Physical Multiscale Modeling of Electrochemical Devices for Energy Storage and Conversion: Concepts, Approaches and Challenges

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In recent years, electrochemical systems such as the Polymer Electrolyte Membrane Fuel Cells and Water Electrolyzers, Lithium-Ion batteries and supercapacitors have attracted much attention due to their potential as clean energy conversion and storage devices for stationary, automotive and portable applications. This resulted on a tremendous technological progress, such as the development of new electrolytes and active materials or the improvement of electrode structures. However, in order to compete within the most attractive markets, these technologies did not reach all the required characteristics yet, in particular in terms of cost and durability.

In this talk I review ongoing efforts on the use of physical multiscale modeling methods to deeply understand the electrochemical mechanisms and numerically simulate the structure and properties of complex media in those electrochemical devices for energy storage and conversion: currently used concepts and adopted approaches within the community are revisited.

More particularly, the multiscale modeling approach developed in the group I am heading is presented: this model (implemented within the in-house numerical package MEMEPhys®) allows resolving simultaneously multiple physicochemical phenomena (e.g. materials aging, contamination reactions, water transport, transport, charge transport, detailed electrochemical reactions...) occurring at multiple spatiotemporal scales and allows predicting the instantaneous performance and durability of the electrochemical devices. The model is supported on ab initio –extracted kinetic databases and structural data representing important prerequisites for engineering practice to understand the synergies and interactions between the aging phenomena, to interpret the electrochemical cell behavior under realistic operating conditions, to predict the components (e.g. electrodes, separator) degradation and durability as a function of the initial nanomaterials composition and nano/microstructure. The capabilities of this model to propose several experimentally-validated innovative procedures (operation strategies and electrodes formulation) to enhance the performance, durability are also illustrated through practical examples. Remaining challenges on this topic are finally discussed.

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