

Theory, Characterization and Modeling

ms. Adoi. org/10.1557/adv.2017.283 Published online by Cambridge University Press



CAMBRIDGE UNIVERSITY PRESS

MRS Advances: Theory, Characterization and Modeling

Associate Editor:

Meenakshi Dutt, Rutgers University

Principal Editor:

Aaron Shugar, SUNY – Buffalo State

MRS Advances Editorial Board:

Editor-in-Chief: David F. Bahr, Purdue University Asa Barber, University of Portsmouth, United Kingdom Meenakshi Dutt, Rutgers University Elizabeth L. Fleischer, Materials Research Society

Marian Kennedy, Clemson University Marilyn L. Minus, Northeastern University Roger J. Narayan, University of North Carolina/North Carolina State University Jeremy Theil, Mountain View Energy

Materials Research Society Editorial Office, Warrendale, PA:

Ellen W. Kracht, Publications Manager Susan Dittrich, Journals Editorial Assistant Kirby L. Morris, Journals Production Assistant Eileen M. Kiley, Director of Communications

Disclaimer

Authors of each article appearing in this Journal are solely responsible for all contents in their article(s) including accuracy of the facts, statements, and citing resources. Facts and opinions are solely the personal statements of the respective authors and do not necessarily represent the views of the editors, the Materials Research Society, or Cambridge University Press.

MRS Advances (EISSN: 2059-8521) is published by Cambridge University Press, One Liberty Plaza, Floor 20, New York, NY 10006 for the Materials Research Society.

Copyright © 2017, Materials Research Society. All rights reserved. No part of this publication may be reproduced, in any form or by any means, electronic, photocopying, or otherwise, without permission in writing from Cambridge University Press. Policies, request forms and contacts are available at: http://www.cambridge.org/rights/permissions/permission.htm. Permission to copy (for users in the USA) is available from Copyright Clearance Center at: http://www.copyright.com, email: info@copyright.com.

Purchasing Options:

²*Premium Subscription-* Premium Subscription includes current subscription and one year's lease access ≥to the full MRS Online Proceedings Library Archive for \$7,219.00 / £4,888.00 / €6,647.00. Subscription- $\frac{5}{2}$ Subscription with perpetual access to the content subscribed to in a given year, including three years 5 of back-file lease access to content from the MRS Online Proceedings Library Archive. The price for Ba 2017 subscription is \$3,019.00 / £1,948.00 / €2,625.00. MRS Members- Access to MRS Advances here is available to all MRS members without charge.

Scontact Details:

E For all inquiries about pricing and access to MRS Advances, please get in touch via the following email addresses: online@cambridge.org (for the Americas); library.sales@cambridge.org (for UK, Europe, and rest of world).

CONTENTS

Comp]	science Applied to Oil Recovery and Mitigation: A Multiscale outational Approach
Scree	matic Search for Lithium Ion Conducting Compounds by ning of Compositions Combined with Atomistic Simulation 483 Daniel Mutter, Daniel F. Urban, and Christian Elsässer
Mater]	rds Reliable Modeling of Challenging <i>f</i> Electrons Bearing rials: Experience from Modeling of Nuclear Materials
ab ini	oressed Crystalline Bismuth and Superconductivity–An tio Computational Simulation
Prope	ic-orbital and Plane-wave Approaches to Ferromagnetic erties of Ni _x Fe _{1-x} Nanowires
Energ on Co	rent Contradiction Between Calculated Kinetic and Potential gy Fractions of Phonons in Molecular Solids with Implications ondensed-phase Chemistry513 Brent Kraczek
Therr	n of Porous Metal-organic Frameworks for Adsorption Driven nal Batteries