

## MAP-fis Essay Proposal, 2015-2016

(please write in English)

### Supervisors

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### Title

**Photoactive nanostructured materials and their application to optoelectronic devices**

### Area

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

Optoelectronics; 2D materials; nanotechnology

### Summary of Proposal

This research proposal is on “Photoactive nanostructured materials and their application to optoelectronic devices”. Two optoelectronic devices will be studied: silicon-based photocathodes decorated with nanocatalysts (metal phosphide nanoparticles) for solar-driven hydrogen production; and, photodetectors based on 2D materials.

As a motivation for the first part of the study one could say that solar energy is by far the largest exploitable renewable source among others (e.g., wind, hydropower, biomass), providing more energy to the Earth in one hour than all of the energy consumed by mankind within one year. Given the intermittent nature of sunlight, if solar energy becomes a major primary energy source in the future, the harvested energy must be able to be stored and dispatched on demand to the end user. Apart from the existing way of storing solar energy using batteries, an especially attractive approach is to store solar-converted energy in the form of chemical bonds, e.g., molecular hydrogen (H<sub>2</sub>), which is considered very promising for small-scale, highly-distributed energy supply. While solar-to-H<sub>2</sub> conversion is already a proven technology, the key challenge facing scientists & engineers is now how to bring materials costs down such that widespread use of solar fuels and up-scale deployment of solar-powered electrolyzers can be made possible. To this end, developing efficient, low-cost, and durable semiconducting photoelectrodes is of paramount importance.

Therefore, this proposal aims to develop silicon (Si) based photocathodes coated with a chemically-inert thin protection layer and decorated with inexpensive, earth-abundant transition metal phosphide (TMP) nano-catalysts. The proposed research must address key challenges to overcome for using Si, the second most abundant element in the Earth’s crust, as a

photocathode material for solar H<sub>2</sub> production: namely, poor chemical stability in electrolytes, small harvestable photovoltage, and the need for precious, scarce platinum (Pt) catalysts.

The motivation to study the type of nanodevices proposed in the second part of the project is the following: recent developments in vertical heterostructures, based on two-dimensional materials, have paved the way to new types of photodetectors. A photodetector of this type is composed by stacking a boron nitride buffer-layer, a graphene sheet, a multilayer transition metal dichalcogenide (TMDC), a second graphene sheet, and a boron nitride encapsulating layer. This architecture is called a vertical photodetector. The two graphene sheets work as conductive electrodes and the active medium is the multilayer TMDC. These devices are interesting because they are extremely thin (only a few atoms thick), flexible and with much better electronic properties than more conventional materials for wearable devices. In order to be economically viable, these devices have to be produced on large area (wafer size), with a method suitable for upscaling. One of the techniques that is compatible with large-area growth of these materials is Chemical Vapor Deposition (CVD), which allows large, reproducible and highly controlled production of very thin (even atomically thin) layers of many different materials.

This proposal entails two types of research tasks: those related with material growth and those related with device design and fabrication.

## References

(to allow students first look at topic)

- Reece, S.Y., Hamel, J.A., Sung, K., Jarvi, T.D., Esswein, A.J., Pijpers, J.J.H., Nocera, D.G. (2011) Wireless solar water splitting using silicon-based semiconductors and earth-abundant catalysts. *Science* 334, 645-648
- Huang, Z.P., Geyer, N., Liu, L.F., Li, M.Y., Zhong, P. (2010) Metal-assisted electrochemical etching of silicon. *Nanotechnology* 21, 465301
- Xiao-Qing Bao, M. Fatima Cerqueira, Pedro Alpuim, and Lifeng Liu, *Chem. Commun.*, Silicon Nanowire Arrays Coupled with Cobalt Phosphide Spheres as a Low-Cost Photocathode for Efficient Solar Hydrogen Evolution (2015) 51 (53), 10742 – 10745
- Lin, Y.J., Battaglia, C., Boccard, M., Hettick, M., Yu, Z.B., Ballif, C., Ager, J.W., Javey, A. (2013) Amorphous Si thin film based photocathodes with high photovoltage for efficient hydrogen production. *Nano Lett.* 13, 5615-5618
- L. Britnell, R. M. Ribeiro, A. Eckmann, R. Jalil, B. D. Belle, A. Mishchenko, Y.-J. Kim, R.V. Gorbachev, T. Georgiou, S. V. Morozov, A. N. Grigorenko, A. K. Geim, C. Casiraghi, A. H. Castro Neto, K. S. Novoselov Strong Light-Matter Interactions in Heterostructures of Atomically Thin Films (2013) *Science* 340, 1311
- G-H Lee, Y-J Yu, X Cui, N Petrone, C-H Lee, M S Choi, D-Y Lee, C Lee, W J Yoo, K Watanabe, T Taniguchi, C Nuckolls, P Kim, J Hone, Flexible and Transparent MoS<sub>2</sub> Field-Effect Transistors on Hexagonal Boron Nitride-Graphene Heterostructures (2013) *ACS Nano* 7, 7931
- Wenjing Zhang, Chih-Piao Chuu, Jing-Kai Huang, Chang-Hsiao, Chen, Meng-Lin Tsai, Yung-Huang Chang, Chi-Te Liang, Yu-Ze Chen, Yu-Lun Chueh, Jr-Hau He, Mei-Yin Chou, Lain-Jong Li, Ultrahigh-Gain Photodetectors Based on Atomically Thin Graphene-MoS<sub>2</sub> Heterostructures (2014) *Scientific Reports* 4, 3826