Special Seminar

Thursday, September 20, 2012

1:30 p.m. in Room 66-319

Multiphysics, multiscale and multiparadigm modeling approaches for the transient analysis of electrochemical devices

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In this talk I will review some of my research activities in the past 11 years on the field of computational electrochemistry for fundamental understanding, diagnostics and design of materials and operation conditions for energy conversion and storage applications. Multiphysics, multiscale and multiparadigm models can reveal very helpful to optimize electrochemical devices, but appropriate mathematical descriptions and simulation algorithms scaling up materials atomistic and microstructural data onto the overall cell performance and durability have to be developed. Once this is achieved, these models can have powerful capabilities to predict experimental observables (e.g. cyclic voltammetries, polarization curves, impedance spectra...) as function of the materials chemical and structural properties at multiple scales.

Several efforts on developing such a type of models will be presented, in particular regarding the performance and materials degradation analysis in water electrolyzers, fuel cells and batteries. Some of the major challenges remaining in the development of these approaches will be also discussed.

[1] A.A. Franco, M.L. Doublet, W. Bessler, Eds., book title: "Multiscale Modeling and Numerical Simulation of Electrochemical Devices for Energy Conversion and Storage", in preparation, Springer (2012).

[2] A.A. Franco, PEMFC degradation modeling and analysis, book chapter in: Polymer electrolyte membrane and direct methanol fuel cell technology (PEMFCs and DMFCs) Vol. 1 : Fundamentals and performance, C. Hartnig and C. Roth Eds. (Woodhead, Cambridge, UK) (2012).

[3] K. Malek, A.A. Franco, *J. Phys. Chem. B*, **115** (25) (2011) 8088.

[4] A. A. Franco et al., *Fuel Cells*, **7** (2007) 99.

[5] L.F. Lopes Oliveira, S. Laref, E. Mayousse, C. Jallut, A.A. Franco, *Phys. Chem. Chem. Phys.*,**14** (2012)10215.