Multiscale Computational Modeling for Energy Conversion and Storage Devices

ABSTRACT

Along with the rapid development of the electrochemical energy storage and conversion devices, such as rechargeable batteries and fuel cells, the demand for multiscale computational modeling has been increasing sharply. It is an efficient tool to benefit the experimentalists in seeking and characterizing new high performance functional materials and bring advantage to the engineers in designing and commercializing the devices. Specifically, for atomic level simulation, it could provide insights between the structure of the materials and their physical and electrical properties; for continuum level multi-physics modeling, it is useful in understanding the rate-limiting mechanisms and optimizing the operating conditions for high performance; for system level analysis, it could project the overall efficiency and monitor the performance when the devices are used for practical applications. This talk introduces the applications of multiscale computational modeling in the field of energy storage and conversion, in order of enhancing the development of new materials and better devices. The specific topics to be covered include: (1) Defect chemistry model of functional materials; (2) Impedance spectroscopy analysis of mixed conducting materials; (3) Modeling and simulation in other scales/applications will also be briefly presented.

BIOGRAPHY

Xinfang Jin is an Research Assistant Professor at University of South Carolina, Columbia. She received her Ph.D. (2014) in Mechanical Engineering from the same university, and then as a Postdoctoral Associate she had been a crucial member of an AparE project entitled, “A Novel Intermediate-Temperature Bi-Functional Ceramic Fuel Cell Energy System”. Her research is focused on multiscale computational modeling and simulation of energy conversion and storage devices.