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PhD project research title:

Development of solid-state electrolytes for optimizing the performances of Li-ion batteries

Abstract:

Nowadays we dwell in a society where the most essential key factor regarding its sustenance and functioning is energy. Climate changes and pollutions impose us a metaphorical coming of ages by taking responsibility through more responsible and overall-sustainable energy production and management. This can also be accomplished by enhancing battery performances and safety. The current market is dominated by Li-ion batteries (LIBs) which are fundamental to a widespread range of applications including electric vehicles and portable consumer electronics. The currently used organic liquid electrolytes (LEs) suffer from several downsides, like flammability, the risk of battery thermal runaway and explosion, the inevitable battery deterioration processes, the possible LEs leakage with safety and environmental implications and last but not the least the restricted electrochemical stability windows and the incompatibility with Li-metal anodes. Currently the most used LEs are lithium salts (like LiPF_6 and LiBF_4) in presence of organic solvents (typically organic carbonates as ethylene carbonate, dimethyl carbonate ...). Solid electrolytes (SEs) offer a promising solution. The ceramic ones possess greater thermal and electrochemical stabilities and relatively high ionic conductivities, however their major issues are the grain boundaries impedance and poor interfacial contact with the electrode material due for the intrinsic rigidity. Solid polymer electrolytes (SPEs) are another valid alternative, consisting on alkali metal salts incorporated into a polymer framework. They display flexibility, lightweight and ease of processing. The main downside here is the conductivity. Gel polymer electrolytes (GPEs, polymeric scaffold entrapping LEs) might be a compromise between the SPEs and the liquid ones, although the current challenges regard the mechanical robustness and potential LEs leakage and flammability.

My PhD project proposal is to investigate the organic-ceramic blended matrices (composite or hybrid solid electrolytes) in order to obtain the best from both sides. An intriguing path is to consider the usage of the single ion electrolytes: anionic counter-ion covalently immobilized to the solid phase constituents in order to virtually have only Li ions leading the ionic current and magnifying so the Li^+ transference number. This should enhance the energy and power performances of the battery system and reduce the dendritic problem at the anode. Another aspect I would explore is the implementation of self-healing properties to enhance the interfacial stability between the electrolyte system and the electrodes and possibly prolong the battery lifespan (through H-bonding and dynamic covalent bonds). In addition, I would take into account the in-situ self-polymerization followed by thermal curing as a functional preparation methodology, for reaching good interfacial electrode-electrolyte contact and ease of processing. The project will contemplate the formulation and screening of the most promising and innovative candidates as solid electrolytes through phase cross-compatibility studies with the most suitable electrode materials; nano- and microstructural investigation; thermal and electrochemical characterizations like flammability tests, thermal behavior analysis, conductivity and impedance studies, symmetric cell tests, cycle life evaluation, post mortem analysis on both electrolytes and electrodes for assessing the aging impact, to count some. The best candidates among the prepared solid electrolytes will be further studied in coin and/or pouch cells for prototype studies in real-world testing scenarios and possibly further optimized.