Current Needs in Electrochemical Engineering Education

by Venkat R. Subramanian and Richard D. Braatz

In recent years, energy research has had a resurgence of interest due to concerns about humanity's environmental footprint, due to issues such as the large-scale production of carbon dioxide and concerns about security and rapid global development. Technological innovations will be essential in addressing this global challenge. For fossil fuel systems, the emphasis has been on carbon dioxide mitigation, and control of fine particle and other pollutant emissions. The development of next-generation biofuels from plant-based sources will require a systems approach to account for all of the associated environmental, human, and economic costs. Advances in materials to accelerate the development and implementation of cost effective solar-based technologies and energy-storage technologies will be essential. The training of a future workforce of broadly educated engineers and scientists, with strong technical skills will be essential. In this important area of research, electrochemists and electrochemical engineers are needed to play an active role in addressing these challenges.

By definition and by its nature, electrochemistry involves reactions that produce current (energy) or use current (energy) to favor reactions. Due to the ubiquity of the electrical potential at the small scale, the electrochemical engineering community is well placed for leading and contributing to current and future technology developments. This is an opportune time to consolidate and enhance the status and role of electrochemistry and electrochemical engineering in chemical and other engineering, chemistry, and materials science curricula and departments across the country.

Electrochemical engineers are in an ideal position to develop technological solutions to the global energy crisis. Some of the unresolved issues and research topics in the energy area relevant for electrochemical engineers are listed in Fig. 1.[1] The range of length scales in these electrochemical applications can range from electronic to atomic to molecular to nanoscale to microscale to macroscale. Figure 2 illustrates some of the computational methods that have been developed to deal with phenomena at different time and length scales to compute properties and model phenomena. These include quantum mechanics for the calculation of electronic and molecular properties; statistical mechanics including molecular dynamics and Monte Carlo methods for developing mechanistic understanding at larger length scales; the mesoscale where relatively new methods such as lattice Boltzmann simulation have emerged that are better suited for the simulation of bubble, droplet, and particle dynamics; and continuum mechanics for macroscopic reaction and transport modeling. Multiscale modeling is the use of distinct methods appropriate for different length and time scales to achieve a comprehensive description of a system.

Progress on the key research challenges, as well as their application to specific electrochemical energy systems will be hampered unless electrochemical engineers have the proper training to address these challenges. While the vision of molecular and multiscale

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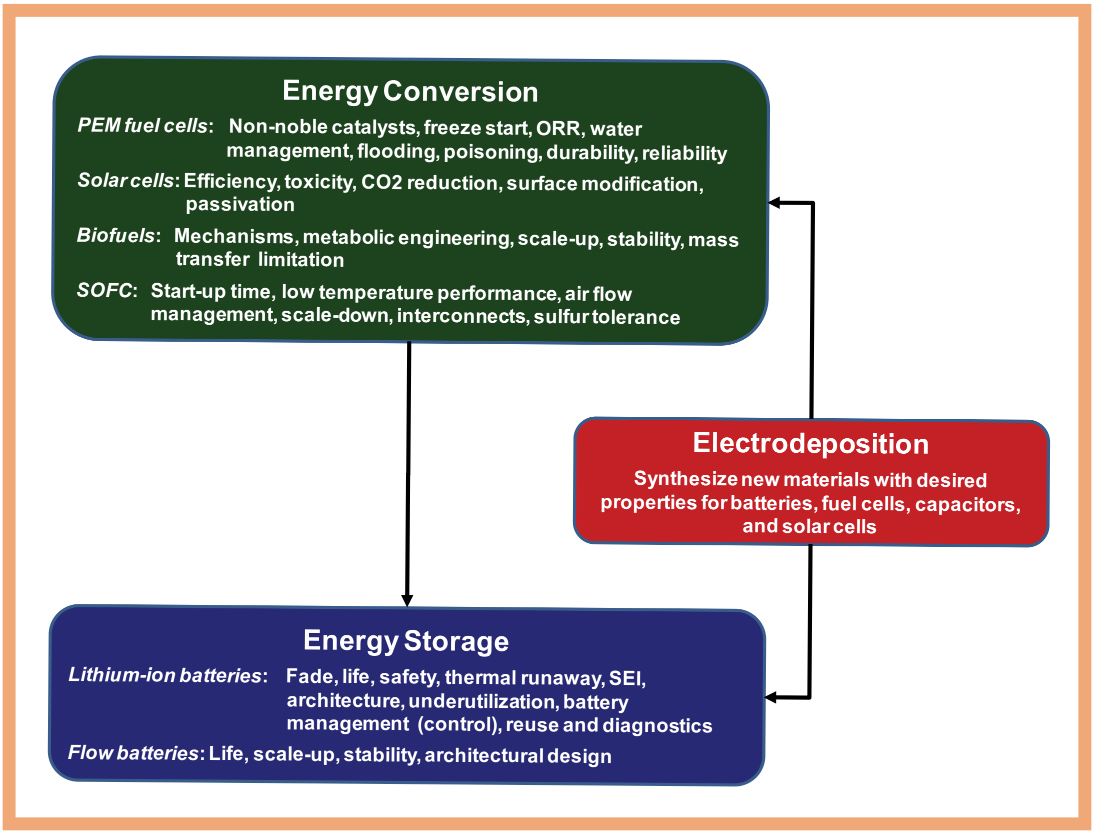

Fig. 1. *Some unresolved issues and topics of relevance in energy systems research for electrochemical engineers.*

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modeling was articulated over a decade ago,[2] undergraduate and graduate curricula do not reflect that vision. Early in the education of electrochemical engineers, students should be taught the fundamental processes at each length scale, associated methods for their modeling and simulation, and the relationships between different scales (see Fig. 2). This education should include the application of software at each of these scales with estimates of the typical accuracy at each scale (*e.g.*, of energy levels in a photovoltaic material computed by density functional theory). Preferably this education should be covered in chemistry, materials science, and chemical engineering curricula, starting with the freshman year. Subsequent electrochemical engineering courses should consider all of the time and length scales for specific electrochemical systems, and imbue students with the ability to accurately assess the relative accuracy needed at each scale in terms of the intended purpose of the model and to make any model simplifications based on well reasoned and thoroughly justified arguments. This is an extension of the education obtained in a good chemical engineering curriculum toward improved understanding of the small length scales and the interaction between scales and how to perform computations to gain understanding or design a particular electrochemical device. These recommendations are motivated by the need to develop molecular-based discoveries into new and improved products and processes.[2-6]

Some care should be taken not to overemphasize advanced multiscale simulation in introductory electrochemical engineering courses. While predictive multiscale models for electrochemical systems are a research need, classical continuum methods should continue to play a major role[7] for analysis in introductory courses. For example, pseudo-2D models with porous electrode theory have been adopted and utilized for the design of various battery electrodes and chemistries in the last few decades.[8,9] While continuum models simplify key interfaces by treating them as known boundary conditions, detailed micro-scale models (including stress-strain analysis and molecular dynamics simulation) have not yet come close to the continuum models for matching the experimental behavior and data. It is important to educate students to have a multiscale perspective while teaching them meaningful and time-tested continuum models, to enable the discovery of new materials and processes.

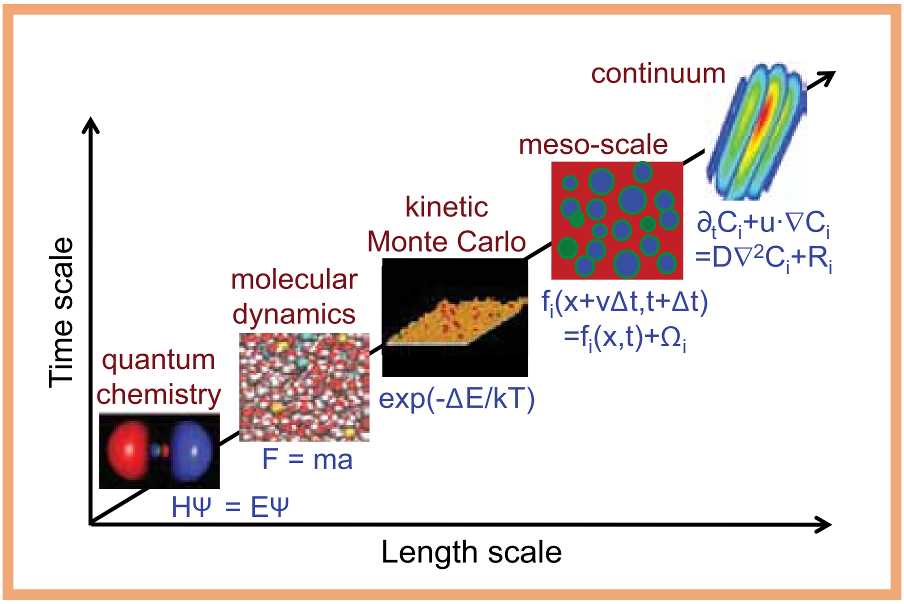

Fig. 2. *Various simulation methods and their suitability for multiple time and length scale.*

Similarly, while commercial software such as FLUENT and COMSOL with graphical user interfaces have enabled the exposure of students to the simulation of many electrochemical systems, these software and modules can be inefficient and non-robust and sometimes erroneous compared to robust FORTRAN or C++ codes developed by numerical modelers of electrochemical systems. A balanced approach of depth and breadth is recommended while training future electrochemical engineers. It is recommended to use commercial software platforms to teach and analyze electrochemical systems, but at the same time the instructors are recommended to provide at least examples of when these software packages can fail and alert the students to be aware of potential pitfalls while using the "black box" approach to analyze an electrochemical system.

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