

Co-design experiments, modelling, and simulations of innovative Li-ion batteries

Greenhouse gas reduction policies with regard to global warming and climate change is one of the leading factors to develop innovative solutions to produce and store energy. Recently, lithium-ion batteries are leading the energy storage market due to high storage density capacity. The developments have not yet reached the desired performance to replace fossil fuel transport systems with Electric Vehicles. The study of electro-chemo-mechanical systems, through theoretical and numerical analysis with particular application to Li-ion batteries is going to be extended regarding the battery geometry and material properties. Furthermore, simulation and experiments are going to be carried out to design a well-performing Lithium-ion battery. Experimental studies are the backbone of the battery investigations, whereas computational modelling could be helpful to predict the results and tailor the materials and conditions in advance. The main perspective of my PhD is to combine and use the advantages of the experimental and computational modelling. Computational simulations are based on a multi-scale and multi-physics approach to enhance the battery performance, tailoring structure and to optimise the materials for better capacity and power release. Furthermore, within the light of the theoretical model, the experiments will be proceeded. Modelling of composite electrodes with different geometries and thickness, the effect of liquid or solid electrolyte on battery performance are the main aspects of the experimental part. More specifically, the collaboration with Prof. Jennifer Schaefer from University of Notre Dame, the investigation of thick electrodes is going to be extended into Ionic Functionalization of Electrode Particles to Enable Ultra-Thick Battery Cathodes.