

Smarter Batteries Based on New Embedded Sensors for In-Live Monitoring of Their Chemical and Physical Evolution

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Introduction

Monitoring the dynamic chemical and thermal state of a cell during operation is crucial in order to make meaningful advancements in battery technology as safety and reliability cannot be compromised. Our group has recently shown the operando decoding of chemical and thermal events in commercial Na(Li)-ion cells via optical sensors. However, key information regarding the chemical nature of the parasitic species and their evolution upon cycling could not be accessed. Therefore, there are two objectives to this project. The first proposes to diversify sensor configuration either by using titled optical fiber grating (TFBG) or Au-coated FBGs to probe the fiber surrounding chemical media. Additionally, we will envision the chemical functionalization of the fiber cladding or the injection of fluorescence or IR probes with optical readout for the identification of chemical species. The second aim deals with the implementation of FBGs within a solid-state battery to monitor strain, pressure, and decomposition reactions developing at interfaces, and to enable the development of this technology, which is a hot topic in today's battery research.

Altogether, these studies, which will involve collaboration with the Hong Kong Polytechnic University, should enable in-live monitoring of the state of health of the battery while increasing its overall performance. They will also offer a second life to the battery. Both are essential to increase battery sustainability and lower their CO₂ footprint.

The benefits of establishing correlations between the FBG optical signal and various battery physical metrics have been exploited over the past few years to determine the state of charge or health of batteries. However, the analysis of such signals was orphaned of chemical inputs. We closed this gap by recently demonstrating how multiple sensors can be used to track the chemical formation of solid electrolyte interface (SEI) and to determine the number of cascade reactions involved in the SEI formation process, hence enabling a rapid screening of the best electrolytes. However, to understand the cascade-reaction mechanism in various electrolytes, a missing link regards the nature and the formulae of the chemical species involved. Therefore, part of this project aims to overcome this limitation by going deeper into the battery chemistry and identifying parasitic chemical species such as alkyl carbonates. Two approaches are envisioned. The first consists of the use of titled TFBG as opposed to uniform FBG sensors. The second is to improve the accuracy and resolution of optical sensing towards chemical species identification, namely Li concentration in the cells – especially in the interfaces – which is relatively difficult to measure.

The development of new sensors with high sensitivity and accuracy along with low cost will definitely offer the possibility of more closely approaching the theoretical performance of the battery in real-time operation. This monitoring of the battery at the component and material levels would allow us to increase its reliability, double its lifetime, and lower its cost per kWh stored. Finally, monitoring could also provide a second life to the battery. All of this will significantly contribute to reducing the battery's environmental footprint, hence ensuring a better planet.

Research Project Details

The Collège de France will be the affiliated institution. Jean-Marie Tarascon will act as Principal Investigator, with Alexis Grimaud acting as deputy supervisor. Two postdocs will be involved in the project, Jiaquiang Huang (Hong Kong Polytechnic University) and Charlotte Gerville, as will PhD student Laura Albera-Blanquer. Balzan funding will be used to staff the present team. A three-year PhD student will

be assigned the task of dealing with the tracking of the battery chemistry species via TFBGs. Additionally, a two-and-a-half year postdoctoral researcher will equally be allocated to the project. Their backgrounds complement the team's expertise. The first postdoc, with dual expertise in batteries and sensing will be recruited at the early stage to work on the task dealing with sensing on solid state batteries. Later, a second postdoc with an optics/physics background will join and overlap with the PhD student to pursue the work on chemical sensing. Throughout the project, it will be decided which one will stay on for the remaining years. Equally co-shared funded students with our collaborating groups either with Hong Kong Polytechnic University or Jinan University will be considered to enhance our staffing.

As Principal Investigator, Tarascon will devote nearly half of the time to the project, namely supervising the team (daily interactions, project meetings, progress management, reporting and coordinating papers). Part of this time will also serve in pursuing well-established, fruitful collaboration with the Polytechnic University of Hong Kong or the Jinan University through the exchange of students and post-docs that could be potential candidates for Balzan PhD or post-doc positions.

The Balzan funding not used for hiring personnel will be used to support research activities in the spirit of the Balzan prize and with direct social impact. This will include not only support for student exchanges (travelling, lodging) with collaborating groups in China, Hong Kong and elsewhere, but also lectures in worldwide universities to disseminate results of the project, and training workshops for young scientists worldwide to arouse their interest in topics mainly related to chemistry and sustainable development. Publications on energy-related topics are also foreseen, especially in high-impact journals like *Science*, *Nature* and *Energy and Environment*.