Towards a multiscale model of conversion reactions in lithium ion and lithium air batteries: concepts, methods and challenges

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Thanks to the growing progress in scientific computational techniques, multiscale modeling approaches and numerical simulation are emerging as powerful tools to bridge the gaps between the chemical and structural properties of the materials, the components, and the efficiency of rechargeable batteries. Development of a deep understanding of rechargeable batteries operation principles will help on achieving significant advances on their controlled design and optimization in both applied science and industry communities.

This lecture first provides an overview of the ongoing efforts worldwide in the field of multiscale modeling of batteries, by discussing the remaining methodological challenges [1]. Then, the lecture presents a new theoretical framework for the numerical simulation of conversion reactions in lithium ion and lithium air batteries, which extends a previous approach extensively developed for the multiscale modeling of fuel cells [2-4]. The framework, based on a modular non equilibrium thermodynamics theory, is designed to take into account the on-the-fly multiscale coupling between continuum models describing ionic transport across the batteries electrodes with Allen-Cahn and Cahn-Hilliard –based phase field electrochemical models parametrized with DFT data [5-6] describing solid phase formation and separation (e.g. CoO/Co°/Li_2O in lithium ion batteries, and $Li_2O/Li_2O_2/LiO_2$ in lithium air batteries) during charge and discharge. Preliminar results are presented, and concepts, methods and challenges of multiscale phase field simulations from both physical and mathematical (numerical resolution techniques) viewpoints are discussed.

Acknowledgements. *AAF gratefully acknowledges Prof. Jean-Paul Chehab and Dr. Youcef Mammeri from the Laboratoire Amiènois de Mathématiques Fondamentales et Appliquées (LAMFA), Amiens, France, for ongoing collaboration on the mathematical aspects of phase field modeling. Prof. Jean-Marie Tarascon and Dr. Mathieu Morcrette (LRCS) are gratefully acknowledged for hosting AAF at LRCS for a very exciting scientific research position in their laboratory.*

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