

Description of the funded research project

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Porous Mesoscopic Assemblies of Non-Oxide Nanoparticles for Photoelectrocatalytic Energy Conversion Applications

Principal Investigator: Gerasimos S. Armatas

Reader-friendly title: NanoFuel-H2

Scientific Area: Environment & Energy

Institution and Country: University of Crete, Greece

Host Institution: University of Crete

Collaborating Institutions: Northwestern University, Nanyang Technological University, Cyprus University of Technology

Project webpage:

https://www.materials.uoc.gr/garmatas/research.html

Budget: 169.983,00 €

Duration: 36 months



Porous Mesoscopic Assemblies of Non-Oxide Nanoparticles for Photoelectrocatalytic Energy Conversion Applications



PI: Prof. Gerasimos Armatas



Photoelectrochemical (PEC) water splitting provides a convenient means of energy storage and production. By utilizing the abundant solar energy to convert water into hydrogen, this method hold promises to address the rising energy demands. PEC process, inspired by natural photosynthesis, involves electrochemical spitting of water into a semiconductor-based device using solar energy. Most recent efforts at improving photon harvesting and solar-to-hydrogen conversion efficiency of PEC cells have boosted the synthesis of new photocatalysts at the nanoscale. Developing semiconductor nanoparticles can provide new opportunities in facing the current challenges in hydrogen production. Small-sized nanoparticles (2–20 nm), unlike to bulk solids, offer great perspectives owing to high photon collection efficiency and low electron-hole recombination yield. However, the practical application of nanoparticles for PEC devices depends on the ability to assemble complex 3D porous architectures. Up to date the synthesis of high-surface-area, open-pore mesostructures from colloidal nanoparticles is an open challenge.

This proposal outlines a research project aiming to gain insight into the PEC properties of mesoporous ensembles from transition-metal chalcogenide nanoparticles. Metal chalcogenides, especially spinel chalcogenides such as $Cdln_2S_4$ and $NiCo_2S_4$, exhibit an electronic band structure that is well suited for water splitting catalysis, excellent charge transport properties, adequate chemical stability especially in alkaline solution, and visible-light response. Moreover, thiospinels are not toxic and are normally inexpensive materials. All these characteristics make them attractive candidates for widespread application in energy conversion. Mesoporous heterojunctional frameworks of metal chalcogenide and transition-metal phosphide nanoparticles (like Ni_2P and CoP) are also of considerable interest to this project. These complex materials are expected to blend disparate functionalities into the inorganic structure such as high mesoporosity and PEC activity, which are difficult to obtained in individual nanoparticles or conventional porous solids. Nanoparticle assemblies will be examined as photoelectrodes in visible-light-driven water splitting at non-bias conditions.



Currently, hydrogen is predominantly produced by fossil fuel reforming, which is an environmentally unfriendly and expensive process. Recently, semiconductor photocatalysis has become an intriguing method for economical and eco-friendly production of hydrogen by using solar energy. Although advantageous, the photocatalytic hydrogen evolution from water is a complex process and usually suffers from low efficiency due to the fast electron-hole recombination and poor visible-light absorption of the catalyst. Nanostructured spinel chalcogenides are the focal point of current investigations for energy applications. They show great promise in overcoming the above-mentioned limitations, demonstrating good perspectives for practical use in photocatalysis, as well as in photovoltaics and energy storage devices. To date, most spinel chalcogenide materials used for energy conversion are in bulk or thin-film forms. Besides, there are seldom publications reporting about transition metal phosphides as photocatalysts for hydrogen evolution. Very recently, some synthetic methods for thiospinel nanoparticles, such as solvothermal reactions, have appeared in literature. These studies describe the synthesis of thiospinel nanoparticles with different size and composition, making them convenient starting materials for assembling extended porous structures.

The idea of combining self-assembled spinel chalcogenide nanoparticles and high porosity for solar fuel production is original and has never been reported until now. This proposal aims to develop a novel family of porous nanomaterials for energy conversion applications. Compared to isolated nanoparticles, 3D ensembles of nanoparticles are expected to elucidate advantageous characteristics such as large and accessible pore surface. Moreover, a tightly bound network of nanoparticles has the potential to exhibits long electron diffusion length by interfacial charge transfer along the assembled structure and, eventually, prolonger electron lifetimes. These characteristics could provide large semiconductor/electrolyte interfacial area and improved charge carrier separation yield. Therefore, the synthesis of these novel semiconductor catalysts can offer new opportunities in facing the current challenges in photoelectrochemical water splitting.



Beyond the state of the art

Focusing on research and advanced synthetic methods and infrastructures for the synthesis of nanostructured materials with improved photoelectrochemical activity, this project will achieve important results in the areas of nanochemistry and nanocatalysis. These findings are expected to provide a tool of knowledge in order to understand the fundamental processes governing the mesoscopic assembly of colloidal nanoparticles and catalytic behavior of complex materials.

Impact on science

The ability to construct low-cost mesoscopic assemblies from colloidal nanoparticles will open a huge number of possibilities for porous materials with a diverse set of multifunctional attributes. Systems that blend disparate features, such as nanoporosity and optical activity, could be of considerable interest for applications in other fields, such as photochemical sensing and light-emitting diodes (LEDs).

Improved knowledge and socio-economic impacts

This proposal aims to contribute to the medium and long-term tackling of energy sufficiency, which is one of the urgent problems of our society. A promising solution to this challenge is to develop novel photocatalytic materials at the nanoscale. These new materials will be useful for practical applications like solar hydrogen production from water.

Potential of gaining professional knowledge

The project is a great opportunity for the member of research group to work in a high-impact technological area within a stimulating, multidisciplinary environment. The research group will gain technical competencies through the project, including experience with state-of-the-art materials processing and characterization techniques. Also, lasting collaboration and important academic interactions within the Host Institution (University of Crete) and world-renowned Universities such as the Northwestern University, Nanyang Technological University and Cyprus University of Technology would be established during the implementation of the project.



The project is a great opportunity for the PI and his research group to work in a high-impact technological area within a stimulating, multidisciplinary environment. The research group will gain technical competencies through the project, including experience with state-of-the-art materials processing and characterization techniques. The results of the project are expected to provide a tool of knowledge in order to understand the fundamental processes governing the mesoscopic assembly of colloidal nanoparticles and catalytic behavior of complex materials. Also, during the implementation of the project, important academic interactions within the Host Institution (University of Crete) and world-renowned Universities such as the Northwestern University, Nanyang Technological University and Cyprus University of Technology would be established. All above qualities will strengthen the applicant's scientific profile and allow him to conduct high-level research during and beyond the project's lifetime.



