CHEMICAL ENGINEERING

MUR DM 117/Stellantis - Experimental and PxD modelling study of sulphur cathode and metallic Li protection for LiS cells

Funded By	CENTRO RICERCHE FIAT [P.iva/CF:07084560015] MINISTERO DELL'UNIVERSITA' E DELLA RICERCA [P.iva/CF:97429780584] Politecnico di TORINO [P.iva/CF:00518460019]
Supervisor	BODOARDO SILVIA - silvia.bodoardo@polito.it
Contact	MARCHISIO DANIELE - daniele.marchisio@polito.it
Context of the research activity	The new e-mobility era requires new solutions from materials to systems. In this framework, topics related to development of new batteries in automotive sector arouses growing interests. The development of new and more efficient materials for energy storage is one these, which can help STELLANTIS to get its target in this field. In particular, the investigation on new materials for solid-state batteries is of high priority.The university doctorate activities will be included in the roadmap for Clean Tech, with strong links to the WCT2 (Clean Tech) and WCT6 (Materials). We have the perfect alignment with catching the target of -50% (2030) up to Carbon net zero in 2038. Progetto finanziato nell'ambito del PNRR - DM 117/2023 - CUP E14D23001980004
	The PhD work is focused on high-capacity electrodes to pursue higher energy density, such as lithium anodes as well as sulfur or oxygen cathodes. Lithium–sulfur (Li–S) batteries highlight as a promising next-generation energy storage system because of the large theoretical gravimetric energy density of 2,600 Wh kg-1 (practical energy density 460 Wh kg-1) and volumetric energy density of 2,800 Wh L-1. The energy of the Li-S battery is stored and released through a series of phase transitions. This is categorized as a conversion mechanism and is not an intercalation process as in Li-Ion batteries. The Li-S battery contains conversion materials in which a full restructuring of the material occurs during the lithiation and delithiation processes, this means that there is a structural rearrangement and a recombination of the chemical conditions. For this reason, the commercial use of the Li-S battery is still slow due to limiting factors in terms of energy

Objectives	efficiency, self-discharge and limited lifetime (cycle and calendar aging). The performance of the Li-S battery is highly dependent on its design, which is reflected in the carbon to sulfur, and electrolyte to sulfur ratios. The PhD will aim at improving the material properties, the sulfur utilization, as well as the control of the complex intermediates. The goal is to find a compromise between all the requirements and challenges. By achieving this goal, the battery technology has the potential to be used in automotive applications or in aerial vehicles that slowly charge their batteries during the day and discharge them overnight, these are likely candidates for the initial adoption of Li-S. Following that, concurrent development paths would target the wider aerospace and other adjacent markets, for which better power and cycle life is required. In the near future and for automotive, Li-S would be suitable for applications where payload is critical, but volume is less important, such as buses and trucks, but there is large room for improvement for consumer vehicles. The timescales associated with these developments are difficult to predict, as they depend on both the speed of development and passing essential regulatory certifications for each market, such as automotive, aircraft and satellites. Therefore, Li-S has the potential to become as widely available as Li-ion cells are today or at least are most likely to enter the markets where mass is the critical factor above all else. Being able to use the Li-S battery in practical applications depends not only on the research of the chemical composition of the battery but also depends on the development of the control algorithms. For this reason, the PhD will develop new computational multiscale modelling with the objective to provide a concrete solution to reduce experimental time, integrate modeling techniques in electrode manufacturing and cell testing, leading to new insights on how to increase the lifetime and safety of such new and emerging battery technologies to reduce the time for production. This will be particularly true for Li-S technology which is closer to market although the proposed solution will be investigated for other battery families (solid state batteries). Several “modules” will be developed and will then be assembled to simulate the entire cell. Two scale are explored: micro- and macro-scales. At the microscale a continuous model will be developed able to describe the involved microstructures, such as for example the pores of the air and sulfur cathodes and dendritic structures of the anode. These are transient, geometrically resolved, three-dimensional simulations, that will inform about the evolution of the micro-structure of the electrodes. These simulations will be based on computational fluid dynamics and will take advantage of the experimental activities based on cathode and anode and full cell production. At the macro-scale instead, the cell will be described with a simplified model, based on the PXD approach. In these models the micro-structure of the electrodes is ignored, and the simulations performed at the micro-scale will be used to develop the macro-scale model and to identify its missing and unknown parameters.

Skills and competencies for the development of the activity	Knowledge in chemical process, electrochemistry, batteries, modelling . Propensity to work in group.- Interest in experimental and modeling activities