SEMINAR SERIES

Department of
Energy Systems Engineering

Boosting rechargeable batteries R&D from multiscale modeling and *in silico* experimentation

- Speaker : **Prof. Alejandro A. Franco**

  Dept. of Chemistry,
  Université de Picardie Jules Verne, France

- Date : **16:00~17:00, Oct. 1(THU.), 2015**
- Venue : **E6 - 626, DGIST**

Abstract

The increasing use of renewable energies and the shift to an electricity-based economy is underway in our societies as a result of the escalating cost of oil, the foreseeable depletion of the finite supply, and severe damage to climate, environment, and human health due to the use of such fossil fuels. This emerging new world blueprint leads into an increasing demand for efficient and sustainable electrical energy storage and conversion devices. Within the spectrum of energy devices, the so-called *rechargeable batteries* and *fuel cells*, are called to play a significant role [1-2]. However, several performance, durability and safety challenges need still to be overcome for their widespread application. Because of the numerous competing mechanisms at multiple materials, their design reveals to be a complex optimization problem where different spatiotemporal scales have to be considered simultaneously.

In this seminar I provide a comprehensive review on the fundamentals and practical aspects of an in-house multiscale modeling approach for the analysis of physicochemical mechanisms in this type of devices. This approach, pioneered by us 14 years ago for the modeling of fuel cells [3-5], allow linking the chemical/microstructural properties of materials and components with their macroscopic efficiency and durability. In combination with "model" experiments, it can provide significant progress in designing and optimizing the next-generation cells [6]. Our approach generally results in bottom-up continuum cell models describing mathematically the physicochemical processes in multiple spatial scales in the components (e.g. ionic transport in porous media, non-equilibrium electrochemical double layer effects, phases separation, elementary kinetic reactions) [7]. The mathematical descriptions translate relevant mass and energy conservations supported on parameters related to the physicochemical and microstructural properties of the components materials, estimated from "mining" simulations based on the Density Functional Theory (e.g. for the determination activation energies of relevant electrochemical reaction steps) and Coarse Grain Molecular Dynamics (e.g. for the determination of pore size distributions and other relevant microstructural features in composite electrodes, together with the associated effective transport properties) [8-9]. These cell models are merged into a single in-house multifaceted simulator called MS LIBER-T [10]. This is a flexible code, supported in Python/C/Matlab, which can also couple on the fly the numerical resolution of continuum transport models with discrete models (e.g. Kinetic Monte Carlo models describing the elementary reaction kinetics on a catalyst surface) [11]. Moreover, by taking into account the on-the-fly feedback between performance models and elementary kinetic models describing materials degradation, our approach is able to predict the cell performance evolution and durability as function of operation conditions (e.g. applied current density or temperature) [9]. The analysis and prediction capabilities of our approach is illustrated in this lecture through concrete examples in relation to the R&D on next-generation lithium ion, lithium air, lithium sulfur and redox flow batteries, fuel cells and dye-synthesized solar cells [11-16]. Finally, I discuss technical dreams and methodological challenges being faced today towards the development of the next-generation computational tools in academia and in industry to stimulate future breakthroughs in battery technologies.

333. Techno Jungang-daero, Hyeonpung-myeon, Dalseong-gun, Daegu, 711-873, KOREA
Contacts : 053-785-6402 / sy.park@dgist.ac.kr

DGIST 대구경북과학기술원