Multiscale Modeling of Electrochemical Reactions and Processes

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PREFACE

Electrochemistry targets the control of the conversion between electrical energy and chemical energy. It represents an exciting field in which long-standing environmental and energy-related issues can be addressed. A comprehensive theoretical understanding of electrochemical reactions and processes is essential for accelerating the development of materials for novel clean-energy-related devices, such as water electrolyzers, fuel cells, batteries, supercapacitors, and solar cells. To achieve this goal, numerical modeling methods have been developed to advance computational studies of the properties of electrocatalysts and the underlying elementary reaction mechanisms. The interests and efforts of scientists active in this hot topic motivate the publication of the collection of computational methods assembled in this book.

Despite the diverse applications of electrochemistry, a holistic understanding of electrochemical reactions and processes occurring at electrode–electrolyte interfaces remains elusive, which is largely attributable to the theory–experiment gap associated with these systems. Experimentalists often spend most of their time optimizing reaction conditions such as the applied bias potential, solvent, electrolyte, support, and dopants to achieve the best material performance. Unfortunately, theoretical investigations of the reaction conditions are still at the fledgling stage. This theory–experiment gap is initially introduced in Chap. 1. Generally, first-principles computations can reveal structural, electronic, and magnetic properties with high accuracy. However, this approach is severely limited when attempting to study large systems owing to its high computational cost, especially when the electrical double layer near the electrode–electrolyte interface must be considered. Classical molecular dynamics and the mean-field method are more computationally affordable and can be used to investigate much larger and more complex systems. On the other hand, the accuracy of these approaches is determined by the quality of available computational parameters. As such, multiscale modeling approaches provide a promising strategy for bridging the theory–experiment gap.

In Chap. 2, the first-principles density functional theory method is introduced, followed by a discussion of its application to the study of two different electrochemical processes: electrocatalysis and batteries. Most DFT studies focus on surface adsorption/desorption and relevant surface reactions. The methodologies for identifying active sites, calculating the energy barriers for the elementary reactions, and elucidating reaction mechanisms at the atomic level are discussed in detail. On the other hand, the influence of the applied bias potential on electrochemical cells deserves serious consideration because this parameter significantly affects the surface processes at electrode–electrolyte interfaces. Several approaches based on the first-principles method and classical molecular dynamics have recently been purposely developed to model these electrified interfaces with consideration of the applied bias potential. These methods are summarized in Chap. 3. In Chap. 4, the constant

potential method of classical molecular dynamics is explored. This method can greatly benefit our understanding of electrode–electrolyte interfaces. However, classical molecular dynamics methods remain too computationally expensive to provide a comprehensive picture of the electrical double layer, which is a crucial factor in electrochemical reactions and processes. Mean-field theory can therefore make valuable contributions to this field. Thus, in Chap. 5, mean-field theory is explored alongside modified Poisson–Boltzmann equations for modeling electrochemical energy storage systems, with an emphasis on the description of concentrated electrolyte solutions, ionic liquids, and electrodes with a high surface charge. Finally, in Chap. 6, organic semiconductors are employed as a model system to introduce the recently developed multiscale modeling strategy for charge transport processes. This is important because the charge transfer efficiency often determines the performance of electrochemical devices.

In addition to providing a glimpse into recently developed multiscale numerical modeling methods and their application to advancing our understanding of electrochemical reactions and processes, this book also demonstrates that the theory–experiment gap has yet to be completely bridged. The efficient and effective integration of simulation methods at different scales of time and space still needs to be improved. In this regard, we hope that the methods described in this book will inspire new ideas and encourage further advances in computational electrochemistry.

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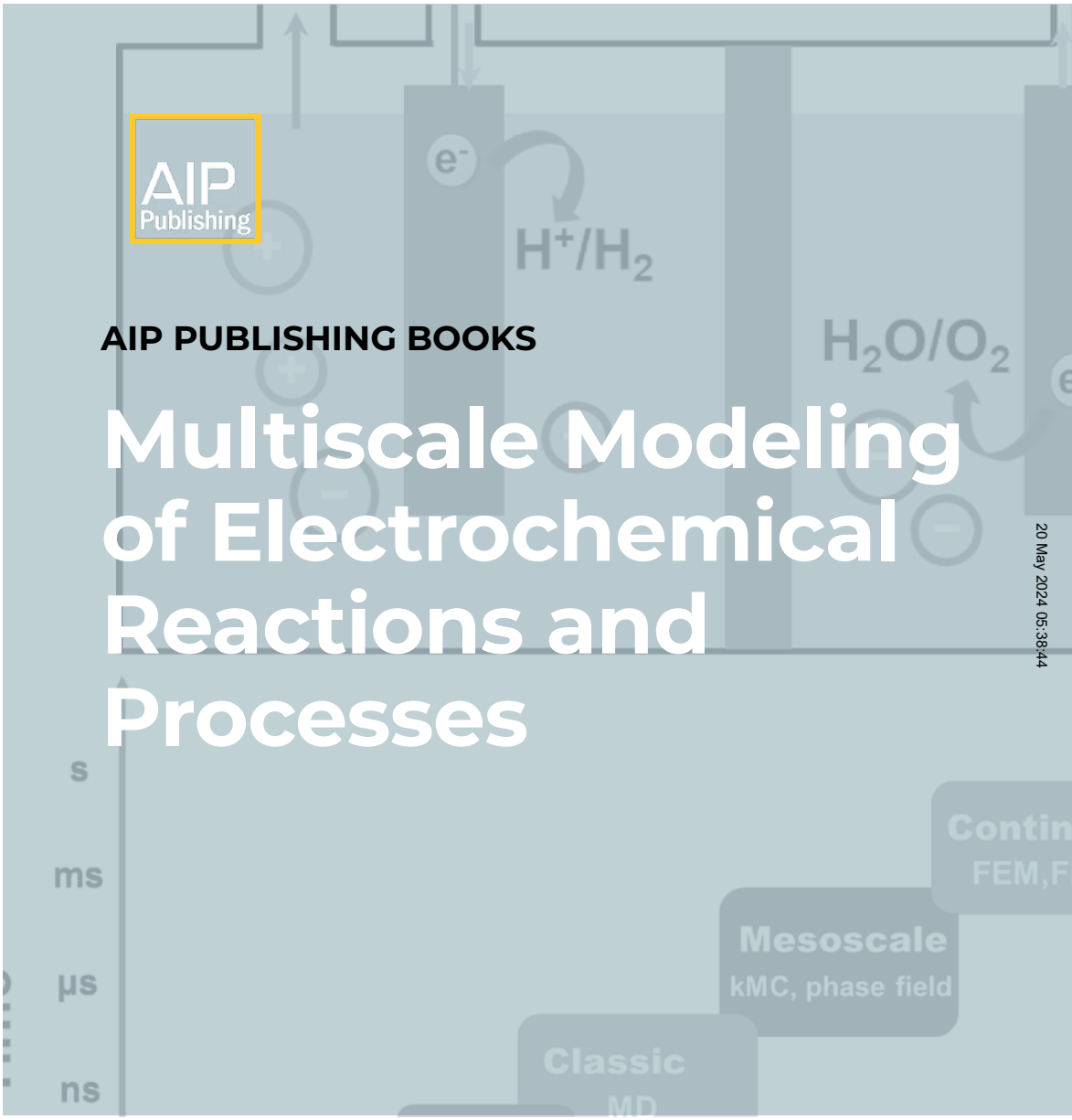
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TABLE OF CONTENTS