PhD opening at CEA Grenoble:

Monitoring systems for organic redox flow energy storage technology using magnetic spectroscopy combined with AI.

The SyMMES/CAMPE laboratory at CEA Grenoble is involved in the "batteries" PEPR project and has several open positions for doctoral candidates in the field of redox flux batteries. In particular, one topic relates to the development of a low-frequency EPR spectrometer to study electrolyte degradation *in operando*.

Due to the importance of energy storage and its links to renewable technologies for the energy transition, the development of redox flow batteries (RFB) is the focus of particular interest (https://en.wikipedia.org/wiki/Flow_battery). Among the various emerging technologies, aqueous organic redox flow batteries (AORFB) are especially interesting in terms of sustainability, cost and safety. The key objectives for these indicators can be achieved thanks to molecular engineering, organometallic and coordination chemistry. Although viable systems are already arriving on the market, improving the energy density while maintaining high stability and power density remains a major preoccupation.

We propose to develop a new type of sensor to better understand and optimise the electrochemical processes in these systems. The student will develop a low-frequency (300 MHz) EPR (Electron Paramagnetic Resonance) spectrometer with a collection of probes to measure the functional state of the complete system by generating microwaves in the presence of a magnetic field. The results will allow us to determine the nature and concentration of chemical species at various points. The information will be exploited with AI algorithms (generative or not) which are being developed thanks to a collaboration with another laboratory specialising in this field (CEA/DRT/LIST). The idea is not just to automate the collection and treatment of these data but also to learn to independently detect any operating anomalies at an early stage. The candidate will work in a highly motivated group with expertise in instrument development and design, spectroscopy, and fabrication of redox flow systems [Caja-Munoz et al., **Analytical Chemistry 2023**, https://doi.org/10.1021/acs.analchem.3c00051; Poizot et al., **Chemical Reviews 2020**, https://doi.org/10.1021/acs.chemrev.9b00482; Sicoli et al., **Science 2016**, https://doi.org/10.1126/science.aad8995]. They will improve an existing EPR spectrometer and will develop probes specifically adapted to the system under study. They will try various strategies to measure concentrations in distinct compartments in the redox flow system (reservoirs, membranes, exchange cell). In collaboration with CEA/DRT/LIST specialists, they will analyse and treat the data by selecting the best AI algorithms. The information obtained will be used to optimise redox flow systems and to develop EPR-based Structural Health Monitoring for energy storage systems.

We are seeking a highly motivated individual capable of working on a high-impact project involving several partners. The successful applicant will have a passion for instrument development and its applications to complex systems, as well as for the use of AI. They will interact with chemists and physicists involved in both basic and applied research. This 3-year PhD will be funded on a CEA contract, and the experiments will be conducted on the CEA-Grenoble centre (Isère, France).

Do you fit this description? Send your CV and cover letter or get in touch for further information; Serge Gambarelli, laboratoire CAMPE (serge.gambarelli@cea.fr) would like to hear from you.

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