

PROCEEDINGS OF SPIE

Solar Hydrogen and Nanotechnology VIII

**Yosuke Kanai
David Prendergast**
Editors

**28–29 August 2013
San Diego, California, United States**

Sponsored and Published by
SPIE

Volume 8822

Proceedings of SPIE 0277-786X, V. 8822

SPIE is an international society advancing an interdisciplinary approach to the science and application of light.

Solar Hydrogen and Nanotechnology VIII, edited by Yosuke Kanai,
David Prendergast, Proc. of SPIE Vol. 8822, 882201 · © 2013 SPIE
CCC code: 0277-786X/13/\$18 · doi: 10.1117/12.2045816

Proc. of SPIE Vol. 8822 882201-1

The papers included in this volume were part of the technical conference cited on the cover and title page. Papers were selected and subject to review by the editors and conference program committee. Some conference presentations may not be available for publication. The papers published in these proceedings reflect the work and thoughts of the authors and are published herein as submitted. The publisher is not responsible for the validity of the information or for any outcomes resulting from reliance thereon.

Please use the following format to cite material from this book:

Author(s), "Title of Paper," in *Solar Hydrogen and Nanotechnology VIII*, edited by Yosuke Kanai, David Prendergast, Proceedings of SPIE Vol. 8822 (SPIE, Bellingham, WA, 2013) Article CID Number.

ISSN: 0277-786X

ISBN: 9780819496720

Published by

SPIE

P.O. Box 10, Bellingham, Washington 98227-0010 USA

Telephone +1 360 676 3290 (Pacific Time) · Fax +1 360 647 1445

SPIE.org

Copyright © 2013, Society of Photo-Optical Instrumentation Engineers.

Copying of material in this book for internal or personal use, or for the internal or personal use of specific clients, beyond the fair use provisions granted by the U.S. Copyright Law is authorized by SPIE subject to payment of copying fees. The Transactional Reporting Service base fee for this volume is \$18.00 per article (or portion thereof), which should be paid directly to the Copyright Clearance Center (CCC), 222 Rosewood Drive, Danvers, MA 01923. Payment may also be made electronically through CCC Online at copyright.com. Other copying for republication, resale, advertising or promotion, or any form of systematic or multiple reproduction of any material in this book is prohibited except with permission in writing from the publisher. The CCC fee code is 0277-786X/13/\$18.00.

Printed in the United States of America.

Publication of record for individual papers is online in the SPIE Digital Library.



SPIDigitalLibrary.org

Paper Numbering: Proceedings of SPIE follow an e-First publication model, with papers published first online and then in print and on CD-ROM. Papers are published as they are submitted and meet publication criteria. A unique, consistent, permanent citation identifier (CID) number is assigned to each article at the time of the first publication. Utilization of CIDs allows articles to be fully citable as soon as they are published online, and connects the same identifier to all online, print, and electronic versions of the publication. SPIE uses a six-digit CID article numbering system in which:

- The first four digits correspond to the SPIE volume number.
- The last two digits indicate publication order within the volume using a Base 36 numbering system employing both numerals and letters. These two-number sets start with 00, 01, 02, 03, 04, 05, 06, 07, 08, 09, 0A, 0B ... 0Z, followed by 10-1Z, 20-2Z, etc.

The CID Number appears on each page of the manuscript. The complete citation is used on the first page, and an abbreviated version on subsequent pages. Numbers in the index correspond to the last two digits of the six-digit CID Number.

Contents

v *Conference Committee*

DRIVING PHOTOELECTROCHEMISTRY USING DEFECTS AND DISORDER IN METAL OXIDES

- 8822 05 **Conductivity and transparency of TiO₂ from first principles (Invited Paper)** [8822-4]
A. Schleife, Lawrence Livermore National Lab. (United States); J. B. Varley, Univ. of California, Santa Barbara (United States) and Lawrence Livermore National Lab. (United States); A. Janotti, C. G. Van de Walle, Univ. of California, Santa Barbara (United States)

UNDERSTANDING AND ENGINEERING INTERFACIAL ELECTRONIC STRUCTURE AND CHEMISTRY FOR WATER SPLITTING

- 8822 0A **Towards a perfect system for solar hydrogen production: an example of synergy on the atomic scale** [8822-9]
R. Nashed, Georgia Institute of Technology (United States) and American Univ. in Cairo (Egypt); F. M. Alamgir, J. Seung Soon, Georgia Institute of Technology (United States); Y. Ismail, American Univ. in Cairo (Egypt); M. A. El-Sayed, Georgia Institute of Technology (United States); N. K. Allam, American Univ. in Cairo (Egypt)
- 8822 0C **Cold gas spraying of semiconductor coatings for the photooxidation of water** [8822-11]
T. Emmeler, Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung (Germany); H. Gutzmann, Helmut-Schmidt Univ. (Germany); P. Hillebrand, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany); M. Schieda, R. Just, Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung (Germany); F. Gärtner, Helmut-Schmidt Univ. (Germany); P. Bogdanoff, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany); I. Herrmann-Geppert, T. Klassen, Helmut-Schmidt Univ. (Germany) and Helmholtz-Zentrum Geesthacht Zentrum für Material- und Küstenforschung (Germany)

COMPLEX OXIDES FOR WATER-SPLITTING

- 8822 0D **Ceria chemistry at the nanoscale: effect of the environment (Invited Paper)** [8822-12]
J. Kullgren, K. Hermansson, P. Broqvist, Uppsala Univ. (Sweden)
- 8822 0E **Development of metal tungstate alloys for photoelectrochemical water splitting** [8822-13]
D. Prasher, M. Chong, Y. Chang, Univ. of Hawaii at Manoa (United States); P. Sarker, M. N. Huda, The Univ. of Texas at Arlington (United States); N. Gaillard, Univ. of Hawaii at Manoa (United States)
- 8822 0F **Photoelectrochemical performance of W-doped BiVO₄ thin-films deposited by spray pyrolysis** [8822-14]
S. K. Holland, M. R. Dutter, D. J. Lawrence, B. A. Reisner, T. C. DeVore, James Madison Univ. (United States)

FUNCTIONAL CHEMISTRY OF SEMICONDUCTOR INTERFACES

- 8822 OM **Water-induced modifications of GaP(100) and InP(100) surfaces studied by photoelectron spectroscopy and reflection anisotropy spectroscopy** [8822-21]
M. M. May, O. Supplie, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany) and Humboldt-Univ. zu Berlin (Germany); C. Höhn, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany); W.-D. Zabka, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany) and Humboldt-Univ. zu Berlin (Germany); H.-J. Lewerenz, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany) and California Institute of Technology (United States); R. van de Krol, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany); T. Hannappel, Helmholtz-Zentrum Berlin für Materialien und Energie (Germany) and Technische Univ. Ilmenau (Germany)

NOVEL MATERIALS AND METHODS FOR HYDROGEN GENERATION

- 8822 OS **Reversible hydrogen evolution and oxidation mediated by molecular ion** [8822-27]
K. Juodkasis, J. Juodkazytė, B. Šebeka, Institute of Chemistry (Lithuania); S. Juodkasis, Swinburne Univ. of Technology (Australia)
- 8822 OU **Nanowires from dirty multi-crystalline Si for hydrogen generation** [8822-29]
X. Li, Univ. Halle-Wittenberg (Germany) and Max-Planck-Institute of Microstructure Physics (Germany); S. L. Schweizer, A. Sprafke, Univ. Halle-Wittenberg (Germany); R. B. Wehrspohn, Univ. Halle-Wittenberg (Germany) and Fraunhofer Institute for Mechanics of Materials (Germany)

Author Index

Conference Committee

Symposium Chair

Martha Symko-Davies, National Renewable Energy Laboratory
(United States)

Conference Chairs

Yosuke Kanai, The University of North Carolina at Chapel Hill
(United States)

David Prendergast, Lawrence Berkeley National Laboratory
(United States)

Conference Program Committee

Hironori Arakawa, Tokyo University of Science (Japan)

Jan Augustynski, University of Warsaw (Poland)

Michael Grätzel, Ecole Polytechnique Fédérale de Lausanne
(Switzerland)

Jinghua Guo, Lawrence Berkeley National Laboratory (United States)

Hicham Idriss, University of Aberdeen (United Kingdom) and SABIC (Saudi
Arabia)

Claude Levy-Clement, Centre National de la Recherche Scientifique
(France)

Yasuhiro Tachibana, RMIT University (Australia)

John A. Turner, National Renewable Energy Laboratory (United States)

Lionel Vayssieres, Xi'an Jiaotong University (China)

Heli Wang, National Renewable Energy Laboratory (United States)

Gunnar Westin, Uppsala University (Sweden)

Upul Wijayantha, Loughborough University (United Kingdom)

Jin Zhang, University of California, Santa Cruz (United States)

Session Chairs

- 1 Material Challenges for Solar Hydrogen
Yosuke Kanai, The University of North Carolina at Chapel Hill (United
States)
- 2 Driving Photoelectrochemistry Using Defects and Disorder in Metal Oxides
Lionel Vayssieres, Xi'an Jiaotong University (China)
- 3 Understanding and Engineering Interfacial Electronic Structure and
Chemistry for Water Splitting
David Prendergast, Lawrence Berkeley National Laboratory (United
States)

- 4 Complex Oxides for Water-Splitting
Marivi Fernandez-Serra, Stony Brook University (United States)
- 5 Understanding and Revealing the Dynamics of Photoelectrochemistry
David Prendergast, Lawrence Berkeley National Laboratory
(United States)
- 6 Functional Chemistry of Semiconductor Interfaces
Feliciano Giustino, University of Oxford (United Kingdom)
- 7 Exploring PEC Materials with X-ray Spectroscopy
Yosuke Kanai, The University of North Carolina at Chapel Hill (United States)
- 8 Novel Materials and Methods for Hydrogen Generation
Tadashi Ogitsu, Lawrence Livermore National Laboratory (United States)