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## Plan Overview

*A Data Management Plan created using DMPonline*

**Title:** Photoelectrochemical system design for CO<sub>2</sub> and CH<sub>4</sub> conversion to valuable products

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**Template:** DMPOnline Template (NWU)

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### Project abstract:

Agribusiness is one of the main financial activities in Brazil, especially the sugar and alcohol sector. Despite the economic relevance of this industrial complex, there is an environmental concern associated to the release of tons of carbon dioxide (CO<sub>2</sub>) and biomethane (CH<sub>4</sub>) per year. As these gases are the main causes of the greenhouse effect, it is necessary to develop technologies and processes to minimize its emission. Photocatalytic processes may be an alternative since they can convert CO<sub>2</sub> and CH<sub>4</sub> into important organic molecules. The photocatalysis efficiency can be further improved by photoelectrocatalytic processes, which separate more efficiently the photogenerated charges. Although there are several studies related to photoelectrocatalysts synthesis, there are few efforts to apply these materials in photoelectrocatalytic reactors with high performance industrial design. In this context, this postdoctoral project has as main objective the development of a photoelectrocatalytic reactor for simultaneous CO<sub>2</sub> and CH<sub>4</sub> conversion to valuable compounds. It will be used a photoanode/photocathode system (TiO<sub>2</sub>/Cu<sub>2</sub>O) and the new reactor will be studied considering micro fluid dynamics elements and process intensification. The reactor will be operated in potentiostatic mode and different process parameters will be analyzed, such as flow, applied potential, and the effects of turbulence promoters, giving special attention to the mass transfer phenomena. Thus, it is expected to be established the best process parameters that provide high selectivity for more valuable products, faster photoelectrocatalysis kinetics, and lower energy consumption.

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# Photoelectrochemical system design for CO<sub>2</sub> and CH<sub>4</sub> conversion to valuable products

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## Data Collection

### What data will you be collecting ?

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: CH<sub>4</sub> conversion in experimental reactors; temperature-programmed gas desorption; surface-acidity titration, etc.

### 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.

### Who will be involved in your data collection ?

The data collection will be made mainly by the Principal Investigator (Jéssica Ariane de Oliveira) but it can also be made by other members of the research group depending on the required equipment since some of them have restricted access.

### 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.

### 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).

### 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, subproposals 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.

## **Ethics**

#### **Give a description of your Ethics**

#### **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 with the final documents in Data Repository.

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

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

#### **How will you share the data?**

Papers and published content will be freely provided on the 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 to keep in contact. These activities will be supported by the Team experience in research networks as well as supporting structures such as AgroNano Network.<sup>3</sup>

To access information about each Project's achievement, Public Yearly Meetings will be promoted, structured for 2-days meetings. The meeting structure will comprise a public part on the 1st day and a closed session on 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 of language (intended to be accessible for all publics) and structure (visually attractive).

On 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 with 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 at the general public. Each investigator will be stimulated to offer short web courses and webinars in related topics using the platform. These platforms will also be useful for 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 Project Coordination. Raw data will be stored in digital format at least for 10 years after Project completion

#### **Who will be responsible for data management?**

Data management will be the 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 the Project Coordinator as a contact point from TI support, researchers, and the 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 the 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 access will be discussed with all investigators. The previous experience of Embrapa Instrumentation in the management of LNNA (Nanotechnology National Laboratory for Agriculture) as a member of SISNano (Brazilian System of Nanotechnology Laboratories) will support this discussion. 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 FAIUFSCar and Embrapa Instrumentation Project Management Office in international acquisitions. In any case, all the equipment financed by this proposal will be offered as a multiuser facility according to FAPESP guidance lines. A wide discussion in the participants institutions will be done to define a specific person for the 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 (RIA), funded by FAPESP, will be enough to achieve the mentioned goals