PhD Proposal 2017

School: Ecole Centrale de Lyon	
Laboratory: Lyon Institute of Nanotechnology	**Web site: http://inl.cnrs.fr/**
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Collaboration with other partner during this PhD: **In France:**	**In China:**

Title: Semiconducting core / functional oxide shell nanowires for water reduction
Scientific field: Nanotechnology, Material science.
Key words: nanowires, core-shell structure, interfaces, semiconductors, functional oxides, photocatalysis

Details for the subject:

Background, Context:

Photocatalytic water splitting is one of the most promising concepts in the context of green energy and CO_2 reduction [1]. This process which can be seen as an artificial photosynthesis mechanism consists in the capture of light energy and its storing into chemical bonds. In the last years, the development of new materials in order to increase the efficiency of hydrogen production in such photoelectrochemical cells has attracted the scientific community.
TiO_2 is the most popular material for photocatalysis [1], however TiO_2 exhibit a large bandgap which do not match perfectly solar spectrum and has low photocurrent density. III-V semiconductors such as GaAs or GaP are among the best materials thanks to their high photocurrent density and narrow band gap. However III-V are not stable during the water splitting process which prevent their utilization. Recently it was shown that surface passivation with thin perovskite oxide layer such as $SrTiO_3$ could dramatically improve the efficiency of silicon photoanode for water reduction [2].
Thanks to their high surface area and efficient charge separation, nanowires are expected to have significantly improved photocatalytic activity compare to thin films [3]. Recently, we developed a methodology allowing the growth of heterogeneous materials on the facet of III-V nanowires leading to the formation of core shell heterostructures [4]. Using this method we grew for the first time $SrTiO_3$ / GaAs nanowires [5] (see figure 1). These newly fabricated semiconducting / functional oxide core-shell nanowires meet all the requirements of highly efficient material for water splitting.

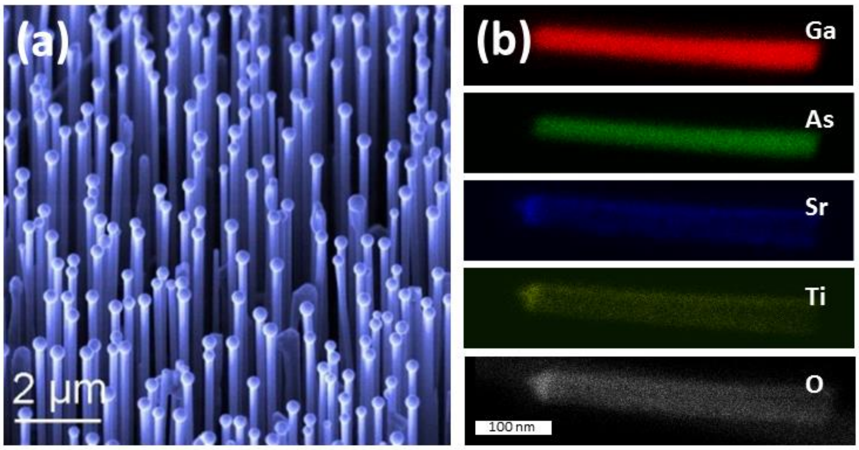

Figure 1: Scanning Electron Microscopy image of GaAs nanowires grown using Vapor Liquid Solid method by Molecular Beam Epitaxy (a). Two-dimensional element mapping for a single GaAs / $SrTiO_3$ nanowire (b) [5].

Research subject, work plan:

The objective of the PhD will be to develop new materials based on core-shell nanowires for water reduction with the objective to obtain the highest device efficiency.

<u>Nanowires growth:</u>
Core-shell hybrid nanowires will be grown on silicon substrate using molecular beam epitaxy facility of the "NanoLyon" clean room. Metallic particle catalyst will be deposited on the nanowires facets using spin coating or physical vapor deposition to obtain a good interfacial transfer between the semiconductor and the electrolyte. Several catalysts will be tested such

as Pt and Rh, a particular emphasis will be given on the size and distribution of the nanoparticles on the nanowires facets.

Structure morphology and interface chemistry:
Standard characterization including (SEM, TEM, XRD, XPS) will be performed in order to design the best nanowires structure and morphology for water splitting (length, diameter, nanowires density etc.). Finally *in situ* measurements will be performed during exposition to water using near ambient pressure XPS and environmental TEM.

Photocatalytic water splitting:
Photocurrent density will be measured as a function of the nanowires main characteristic, results will be compared with thin films grown in the laboratory [6]. Finally the water splitting efficiency for hydrogen production will be measured.

References:

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[3] A. Standing, S. Assali, L. Gao, M. A. Verheijen, D. van Dam, Y. Cui, P. H. L. Notten, J. E. M. Haverkort, E. P. A. M. Bakkers, *Efficient water reduction with gallium phosphide nanowires*, **Nature Communications** 6, 7824 (2015)
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