Plan Overview

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Title: Development of heterostructured semiconducting nanoparticles for methane conversion by photoelectrocatalytic process

Creator: Ricardo Marques e Silva

Principal Investigator: Ricardo Marques e Silva, Caue Ribeiro de Oliveira

Data Manager: Ricardo Marques e Silva

Project Administrator: Caue Ribeiro de Oliveira

Affiliation: Other

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ORCID iD: 0000-0002-3652-7408

ORCID iD: 0000-0002-8908-6343

Project abstract:

Global warming and wastes disposal are among the main environmental concern that we face today. Livestock (especially cattle) and diverse agro-industrial wastes can generate and, therefore, release large tones of carbon dioxide and methane into the atmosphere per year. After carbon dioxide, methane is regarded as the second most important greenhouse gas in terms of impact on the climate. There is a great interest in developing capable and feasible technologies that can convert these available greenhouse gases into value-added products, thus reducing their emission into the atmosphere. Carbon dioxide has often been more studied than methane. As a result, some materials such as copper, silver, tin, and bismuth have already exhibited good performance. However, methane recovery and conversion strategies have demanded a high quantity of energy and, hence present cost-prohibitive. Electrochemical techniques are particularly desirable to replace the limitations of traditional thermal catalysis as they are fossil-free and sustainable. Some of the electricity required to conduct methane electrocatalysis may be supplied by solar energy, a sustainable and inexpensive energy source. This hybrid photo/electron-driven combined with suitable catalysts can overcome such energetic barriers even at low temperatures (<100 °C) and enable better control of the selectivity, that is, turning methane into profitable organic molecules. Semiconductor structures are the most favorable for these types of reactions, although most of them have achieved low efficiency for partial or selective oxidation of methane into value-added products. On the other hand, complex heterostructures have demonstrated successful results for heterogeneous photoelectrocatalytic reactions since part of the structure acts as a cathode (typically a p-type semiconductor), while the other part acts as an anode (n-type semiconductor). A proper understanding of the different system parts is essential to boost efficiency. Nevertheless, it is still poorly explored in the literature. Factors such as photoelectrocatalyst role, reactions at interfaces (electrode/electrolyte), and reaction mechanism may provide essential information to control the reaction extension. This control may enable the production of hydroxyl radicals (•OH) that react in specific methane sites with

a determined energy rate to produce particular chemicals (liquid fuel, for example). Along these lines, an electrochemical cell comprised of complex nanoparticulate photoelectrocatalysts composed of two aligned epitaxially attached phases is desired. In previous studies, the heterostructured nanoparticles TiO2:SnO2, WO3:TiO2, and g-C3N4/Nb2O5 were revealed to be efficient for the oxidation of different emerging pollutants in water and it possess sufficient potential to oxidize methane. From this perspective, this type of material can be a strong candidate to achieve an economical, more efficient, and environmentally attractive conversion of methane into value-added products. In this context, this project aims to unveil the role of each catalyst mentioned and its reaction mechanisms. The catalysts will be synthesized, and some predefined conditions, such as potentials, presence of oxidants agents, and electron acceptor use will be assessed. Advanced characterization techniques as XRD, N2 physisorption, SEM-FEG, and *in situ* TEM will be employed to support the studies of the catalysts. Techniques such as XPS and FTIR will be carried out to understand kinetic reactions of product formation. Lastly, NMR and CG will be used to identify the formed compounds. The outcome of the proposed research will be essential to understanding the methane oxidation facets under mild conditions and thus indicate the best photoelectrocatalyst to obtain gainful both liquid and gas products.

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Development of heterostructured semiconducting nanoparticles for methane conversion by photoelectrocatalytic process

Data Collection

What data will you collect or create?

In the Project Scope, data will refer to any equipment result, including those intended for graphical plots (e.g., spectroscopic data) or images (e.g. transmission electron microscopy). These data will be collected in different experiments regarded to the produced samples and their characterizations, mainly in digital format.

How will the data be collected or created?

• Catalyst characterizations: scanning and transmission electron microscopies; X-ray diffraction patterns; infrared, Raman and UV-Vis spectroscopies; analytical elemental determination; etc
• Catalysis-related data: CH4 conversion in experimental reactors; temperature-programmed gas desorption; surface-acidity titration, etc.

Documentation and Metadata

What documentation and metadata will accompany the data?

Along to Storage and Backup and Selection and Preservation procedures, all information about equipment model, experiment setup, calibration and accessory data will be kept in Repository. Information management will be done by the Project software using the structure of Laboratory digital notebooks.

Ethics and Legal Compliance

How will you manage any ethical issues?

Each project member should sign an Ethical and Legal Responsibility term, which will be kept by Project Coordination. This term will follow the general guidelines promoted by FAPESP, including data ownership, responsibility and absence of plagiarism declarations. Plagiarism software support will be provided by Project Coordination using Technical Reserve resources. Plagiarism reports for each produced document will be kept together to the final documents in Data Repository.

How will you manage copyright and Intellectual Property Rights (IPR) issues?

Core IT systems to secure IP, includes all input/output devices that store the documents they process, and they are typically networked and connected to remote management systems. Also, cloud applications and file-sharing services.

Storage and Backup

How will the data be stored and backed up during the research?

All produced data will be stored in a Data Repository, based in digital servers (to be acquired using Technical Reserve resource)

provided by the Project Coordination and located in UFSCar TI Support, with remote backup in Embrapa TI Support. For data organization, project management software will be provided to all users keeping basic information about acquisition date, equipment and measurement conditions. Free software alternatives will be analyzed by Project Coordination but keeping all the information encrypted in a physical server, for data reliability and confidentiality.
Management software will include a digital Laboratory Notebook, which will be used by all project members. Related sub-projects (e.g. PhD thesis, posdoc projects, etc) will be registered using the same system. Raw data from equipments will be linked to the digital Notebook and physical versions (paper-based) will be scanned and also stored in digital format. Project Coordination will keep physical notebooks after each sub-project ending at least for 3 years after Project completion.

How will you manage access and security?

All data will be registered in a standard Laboratory Notebook, to be provided by the Project Coordination to all project members. This Laboratory Notebook (see below), in both physical and digital format, is aimed to keep all the information protected and easily available for Coordinators (for checking or validation).

Selection and Preservation

Which data are of long-term value and should be retained, shared, and/or preserved?

Several experiments proposed in this Project are destructive analyses and, in some cases, as-produced catalysts are unstable for a long-term storage. Therefore, methods for sample preparation and characterization will be preserved in digital server for experiment reproduction in a detailed format. When possible, representative samples will be stored and classified by Project Coordination for cross-checking and validation if necessary. As described above, data and methods should be preserved in Repository at least for 10 years.

What is the long-term preservation plan for the dataset?

A Project webpage will be built for public information about main proposal, members, sub-proposals and achievements. A contact email will be provided in webpage. This webpage will be prepared using support from UFSCar and Embrapa TI services and features will be used to help accessing of project members to restricted areas.

Data Sharing

How will you share the data?

Papers and published content will be freely provided in Project webpage using preprint documents or final papers in case of open access options. These will strictly follow Journals' policies and, in cases of restricted data access, Project Coordination will ask FAPESP about any specific event. Raw data will be provided by request to Project Coordination, in Project contact email.
The wide range of possible new knowledge requests a continuous approach of integration and discussion among researchers, which is only possible through regular meetings. Since all the groups are based in Sao Paulo state, dislocations and travels are not a major problem to the group keep in contact. These activities will be supported by the Team experience in research networks as well as supporting structures such as AgroNano Network.3
To access information about each Project achievements, Public Yearly Meetings will be promoted, structured for 2-days meeting. The meeting structure will comprise a public part in the 1st day and a closed session in the 2nd day with project members.
During the 1st day each principal investigator will be invited to present to the general public the main achievements through oral presentations and poster discussion about specific topics. The events will follow the general structure of scientific meetings, with invited presentations (generally by important researchers in related areas, not necessarily working on the project) and regular talks.
A public document will be produced reporting the main achievements and highlights of the research, such as important papers (in high impact factor journals), patents or technology transfer processes. In this document only the public information will be widespread taking care about language (intended to be accessible for all publics) and structure (visually-attractive).
In the 2nd day, the closed meeting will take place to discuss the main problems in the course of research activities and present technologic achievements under protection processes. This closed meeting is intended to help researchers to share their experience in confidential topics and, also, to avoid any unintentional information disclosure which may compromise patent requests.
The Public Yearly Meetings will be important to start cooperation among groups but this will be stimulated by other means, such as regular web-based forums. To that a project webpage will be developed with thematic forums to promote continuous discussion about specific topics and sharing of research results.

The presence in social media will be stimulated, starting a project Facebook page and YouTube channel. These platforms will also help on project webpage development (see above), since information posted there may be widespread by the page and vice-versa. Especially for the YouTube channel, the researchers will be invited to post short videos and short tutorial videos aimed to general public. Each investigator will be stimulated to offer short webcourses and webinars in related topics using the platform. These platforms will also be useful to widespread information about yearly meetings, such as posting news or recorded presentations.

Are any restrictions on data sharing required?

Access will be restricted to project members until paper publication or any other information disclosure (patent, meetings, etc). As published, raw data will be available to anyone who formally requests to Project Coordination. Raw data will be stored by digital format at least for 10 years after Project completion.

Responsibilities and Resources

Who will be responsible for data management?

Data management will be responsibility of Project Coordination (Coordinator and PIs). TI support from institutions will be provided as Institutional Support. A Data curator will be yearly indicated by Project Coordinator as a contact point from TI support, researchers and community. To help the Proponent to organize information about equipment and data
sources, a project secretariat will be provided with general support for project management (acquisitions, payments, etc) and to provide information about multiuser facility. All the equipment acquired in this proposal will be asked to operate as multiuser facilities and the Secretariat will be responsible to propose and manage a system for easy access. The involved costs (including maintenance, consumables and operational people) of each technique will be studied by the Secretariat aiming to support researchers to propose sustainable conditions for shared usage. A general web-based scheduling system for equipment accessing will be discussed with all investigators. The previous experience of Embrapa Instrumentation in the management of LNNA (Nanotechnology National Laboratory for Agriculture), as member of SISNano (Brazilian System of Nanotechnology Laboratories) will support this discussion.2
The equipment, book and database acquisition processes will be preferably done by the project secretariat. The Secretariat will be supported by the previous experience of FAI-UFSCar and Embrapa Instrumentation Project Management Office in international acquisitions. In any case, all the equipments financed by this proposal will be offered as multiuser facility according to FAPESP guidance lines. A wide discussion in the participants institutions will be done to define a specific person for secretariat, according to the local availability and as an additional resource (not paid by FAPESP).

What resources will you require to deliver your plan?

The approval of the Research Internship Abroad Scholarship (BEPE), funded by FAPESP will be enough to achieve the mentioned goals.