

MATERIALS RESEARCH SOCIETY
SYMPOSIUM PROCEEDINGS VOLUME 1263

Computational Approaches to Materials for Energy

April 5 – 9, 2010
San Francisco, California, USA

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571
www.proceedings.com

ISBN: 978-1-61782-223-0

Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2010) by the Materials Research Society
All rights reserved.

Printed by Curran Associates, Inc. (2010)

For permission requests, please contact the Materials Research Society
at the address below.

Materials Research Society
Proceedings
506 Keystone Dr.
Warrendale, PA 15086

Phone: 724-779-3004 x 531
Fax: 724-779-4396

eproceedings@mrs.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

CURRAN ASSOCIATES INC.
proceedings
.com

TABLE OF CONTENTS

Organic Heterojunctions for Photovoltaic Applications: C₆₀ Growth on Pentacene	1
<i>Rebecca A. Cantrell, Paulette Clancy</i>	
Visible-Light Photoresponse of Nitrogen-Doped TiO₂: Excited State Studies Using Time-Dependent Density Functional Theory and Equation-of-Motion Coupled Cluster Methods	7
<i>Niranjan Govind, Roger Rousseau, Amity Andersen, Karol Kowalski</i>	
Kinetic Monte Carlo Simulation of the Aging of Nanoporous Metals	13
<i>Gregory J. Wagner, Dariush Seif, Markus Ong</i>	
Mechanism of Ultrafast (Dis)charging of Li Ion Batteries by Heterogeneous Doping of LiFePO₄	19
<i>Stefan Adams, R. Prasada Rao, Haiping Choo</i>	
Quantum Chemical Molecular Dynamics Simulation of Oxidation Process on Clean Metal Surface in High Temperature Water	25
<i>Ken Suzuki, Hideo Miura</i>	
Author Index	