POLITECNICO DI MILANO

PhD in SCIENZE E TECNOLOGIE ENERGETICHE E NUCLEARI / ENERGY AND NUCLEAR SCIENCE AND TECHNOLOGY - 40th cycle

INTERDISCIPLINARY Research Field: IN SITU ELECTROCHEMICAL SUM-FREQUENCY GENERATION MICROSCOPY FOR BATTERY STUDIES

Monthly net income of PhDscholarship (max 36 months)
€ 1300.0 In case of a change of the welfare rates during the three-year period, the amount could be modified.

Context of the research activity	
Motivation and objectives of the research in this field	Electrolyzer demand is heavily increasing, pushed by the necessity to produce hydrogen from the electricity to decarbonize the hard-to-abate sectors and have a long-term energy storage strategy (up to seasonal storage). Several sectors are interested in hydrogen exploitation, like industries in which heat at high temperatures is mandatory in their processes or the transport sector, in which hydrogen can be directly used or is a feedstock to create synthetic fuels. Among different types of electrolyzers, the anion-exchange membrane (AEM) is a promising technology. AEM electrolysis works in a highly diluted alkaline environment and is, therefore, much safer to handle. It can use similarly cost-efficient materials while making much purer hydrogen at higher efficiency. It is fully scalable and is ideal for linking up with variable renewable energy sources. A comparison with other available technologies should be made for greater awareness of the benefits. In addition to a comparison on a technical and performance basis, it is necessary to take a holistic approach to determine convenience in addition to techno-economic evaluations, so an analysis for estimating the carbon footprint using a Life Cycle Assessment (LCA) approach will be adopted. With this approach, some issues related to materials that may be critical in electrolyzers will be learned in addition to greenhouse

	gases.
Methods and techniques that will be developed and used to carry out the research	The research is highly interdisciplinary, combining non-linear spectroscopy and electrochemistry to achieve otherwise inaccessible molecular-level information on the reacting electrodic interface. Sum Frequency Generation (SFG) is a second-order nonlinear optical process where two incident laser beams interact with the sample to generate a new beam at the sum frequency. SFG can arise only in a medium lacking centro-symmetry: the functionally crucial interfaces present in a battery (electrode/electrolyte, separator/electrode, active material/additives) meet this requirement, so that their molecular properties can be addressed selectively. Specifically, SFG hyperspectral imaging with micrometer resolution is ideally suited to explore battery interfaces. Finally, our approach to SFG will employ a broadband input, enabling time-resolved work on the battery-evolution timescale and will implement both VIS-IR and VIS-VIS modes, allowing to monitor molecular and electron-structure aspects of the electrochemical interface.
Educational objectives	Currently, in battery science and technology, the properties of the electrode/electrolyte interface – the functionally crucial element for electrochemical energy conversion – are optimized by trial-and-error, relying on the properties of the combined phases, without access to interface information. This proposal uses a different approach. By second-order nonlinear spectroscopy in a dedicated electrochemical cell, we aim at the molecular characterization of the processes occurring at the electrified reacting interface, controlling electrochemical charge-transfer through the formation and adsorption of intermediates. This will provide guidelines for knowledge-based interface engineering, explicitly addressing the formation, the structural and electronic properties and the Solid-Electrolyte and Cathode Electrolyte Interphases. The Dept. of Physics has a world-level competence in non-linear optical spectroscopy. The Battery Materials Engineering Laboratory at the Dept. of Energy has long-

	standing expertise in spectroelectrochemistry, as well as in the fabrication, characterization and functional testing of battery materials and devices. The PhD candidate will collaborate with the two groups, merging competences in electrochemistry and optics, that are traditionally well separated.
Job opportunities	The PhD candidate will develop a joint approach for tackling battery studies from materials synthesis to *in operando* characterization, and will consolidate battery-oriented scientific and technological skills, including electrochemical cell fabrication, experimental protocols, data analysis and modelling. The candidate's profile will be highly attractive both in the research environment, where cross-disciplinary skills are more and more appreciated, and in the rapidly expanding industrial field of battery design, production and management.
Composition of the research group	2 Full Professors 4 Associated Professors 2 Assistant Professors 10 PhD Students
Name of the research directors	Giulio Cerullo, Benedetto Bozzini

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Additional support - Financial aid per PhD student per year (gross amount)	
Housing - Foreign Students	--
Housing - Out-of-town residents (more than 80Km out of Milano)	--

Scholarship Increase for a period abroad	
Amount monthly	650.0 €
By number of months	6

Additional information: educational activity, teaching assistantship, computer availability, desk availability, any other information
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