Preface

World-scale challenges such as climate change, depletion of fossil resources, and the fast increasing energy demand has significantly boosted the R&D on alternative devices for energy conversion and storage. In this context, emerging technologies such as fuel cells and batteries are called to play an important role in any sustainable scenario. However, the successful large-scale implementation of these devices in realistic applications is subjected to numerous constraints in terms of cost, efficiency, durability, safety and impact on the environment. Precise design of cells and stacks is then required, and production cost constraints drive more and more the R&D to go beyond trial-error approaches: the use of numerical simulation and mathematical modeling arises as a natural approach to deal with the design optimization problem.

Since almost 60 years numerous mathematical models of fuel cells and batteries have been reported showing powerful capabilities for *in silico* studies of a large diversity of mechanisms and processes. These models are generally devoted to link the chemical and microstructural properties of materials and components with their macroscopic efficiency. In combination with dedicated experiments, they can potentially provide tremendous progress in designing and optimizing the next-generation cells. The available spectrum of approaches already available is wide: quantum mechanics, nonequilibrium thermodynamics, Monte Carlo and molecular dynamics methods, continuum modeling, and more recently, multiscale and/or multiparadigm models connecting multiple simulation techniques and describing the interplay of mechanisms at multiple spatiotemporal scales.

Through several comprehensive chapters written by recognized scientists in the field, we aim at reviewing the latest progresses in the development and deploy of innovative physical modeling methods and numerical simulations to better understand, rationalize, and predict the electrochemical mechanisms involved in electrochemical devices for energy storage and conversion. Concepts, methodologies, and approaches connecting *ab initio* with micro, meso, and macroscale modeling

of the components and cells are revisited, jointly with appropriate illustrations and application examples. Major remaining scientific challenges are also discussed. We hope this book will provide an interesting support to students, researchers and engineers from the industry and academic communities.

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From Theory to Engineering to Practice

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