

## MAP-fis Essay Proposal, 2015-2016

(please write in English)

### Supervisor

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### Title

Photoelectrochemical cells for hydrogen production from solar energy

### Area

(Materials, Optics, Condensed Theory, High Energy Theory,...);

Materials

### Summary of Proposal

Hydrogen energy has become of utmost importance due to the imperative requirements of solving the global energy demand and environmental problems, representing also a clean and low-cost fuel. Photoelectrochemical cells (PECs) for water splitting are one of the most promising ways to convert solar energy into chemical energy [1]. In particular, hematite ( $\alpha\text{-Fe}_2\text{O}_3$ ) presents attractive properties as photoanode for this type of devices, as demonstrated by Graetzel's group that succeeded in building a tandem PEC cell based on a hematite photoanode [2]. On semiconductor photoanodes, the path travelled by the hole to reach the surface, avoiding electron-hole recombination, is the most important factor of the photoresponse. Self-ordered  $\alpha\text{-Fe}_2\text{O}_3$  nanotubes (NTs) with 1D architecture, obtained by electrochemical anodization techniques, have been considered the most suitable way to achieve the largest enhancement of specific surface area without an increase of the geometric area, leading to enhanced PEC performances. Due to the ultra-thin walls of the NTs, holes can reach the surface faster, which reduce electron-hole recombination losses; also the 1D nature of the NTs leads to faster electron transfer of the electrodes ensuring that holes can reach the surface faster than in other architectures . (

This essay proposal targets a review of the fabrication methods of nanostructured photoanodes based in hematite NT arrays for application in PECs, with main focus on the electrochemical anodization process and its optimization for achieve highly organized arrays of NTs.

The main techniques for the morphological, electrical and magnetic characterization of these nanostructures will be also discussed.

The review will be performed having as long term goal of the Phd work the development of

innovative and more efficient hematite based photoelectrodes for solar water splitting, with efficiencies significantly above the present state-of-the-art value of 4.32 mA/cm<sup>2</sup> (for hematite thin films, at 1.23VRHE) and towards the 10% demands for commercialization [5-7].

## References

*(to allow students first look at topic)*

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- [2] A. Duret, M. Gratzel, Visible Light-Induced Water Oxidation on Mesoscopic alpha-Fe<sub>2</sub>O<sub>3</sub> Films Made by Ultrasonic Spray Pyrolysis, J. Mater. Chem. B, 109 (2005) 17184-17191.
- [3] S. K. Mohapatra et al., Water Photooxidation by Smooth and Ultrathin  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Nanotube Arrays, Chem. Mater., 21 (2009) 3048-3055.
- [4] T.J. LaTempa et al., Temperature-Dependent Growth of Self-Assembled Hematite (alpha-Fe<sub>2</sub>O<sub>3</sub>) Nanotube Arrays: Rapid Electrochemical Synthesis and Photoelectrochemical Properties, J. Phys. Chem. C, 113 (2009) 16293-16298.
- [5] J. Y. Kim et al., Single-crystalline, wormlike hematite photoanodes for efficient solar water splitting, Sci. Rep., 3 (2013).
- [6] T. Lopes et al., An innovative photoelectrochemical lab device for solar water splitting, Sol. Energ. Mat. Sol. Cells, 128 (2014) 399-410.
- [7] Gratzel, M., NanoPEC. <http://www.fch.europa.eu/sites/default/files/FCH%20Programme%20review%202011-%20Project%20NanoPEC.pdf>