Multiscale computational modeling of rechargeable batteries : concepts and practice

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Multiscale modeling is emerging as a promising discipline for supporting the design and optimization of the next-generation of rechargeable batteries, including advanced lithium-ion and post-lithium technologies. This theoretical discipline aims at simultaneously describing physicochemical mechanisms taking place at different spatial scales, from the material to the cell level.

This tutorial provides a comprehensive review on cutting-edge methods for the computational multiscale modeling and numerical simulation of rechargeable batteries. Both theoretical and practical aspects are presented for the modeling of transport processes and electrochemical reactions in porous composite electrodes, together with concrete application examples for advanced lithium ion, lithium sulfur, lithium-O_2 and redox flow batteries with Si/C solid suspensions.

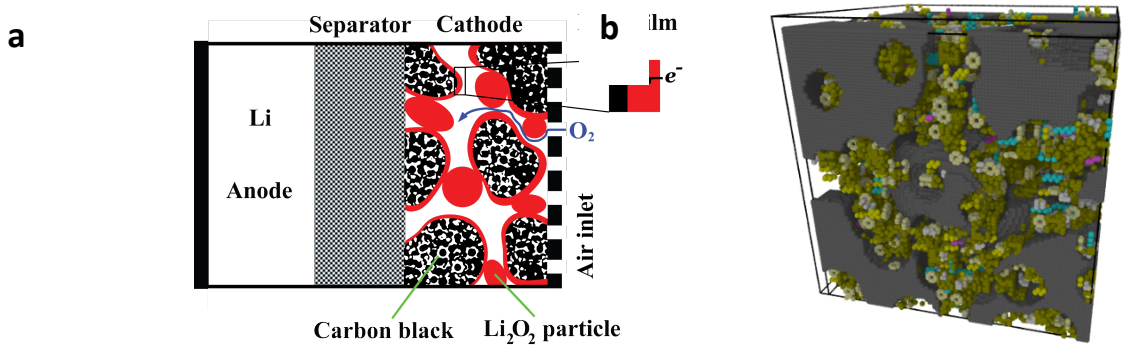

Figure. Examples of modeling approaches developed by us : a) continuum modeling of lithium-O_2 batteries ; b) mesoscopic modeling of iithium sulfur batteries.

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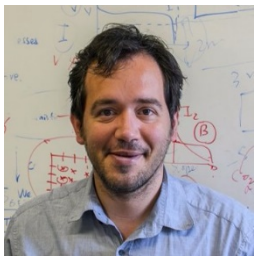

Alejandro A. Franco is now Full Professor at LRCS, and since October 2016 Junior member of the Institut Unversitaire de France. He headed the Modelling Group of Electrochemical Systems at CEA (Grenoble) in the period January 2006-January 2013. For more than 14 years, his research consists in developing multiscale models for the numerical simulation of electrochemical devices for energy storage and conversion, such as lithium air and lithium sufur batteries, redox flow and lithium ion batteries, polymer electrolyte membrane fuel cells and electrolyzers. These models, based on theoretical approaches pioneered by himself, allow to perform *in silico* studies of the physicochemical mechanisms taking place at multiple spatiotemporal scales in these devices during their operation In addition, they allow to establish links between chemical and microstructural properties of the materials, and their performance and durability. In combination with dedicated experiments, and thanks to their predictive nature, these models prove to be very helpful to optimize the design of the next generations of batteries and fuel cells.

Prof. Franco was/is coordinator and/or Work Package leader in several national and european projects (7 as PI, 11 as a partner), and has ongoing collaborative projects with companies such as Renault, SAFT and IRT-Saint Exupery/Airbus. He is author of 53 publications, 10 invited book chapters, 19 granted patents, and edited 3 books and 2 journal special issues. He delivered more than 57 Invited Presentations (more than 17 keynotes) in international conferences and in first class institutions (e.g. MIT, ANL, LBNL, Stanford Univ.). He organized 9 international conferences and 2 international schools. He is the recipient of the P.E.D.R. and of the Chercheur Haut Niveau Laureate (Region Picardie). His teaching activities include two lecture-series he created (44 h/y) where he implements cutting-edge teaching methods: one on fuel cells (M.E.S.C.) and one on non-equilibrium thermodynamics (UPJV Doctoral School).