

Research Topic for the ParisTech/CSC PhD Program

Field: Energy, Processes, Materials Science, Physics, Design, Industrialization

Subfield: (Applied Physics, Chemistry, Mathematics, Mech. Eng. etc...)

Title: Hierarchically assembled nanostructures for energy and environmental sustainability applications

ParisTech School: LPICM-Ecole Polytechnique/ CNRS

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Short description of possible research topics for a PhD:

The effect of global warming as a consequence of continuous consumption of energy resulted from burning of fossil fuels, raised the challenge for both fundamental and industrial research to find sustainable solutions to tackle the problem, with emphasis on topics related to the energy storage devices like supercapacitors, Li-ion and/or Na-ion batteries, and on the photocatalytic reduction of CO₂ and H₂ production. A raising hot topic in the field of new advanced materials for energy applications, focus on the Transition Metal Dichalcogenides (TMDCs) in nanostructured form that receive a still increasing attention as potential candidates for applications in the area of energy storage and nanocatalysis. [L. Peng, *et al. Adv Energy Mat.* 6 (2016) 1600025]. For Electrochemical Energy Storage devices (as for example Li-ion batteries), depending on their chemical composition, TMDCs can be used either as cathode or anode material and exhibit theoretical specific capacities larger than the commercially available graphite anode or transition layered metal oxides [H. Hwang, *et al. Nano Lett.* 11 (2011) 4826]. At the same time their large interlayer Van der Waals gaps allow the intercalation of Li ions (or larger size Na ions for use in Na-ion batteries) in their structure alleviating the large volume expansion presented in common alloying type materials. However this area of research is still in its infancy and extensive studies need to be pursued for improving the light harvesting and the conversion efficiency in 2D layered TMDs as well as further understanding of the complex photocatalytic mechanism on these materials. The goal of this thesis project is to develop hierarchically assembled nanostructures in forms of electrodes based on dense, thin walled carbon nanotubes (CNTs) carpets used as current collectors and decorated with various TMDC nanomaterials. The role of the CNTs is to: i) increasing the specific electrode surface area ii) insure the fast charge transfer and III) promote good crystallinity of the deposited active material. The functionalization of vertically aligned CNT by TMDs offers an unprecedented opportunity for their use in energy storage devices and photocatalytic reactions. These hierarchical nanoarchitectures, due to their unique combination of redox chemistry, rapid ionic-transport channels, short-distance interactions between charge carriers, as well as between carriers and ions, and their earth-abundance, will play a key role in the successful implementation in the area of rechargeable batteries, photocatalytic water splitting and environmental sustainability applications.

Required background of the student: We are seeking an excellent young scientist, eager to carry out leading edge research in a multidisciplinary field at interface of materials science, surface science and electrochemistry. The candidate should have a good background in (electro) chemistry and/or condensed matter physics. He (she) will work in strong interaction with a multi-disciplinary team made up of physicists, chemists and engineers.