

International Conference

nanoGe September Meeting 2017 (SeptemberMeeting17)

SF1: Material and Device Innovations for the Practical Implementation of Solar Fuels (SolarFuel17)

Barcelona, Spain, 2017 September 4th - 6th

Conference Chairs: Wilson Smith and Ki Tae Nam

Conference Program

September 4th - Day 1 (Monday)	
08:00 - 09:30	Registration
09:30 - 09:45	Opening
	SF1.1 Chair: Wilson Smith
09:45 - 10:20 SF1.1-I1	<u>James Durrant</u> (<i>Imperial College London</i>) The kinetics of charge separation, recombination and catalysis on photoelectrodes for water oxidation and reduction
10:20 - 10:30	Discussion
10:30 - 11:05 SF1.1-I2	James Thorne, Wei Li, Erik Liu, Yanyan Zhao, <u>Dunwei Wang</u> (<i>Boston College</i>) Co-Catalysts on Photoelectrodes: Catalyst or Passivation?
11:05 - 11:15	Discussion
11:15 - 11:45	Coffee Break
11:45 - 12:20 SF1.1-I3	<u>Kevin Sivula</u> (<i>École Polytechnique Fédérale Lausanne</i>) Engineering solution-processed semiconductor materials for photoelectrochemical solar fuel production
12:20 - 12:30	Discussion
12:30 - 13:05 SF1.1-I4	<u>Ib Chorkendorff</u> (<i>The Villum Center for the Science of Sustainable Fuels and Chemicals</i>) Water splitting and the making of renewable chemicals.

13:05 - 13:15	Discussion
13:15 - 14:45	Lunch
	SF1.2 Chair: Shane Ardo
14:50 - 15:00 SF1.2-S1	<u>Kwangsun Ji</u> (<i>LG TCM, LG Electronics</i>) LG Materials & Devices Advanced Research
15:00 - 15:35 SF1.2-I1	<u>Daniel Esposito</u> (<i>Columbia University, US</i>) Oxide-Encapsulated Electrocatalysts for Solar Fuels Production
15:35 - 15:45	Discussion
	SF1.2.1 Chair: Shane Ardo
15:45 - 16:00 SF1.2.1-O1	<u>Sixto Gimenez</u> (<i>Institute of Advanced Materials, Universitat Jaume I, Spain</i>), Drialys Cardenas-Morcoso Tuning the functionalities of Bismuth Vanadate. From water splitting photoanodes to photocapacitive devices
16:00 - 16:15 SF1.2.1-O2	<u>Morgan Stefik</u> (<i>University of South Carolina, Department of Chemistry and Biochemistry</i>) Bismuth Vanadate : SF-ALD and Remarkable Post-Synthetic Treatments
16:15 - 16:30 SF1.2.1-O3	Rajiv Ramanujam Prabhakar, Wilman Septina, Sebastian Siol, René Wick, Thomas Moehl, <u>David Tilley</u> (<i>University of Zurich, Department of Chemistry</i>) Highly Active Sb ₂ Se ₃ -based Photocathodes for Solar Hydrogen Production
16:30 - 16:45 SF1.2.1-O4	<u>Silvan Suter</u> , Yannick Gaudy, Sophia Haussener Quantitative Structural and Transport Analysis of Morphologically-Complex Photoelectrodes
16:45 - 17:00 SF1.2.1-O5	<u>Laia Francas Forcada</u> (<i>Department of Chemistry, University of Wisconsin–Madison, Madison, WI 53706, USA.</i>), Sacha Corby, Shababa Selim, Camilo Mesa, Yimeng Ma, Dongho Lee, Kyoung-Shin Choi, James Durrant Shining light on the role of catalysts layers on BiVO ₄ for water oxidation.
17:00 - 17:15 SF1.2.1-O6	<u>Martin Rohloff</u> (<i>Institut für Anorganische und Analytische Chemie, Albert-Ludwigs-Universität Freiburg</i>), Björn Anke, Martin Lerch, Anna Fischer Fluorinated BiVO ₄ – Enhancement of Photoelectrochemical Performance for Water Oxidation by Fluorine Incorporation
	SF1.2.2 Chair: Curtis Berlinguette

15:45 - 16:00 SF1.2.2-O1	<u>Jara Garcia Santaclara</u> (<i>Chemical Engineering, Delft University of Technology</i>), Alma Olivios-Suarez, Sonia Castellanos, Freek Kapteijn, Monique van der Veen, Jorge Gascon Design Guidelines of MOFs for Photocatalytic H ₂ Production
16:00 - 16:15 SF1.2.2-O2	<u>Idan Hod</u> (<i>Ben-Gurion University of the Negev</i>) Metal-Organic Frameworks as an Enzyme-Inspired Heterogeneous Platform for Electrocatalytic CO ₂ Reduction
16:15 - 16:30 SF1.2.2-O3	<u>Franziska Hegner</u> , Nuria Lopez, Galán Jose-Ramon, Gimenez Sixto Enhanced Photoanode Activity with Co-Fe Prussian blue as genuine Water Oxidation Catalyst
16:30 - 16:45 SF1.2.2-O4	<u>Yihui Zhao</u> (<i>DIFFER – Dutch Institute for Fundamental Energy Research, the Netherlands, www.differ.nl</i>), Shashank Balasubramanyam, Ageeth Bol, Anja Bieberle-Hütter Tungsten trioxide Thin Films Fabricated by Radio Frequency Sputtering and by Atomic Layer Deposition for Water Splitting
16:45 - 17:15 SF1.2.2-I1	<u>Sophia Haussener</u> (<i>École Polytechnique Fédérale de Lausanne EPFL</i>) Modelling approaches to guide best conceptual device classes and research pathways for photo-driven processing of chemical commodities
17:15 - 18:45	Poster Exhibition

September 5th - Day 2 (Tuesday)

SF1.3

Chair: Kevin Sivula

09:00 - 09:35 SF1.3-I1	William White, Christopher Sanborn, David Fabian, Ronald Reiter, <u>Shane Ardo</u> (<i>Department of Chemistry, University of California, Irvine, CA 92617 USA</i>) Engineering Bipolar Ion-Exchange Membranes to Enable New Functions Relevant to Photoelectrochemical Applications
09:35 - 09:45	Discussion
09:45 - 10:20 SF1.3-I2	<u>Jihun Oh</u> (<i>Korea Advanced Institute of Science and Technology (KAIST)</i>) Silicon Photosynthetic Cells for Efficient and Selective Solar Chemical Production
10:20 - 10:30	Discussion
10:30 - 11:05 SF1.3-I3	<u>Leif Hammarström</u> (<i>Uppsala University, Dept. Chemistry Ångström Laboratory</i>) Molecular Approaches to Solar Fuels
11:05 - 11:15	Discussion

11:15 - 11:45	Coffee Break
11:45 - 12:20 SF1.3-I4	<u>Byoung Koun Min</u> (<i>Clean Energy Research Center, Korea Institute of Science and Technology</i>) Bifunctional photoelectrode by bilateral fabrication of photovoltaics and electrocatalyst
12:20 - 12:30	Discussion
12:30 - 12:45 SF1.3-O1	<u>Wei Cui</u> (<i>Department of Chemistry, University of Zurich</i>), David Tilley Deconvolution of Photovoltaic and Electrocatalytic Performance in Water Splitting Photocathodes by Dual Working Electrode Photoelectrochemistry
12:45 - 13:00 SF1.3-O2	<u>Dariusz Mitoraj</u> , Radim Beranek Ultrasmall Cocatalyst Nanoparticles for Efficient Photoelectrocatalysis: Optical Properties and Electrolyte Effects
13:00 - 13:15 SF1.3-O3	<u>Ming Ma</u> (<i>Department of Chemical Engineering, Delft University of Technology</i>), Heine Hansen, Marco Valenti, Wilson Smith Electronic Effects on the Electrochemical Reduction of CO ₂ on Compositionally Variant Au-Pt Bimetallic Films
13:15 - 15:00	Lunch
	SF1.4.1 Chair: Daniel Esposito
15:00 - 15:15 SF1.4.1-O1	<u>bruce Parkinson</u> (<i>University of Wyoming</i>) Solar Fuels: Future Prospects?
15:15 - 15:30 SF1.4.1-O2	<u>Yannick Hermans</u> (<i>UBordeaux</i>), Wolfram Jaegermann, Andreas Klein, Thierry Toupance PES band alignment study of BiVO ₄ with common oxidation cocatalysts
15:30 - 15:45 SF1.4.1-O3	<u>Teresa Andreu</u> (<i>Catalonia Institute for Energy Research (IREC), Jardins de les Dones de Negre 1, Sant Adrià del Besòs, 08930 Barcelona</i>), Erdem Irtem, Nina Carretero, Felix Urbain, Carles Ros, Maria Dolores Hernández-Alonso, Germán Penelas-Pérez, Joan Ramon Morante A photoelectrochemical flow cell design for the efficient CO ₂ conversion to fuels
15:45 - 16:00 SF1.4.1-O4	<u>Pieter Westerik</u> (<i>MESA+ Institute for Nanotechnology, University of Twente</i>), Wouter Visselaar, Erwin Berenschot, Juriaan Huskens, Han Gardeniers Silicon membrane architecture for unassisted solar water splitting with separate product gasses

16:00 - 16:15 SF1.4.1-O5	<u>Rajiv Ramanujam Prabhakar</u> (<i>Department of Chemistry, University of Zurich</i>), Wilman Septina, David Tilley Efficient Earth Abundant Copper Sulphide Photocathodes for Solar Water Splitting
16:15 - 16:30 SF1.4.1-O6	Anton Litke, Yaqiong Su, Emiel J.M. Hensen, <u>Jan Philipp Hofmann</u> (<i>Eindhoven University of Technology, NL</i>) Stabilization of trapped charge carriers in TiO ₂ by adsorbed water: a combined time-resolved FTIR spectroscopy and DFT+U study
16:30 - 16:45 SF1.4.1-O7	Akihiro Nakamura, Hiroaki Maruyama, Yoshiaki Nakano, Katsushi Fujii, <u>Masakazu Sugiyama</u> (<i>The University of Tokyo</i>) Polarization engineered photocathode using InGaN/AlN heterostructure for zero-bias solar water splitting
16:45 - 17:00 SF1.4.1-O8	<u>Rahman Daiyan</u> (<i>Particles and Catalysis Research Group, School of Chemical Engineering,</i>) Tin catalysts for Conversion of Carbon Dioxide into Formate
SF1.4.2 Chair: Yogesh Surendranath	
15:00 - 15:15 SF1.4.2-O1	<u>Dowon Bae</u> (<i>Department of Physics, Technical University of Denmark</i>), Brian Seger, Thomas Pedersen, Ole Hansen, Peter Vesborg, Ib Chorknedorff Strategies for photoelectrode protection: A case study of an extremely stable TiO ₂ protected c-Si device
15:15 - 15:30 SF1.4.2-O2	<u>Thomas Moehl</u> (<i>Department of Chemistry, University of Zurich</i>), Jihye Suh, Laurent Sévery, René Wick, David Tilley Investigation of ALD TiO ₂ Protection Layers for Water Splitting Photoelectrodes
15:30 - 15:45 SF1.4.2-O3	<u>Kayo Koike</u> (<i>Photonics Control Technology Team, Advanced Photonics Technology Development Group, RIKEN, Wako, Japan</i>), Kazuhiro Yamamoto, Satoshi Ohara, Masakazu Sugiyama, Satoshi Wada, Katsushi Fujii Role and model of NiO on n-type GaN Photoanode for Water Splitting
15:45 - 16:00 SF1.4.2-O4	<u>Shun Kashiwaya</u> (<i>TU Darmstadt, Surface Science</i>), Andreas Klein, Wolfram Jaegermann Work function of the anatase (001) and (101) facet in different surface states
16:00 - 16:15 SF1.4.2-O5	<u>Hiroaki Maruyama</u> (<i>The University of Tokyo</i>), Akihiro Nakamura, Yoshiaki Nakano, Katsushi Fujii, Masakazu Sugiyama Pt co-catalyst by photo-electrodeposition on tandem nitride semiconductor photocathode for zero-bias solar water splitting
16:15 - 16:30 SF1.4.2-O6	<u>Andreas Zeidler</u> , Viktoria Kunzelmann, Martin Stutzmann Photo-catalytic carbon dioxide reduction with InGaN photo-electrodes

16:30 - 17:05 Todd Deutsch (*National Renewable Energy Laboratories*)
SF1.4.2-I1 Over 16% Solar-to-Hydrogen Photo-Electrochemical Water Splitting on III-V Multijunction Semiconductors

17:05 - 17:15 Discussion

20:00 - 22:00 **Social Dinner**

September 6th - Day 3 (Wednesday)

SF1.5

Chair: Dunwei Wang

09:00 - 09:35 Curtis Berlinguette (*The University of British Columbia*)
SF1.5-I1 Converting CO₂ into something useful

09:35 - 09:45 Discussion

09:45 - 10:20 Marc Koper (*Leiden University*)
SF1.5-I2 Mechanisms of electrocatalytic CO₂ reduction

10:20 - 10:30 Discussion

10:30 - 11:05 Yogesh Surendranath (*Massachusetts Institute Of Technology*), Anna Wuttig,
SF1.5-I3 Youngmin Yoon, Sahr Khan
Mechanistic Insights Into Selective CO₂-to-Fuels Catalysis

11:05 - 11:15 Discussion

11:15 - 11:45 **Coffee Break**

11:45 - 12:20 ryuhei nakamura (*RIKEN Center for Sustainable Resource Science*)
SF1.5-I4 Element Strategy of Oxygen Evolution Electrocatalysis Based on in-situ Identification of Intermediate Species

12:20 - 12:30 Discussion

12:30 - 13:05 Heinz Frei (*Molecular Biophysics and Integrated Bioimaging Division Lawrence Berkeley National Laboratory Berkeley, CA 94720*)
SF1.5-I5 Nanoscale Oxide Based Core-Shell Assembly for Photocatalytic Reduction of CO₂ by H₂O

13:05 - 13:15 Discussion

13:15 - 13:25 **Closing**

Poster Contribution

015	<u>Michael Nagli</u> (<i>Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Haifa 3200003, Israel</i>), Maytal Caspary-Toroker M(OH) ₂ (M = Ni, Fe, Co) two-dimensional materials and investigation of their electronic properties through computational methods
016	<u>Yannick Gaudy</u> (<i>EMPA</i>), Stefan Dilger, Steve Landsmann, Ulrich Aschauer, Simone Pokrant, Sophia Haussener Coupled Experimental-Numerical Analysis of LaTiO ₂ N Particle-Based Water-Splitting Photoelectrodes
026	<u>Pramod Patil Kunturu</u> (<i>University of Twente</i>), Jurriaan Huskens Efficient solar water splitting copper(I) oxide photocathodes protected by carbon materials
028	<u>Daniel Esposito</u> (<i>Columbia University, US</i>) 3D Printed Membraneless Electrolyzers for Hydrogen Production
032	<u>Wouter Vijsselaar</u> (<i>University of Twente</i>), Pieter Westerik, Janneke Veerbeek, Roald Tiggelaar, Erwin Berenschot, Jurriaan Huskens, Han Gardeniers Spatial Decoupling of Light Absorption and Catalytic Activity of Nickel-Molybdenum on High-Aspect-Ratio Silicon Microwire Arrays
036	<u>Katsushi Fujii</u> (<i>Research Cluster for Innovation, Nakamura Lab., RIKEN, Wako, Japan</i>), Takenari Goto, Shinichiro Nakamura, Kayo Koike, Takafumi Yao In-situ Photoluminescence Observation Trial for Photoelectrochemical Water Splitting using with n-type GaN as an Photoanode
061	<u>Huu Chuong Nguyen</u> (<i>Institute of Chemical Research of Catalonia (ICIQ)</i>) Catalytic properties of doped Fe ₂ O ₃ using DFT+U approach
073	<u>Divya Bohra</u> (<i>Delft University of Technology, Department of Chemical Engineering, Materials for Energy Conversion and Storage</i>), Wilson Smith Rational design of carbon dioxide electroreduction catalysts using multiscale modeling
156	<u>Rochan Sinha</u> (<i>DIFFER – Dutch Institute for Fundamental Energy Research, the Netherlands, www.differ.nl</i>), Valerio di Palma, Reinoud Lavrijsen, Mariadriana Creatore, Anja Bieberle-Hütter Improvement In The Water Splitting Activity Of Hematite Thin Films with ZnO Underlayer



157	<u>Jin-Young Yu</u> (<i>Departments of Chemical Engineering, Hanyang University</i>), Jin-Young Jung, Jung-Ho Lee High open-circuit potential obtained by ion-permeable NiOx on n-Si photoanode for efficient water oxidation
159	<u>Nienke Firet</u> (<i>Delft University of Technology, Department of Chemical Engineering</i>), Wilson Smith The role of crystal structure in oxide-derived Ag catalysts for CO2 reduction
160	<u>Yuya Uzunaki</u> (<i>NTT Device Technology Labs, NTT Corporation</i>), Yoko Ono, Kazuhide Kumakura, Takeshi Komatsu Impedance Analysis of Water Oxidation Reaction with a GaN-based Photoanode for Artificial Photosynthesis
164	<u>Yoko Ono</u> (<i>NTT Device Technology Labs, NTT Corporation</i>), Yuya Uzunaki, Kazuhide Kumakura, Takeshi Komatsu Suppression of Photocurrent Degradation in an Artificial Photosynthesis System with GaN-based Anode by NiO Protective Layer
165	<u>Dennis Friedrich</u> (<i>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institute for Solar Fuels</i>), Mario Borgwardt, Sönke Müller, Hannes Hempel, Roel van de Krol, Rainer Eichberger Carrier dynamics in metal oxide absorbers for solar fuel production
169	<u>Bartek J. Trzeźniowski</u> (<i>Delft University of technology</i>), Ibadillah A. Digdaya, Sandheep P. Ravishankar, Isaac Herraiz-Cardona, Sixto Gimenez, Wilson A. Smith Photocharged BiVO4 photoanodes for solar water splitting
170	<u>Shababa Selim</u> (<i>Chemistry Department, Imperial College London</i>), Laia Francas, Andreas Kafizas, James Durrant Charge carrier separation in the BiVO4/WO3 heterojunction
171	<u>Serena Berardi</u> (<i>Dept. of Chemical and Pharmaceutical Sciences - University of Ferrara, Via Fossato di Mortara 17-19, 44121 – Ferrara, Italy</i>), Michele Orlandi, Alberto Mazzi, Nicola Bazzanella, Antonio Miotello, Stefano Caramori, Carlo Alberto Bignozzi Nickel-Iron oxide-modified Hematites as efficient earth-abundant photoanodes
173	<u>Ludmilla Steier</u> (<i>Chemistry Department, Imperial College London</i>), Matthew Mayer, Sebastiano Bellani, Hansel Comas, Laia Francas, James Durrant, Maria-Rosa Antognazza, Michael Grätzel Low-temperature Atomic Layer Deposition of TiO2 for Stable High-performance Organic Photocathodes



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| 174 | <u>Kai Liu</u> (<i>Chemical Engineering, Delft University of Technology</i>), Ming Ma, Sixto Gimenez Julia, Wilson Smith
Au-Cu bimetallic thin film for CO ₂ reduction |
| 176 | <u>Sacha Corby</u> (<i>Department of Chemistry, Imperial College London</i>), Laia Francas Forcada, Andreas Kafizas, James Durrant
Evaluation of water oxidation kinetics and charge trapping in nanostructured WO ₃ photoanodes |
| 178 | <u>Dong-Hyung Kim</u> (<i>Department of Materials and Chemical Engineering, Hanyang University, Ansan, Kyunggido, 426-791, Republic of Korea.</i>), Sambhaji S Shinde, Jin-Young Jung, Jin-Young Yu, Sung-Hae Kim, Jung-Ho Lee
Noble metal free Co-Sn-Sx chalcogel hybrids for high performance hydrogen evolution |
| 180 | <u>Jin-Young Jung</u> (<i>Departments of Materials and Chemical Engineering, Hanyang University, 55 Hanyangdaehak-ro, Sangnok-gu, Ansan, Kyeonggi-do 426-791, Republic of Korea</i>), Jin-Young Yoo, Jung-Ho Lee
Photoelectrochemical hydrogen evolution reactions using electrolyte-permeable NiOx coated Si photocathodes |