
Multiscale Modeling, Simulation and Design – From Conventional Methods to the Latest in Data Science

Editors:**J. N. Harb****M. Lowe****G. Botte****J. St-Pierre****V. R. Subramanian****Sponsoring Divisions:** **Industrial Electrochemistry and Electrochemical Engineering** **Energy Technology**

Published by
The Electrochemical Society

65 South Main Street, Building D
Pennington, NJ 08534-2839, USA

tel 609 737 1902

fax 609 737 2743

www.electrochem.org

ecsttransactions™

Vol. 85, No. 5

Copyright 2018 by The Electrochemical Society.
All rights reserved.

This book has been registered with Copyright Clearance Center.
For further information, please contact the Copyright Clearance Center,
Salem, Massachusetts.

Published by:

The Electrochemical Society
65 South Main Street
Pennington, New Jersey 08534-2839, USA

Telephone 609.737.1902
Fax 609.737.2743
e-mail: ecs@electrochem.org
Web: www.electrochem.org

ISSN 1938-6737 (online)
ISSN 1938-5862 (print)
ISSN 2151-2051 (cd-rom)

ISBN 978-1-62332-485-8 (CD-ROM)
ISBN 978-1-62332-498-8 (USB)
ISBN 978-1-60768-833-4 (PDF)

Printed in the United States of America.

ECS Transactions, Volume 85, Issue 5

Multiscale Modeling, Simulation and Design – From Conventional Methods
to the Latest in Data Science

Table of Contents

<i>Preface</i>	<i>iii</i>
----------------	------------

Chapter 1
Multiscale Modeling – Fundamental Systems

Electrochemical Properties of Anatase-Type TiO ₂ Nanoparticles with Different Morphology <i>G. Juhasz</i>	3
---	---

Orthogonal Collocation on Finite Element Method for Lid-Driven Cavity Flow <i>T. Jang, C. Pathak, V. R. Subramanian</i>	11
--	----

Chapter 2
Multiscale Modeling – Batteries

A Pulse Voltammetry Analysis Toolkit for Battery and Fuel Cell Material <i>P. W. C. Northrop, J. V. Cole</i>	23
---	----

Estimation of Transport and Kinetic Parameters of Vanadium Redox Batteries Using Static Cells <i>S. B. Lee, H. D. Pratt III, T. M. Anderson, K. Mitra, B. R. Chalamala, V. R. Subramanian</i>	43
--	----

Chapter 3
Multiscale Modeling – Fuel Cells

Nonlinear Impedance Spectra Analysis of CO Poisoning on PEM Fuel Cell Performance <i>R. Pachimatla, R. Srinivasan</i>	67
--	----

A Multiscale Method for Multiphase Pore-Scale Simulation of the Polymer
Electrolyte Fuel Cell Catalyst Layer
W. Zheng, S. H. Kim

77

Author Index

87