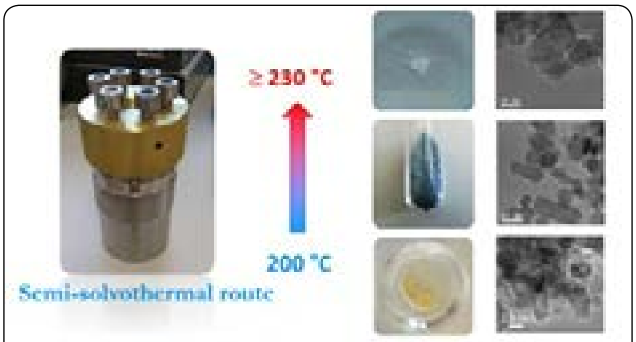

Figure 1: Different TiO_2 anatase nanoparticles with controlled band-gap and morphology obtained by a semi-solvothermal route. (scale bar: 10, 20 and 10 nm, respectively)

Recent Publications

1. Xu H, Ouyang S, Liu L, Reunchan P, Umezawa N, Ye J (2014) Recent advances in TiO_2-based photocatalysis. J. Mater. Chem. A 2: 12642-12661.
2. Sclafani A, Herrmann J M (1996) Comparison of the Photoelectronic and Photocatalytic Activities of Various Anatase and Rutile Forms of Titania in Pure Liquid Organic Phases and in Aqueous Solutions. J. Phys. Chem. 100: 13655-13661.
3. Carp O, Huisman C L, Reller A (2004) Photoinduced reactivity of titanium dioxide. Prog. Solid State Chem. 32: 33-177.

4. Calatayud D G, Jardiel T, Peiteado M, Illas F, Giamello E, Palomares, F J, Fernández-Hevia D, Caballero A C (2015) Synthesis and Characterization of Blue Faceted Anatase Nanoparticles through Extensive Fluorine Lattice Doping. J. Phys. Chem. C 119: 21243-21250.
5. Calatayud D G, Jardiel T, Peiteado M, Rodríguez C F, Espino Estévez M R, Doña Rodríguez J M, Palomares F J, Rubio F, Fernández-Hevia D, Caballero A C (2013) Highly photoactive anatase nanoparticles obtained using trifluoroacetic acid as an electron scavenger and morphological control agent. J. Mater. Chem. A 1: 14358-14367.

Biography

Dr. David G. Calatayud received his doctorate in Chemistry from the University of Autonoma de Madrid in 2004 where he studied new asymmetric double-Schiff-bases containing a thiosemicarbazone moiety and their complexes. After completing his PhD he worked as a postdoctoral researcher in the Spanish National Research Council – CSIC, focusing on novel materials, nanotechnology, photocatalytic nanoparticles and crystal engineering. In 2014 he joined Sofia Pascu's group at the University of Bath (UK) as a Research Associate developing on 'smart' all-in-one multimodal imaging probes as novel synthetic platform systems for personalised diagnosis and treatment of diseases such as cancer. In 2016 he moved to the Funceramics group at Instituto de Ceramica y Vidrio – CSIC, his current research is focused on the development of new experimental techniques to assemble functional materials for advanced micro and nanoelectronics, biosensing, molecular imaging and drug delivery applications.

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