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Preface—Mathematical Modeling of Electrochemical Systems at Multiple Scales In Honor of Professor Richard Alkire

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Advancing our understanding of electrochemical phenomena, and ultimately improving the operation and design of electrochemical systems, is aided by the use of advanced simulation tools which enable researchers to deconvolute complex, interacting phenomena. The challenge in developing these tools is that relevant length scales in electrochemical applications can range from subatomic to macroscale. Figure 1 illustrates some of the computational methods that have been developed to deal with phenomena at these disparate length scales and corresponding time scales to compute properties and model phenomena.1 This focus issue of the Journal of The Electrochemical Society is devoted to the mathematical modeling of electrochemical systems across multiple scales, and is aligned with two previous focus issues.2,3 It is dedicated to Professor Richard Alkire from the University of Illinois in recognition of his contributions in this area, which include the introduction of Kinetic Monte Carlo methods for electrochemical systems (electrodeposition) and advanced numerical methods for electrochemical systems. For example, he pioneered finite element methods for simulating shape changes during electrodeposition.4 This method and paper remain relevant today for the analysis of lithium metal batteries that still pose numerical challenges for commercial solvers. Professor Richard Alkire dedicated a significant portion of his career to this topic, and has played a critical role in defining and running multiscale symposia for the ECS community. He has trained numerous researchers over the years to analyze, simulate, and optimize electrochemical systems using detailed, quantitative mathematical models of essential physical phenomena, and has influenced countless others. His impact cuts across different electrochemical systems as evidenced by the wide variety of topics in this focus issue including lithium-ion batteries, fuel cells, corrosion, molten salts, etc. We hope that these papers, together with Professor Alkire’s perspective article and influence, continue to inspire readers to add mathematical modeling and numerical simulation of multiscale models to their toolbox to accelerate the development of electrochemical systems and technologies.

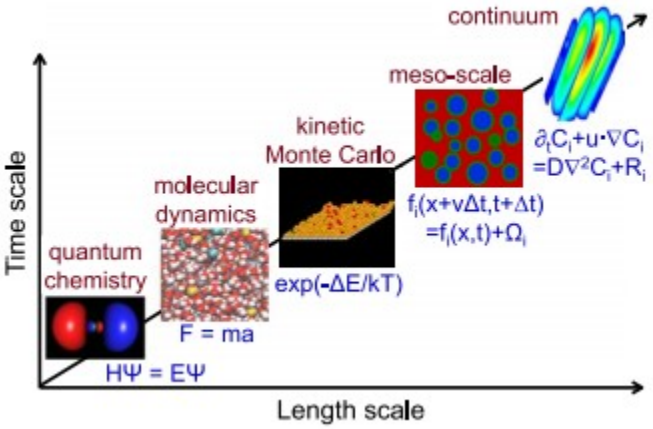

Figure 1. Various simulation methods and their suitability for multiple time and length scales.

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