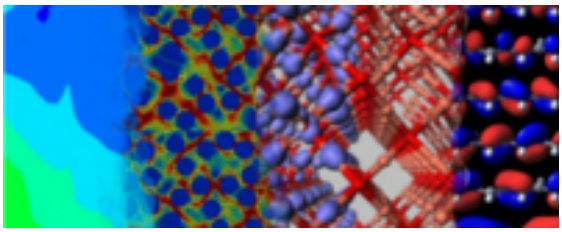

Contribution ID: **6** Type: **Talk**

Top-down and bottom-up modeling paradigms for the simulation of batteries and supercapacitors

Friday, November 9, 2012 11:00 AM (25 minutes)

Electrochemical devices for electric energy storage, such as lithium ion batteries, lithium air batteries and super-capacitors, are expected to play an important role in the future widespread development of a sustainable energy network for a large diversity of applications. However, several technical challenges related to the materials chemical and structural properties as well as operation conditions should be still solved to enhance their speicific capacity and durability. The development of physical models and numerical methods to simulate these devices operation by connecting the materials properties with the experimental observables (e.g. charge discharge curves) can reveal helpful tools for achieving this.

In this talk I will review some of the ongoing efforts within the community to develop top-down cell models (connecting detailed macroscopic descriptions of mechanisms with global parameters representing microscopic mechanisms) and bottom-up cell models (scaling up detailed descriptions of microscopic mechanisms onto global parameters to be used in macroscopic models) to simulate electrochemical storage devices. The importance of developing a multiparadigm approach synergetically connecting these two complementary views will be highlighted and some of the remaining methodological and numerical challenges will be discussed on the basis of analogies with past modeling works for fuel cells.

///// References:

[1] Multiscale modeling and numerical simulation of electrochemical devices for energy conversion and storage, A.A. Franco, M.L DOublet, W. Bessler, Eds., book in preparation (2012).

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

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Session Classification: Session: Energy storage (Click for details or select 'Detailed view')

Track Classification: Energy storage