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Physical Multiscale Modeling and Numerical Simulation of Electrochemical Devices for Energy Conversion and Storage

From Theory to Engineering to Practice

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- Reviews the ongoing efforts within the scientific community to develop and apply innovative multiscale modeling methods through contributions from world-class experts in the field
- Explores concepts, methodologies and approached across different scales of modeling cells and components with a range of illustrations and examples to provide clear and comprehensive explanations
- Discusses remaining and future challenges such as the transferability of technique, the capabilities and the economic impact of these applied methods

Through comprehensive chapters written by world-class experts in the field, this book will review ongoing efforts within the scientific community on the use of innovative physical multiscale modeling methods to deeply understand the electrochemical mechanisms and numerically simulate the structure and properties of 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 will be revisited, jointly with appropriate illustrations and application examples. Major remaining scientific challenges will be discussed, and the transferability of these techniques, well established for polymer electrolyte fuel cells, to batteries will be demonstrated. The promising capabilities of such approaches for inexpensive virtual experimentation will be highlighted. The book is expected to have a strong impact as a reference book for industry engineering and academic communities.

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