

# SYMPOSIUM ES7

(Photo)electrocatalytic Materials and Integrated Assemblies for Solar Fuels Production—Discovery, Characterization and Performance

April 17 - April 21, 2017

## Symposium Organizers

Akihiko Kudo, Tokyo University of Science  
Francesca Maria Toma, Lawrence Berkeley National Laboratory  
Roel Van de Krol, Helmholtz-Zentrum Berlin  
Lianzhou Wang, University of Queensland

## Proceedings Statement

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\* Invited Paper

## SESSION ES7.1: CO<sub>2</sub> Reduction

Session Chairs: Harry Atwater, Francesca Maria Toma and Roel Van de Krol  
Monday Morning, April 17, 2017  
PCC North, 200 Level, Room 222 BC

### 8:30 AM \*ES7.1.01

**Artificial Photosynthesis—The Selective CO<sub>2</sub> Reduction Challenge** [Harry A. Atwater](#); California Institute of Technology, United States.

### 9:00 AM ES7.1.02

**Optimizing C-C Coupling on Oxide Derived Copper Catalysts for Electrochemical CO<sub>2</sub> Reduction** [Yanwei Lum](#)<sup>1,2</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory, United States; <sup>2</sup>University of California, Berkeley, United States.

### 9:15 AM ES7.1.03

**Strain Induced Changes in CO<sub>2</sub> Electro-Reduction Pathway at Au-Pd Core-Shell Nanostructures** [David J. Fermin](#); University of Bristol, United Kingdom.

### 9:30 AM ES7.1.04

**Surface Science Insights into the Role of the Electrode Surface in Solar-Driven Pyridine-Catalyzed CO<sub>2</sub> Reduction** [Bruce E. Koel](#); Princeton University, United States.

### 9:45 AM ES7.1.05

**Investigations of Heterogeneous Processes for CO<sub>2</sub> Reduction Involving Molecular Co-Catalysts** [Coleman X. Kronawitter](#); University of California, Davis, United States.

## 10:00 AM BREAK

### 10:30 AM \*ES7.1.06

**Solar CO<sub>2</sub> Reduction Coupled with Water Oxidation—Semiconductor/Metal-Complex Hybrid System** [Takeshi Morikawa](#); Toyota Central R&D Labs, Japan.

### 11:00 AM ES7.1.07

**High Efficiency Solar-Fuel Devices** [Chengxiang \(CX\) Xiang](#); California Institute of Technology, United States.

### 11:15 AM ES7.1.08

**Highly Efficient Artificial Photosynthesis with Low-Cost Transition Metal Electrocatalysts in Aqueous Solution** [Haotian Wang](#); Harvard University, United States.

### 11:30 AM ES7.1.09

**Fabrication of Copper Oxide Photocathode for CO<sub>2</sub> Reduction** [Guiji Liu](#); Lawrence Berkeley National Laboratory, United States.

### 11:45 AM ES7.1.10

**Photocatalytic Conversion of CO<sub>2</sub> over Nanostructures into Solar Fuels** [Yong Zhou](#); Nanjing University, China.

## SESSION ES7.2: Advanced Architectures for Solar Fuels

Session Chairs: Takeshi Morikawa and Bruce Parkinson  
Monday Afternoon, April 17, 2017  
PCC North, 200 Level, Room 222 BC

### 1:30 PM \*ES7.2.01

**Sunlight-Driven Hydrogen Formation by Membrane-Supported Photoelectrochemical Water Splitting** [Nathan S. Lewis](#); California Institute of Technology, United States.

### 2:00 PM ES7.2.02

**Nano-Photoelectrochemical Cell Arrays with Spatially Isolated Oxidation and Reduction Channels** [Mohammad F. Islam](#); Carnegie Mellon University, United States.

### 2:15 PM ES7.2.03

**Core-Shell Micro-Tube Array for Closing the Artificial Photosynthesis Cycle on a Nanometer Scale** [Eran Edri](#); Lawrence Berkeley National Lab, United States.

### 2:30 PM ES7.2.04

**Design of Photonic and Plasmonic Materials for Photocatalytic CO<sub>2</sub> Reduction** [Ashley Gauding](#); Lawrence Berkeley National Lab, United States.

### 2:45 PM ES7.2.05

**Solid-State Architecture for a High-Current, Elevated-Temperature Photoelectrochemical Cell** [Madhur Bloor](#); Stanford University, United States.

## 3:00 PM BREAK

SESSION ES7.3: Novel Concepts  
Session Chairs: Nathan Lewis and Lianzhou Wang  
Monday Afternoon, April 17, 2017  
PCC North, 200 Level, Room 222 BC

### 3:30 PM ES7.3.01

**Photoelectrochemical Tandem Configuration for Solar Water Splitting Exceeding 7% Using Photon Recycling** [Jong Hyeok Park](#); Yonsei University, Korea (the Republic of).

### 3:45 PM \*ES7.3.02

**Photoelectrochemical Solar Energy Storage—Hydrogen Production vs Direct CO<sub>2</sub> Reduction and Photoredox Flow Batteries** [Bruce A. Parkinson](#); University of Wyoming, United States.

SESSION ES7.4: Advanced Characterization and Operando Studies  
Session Chairs: Rainer Eichberger and Dunwei Wang  
Tuesday Morning, April 18, 2017  
PCC North, 200 Level, Room 222 BC

### 10:30 AM \*ES7.4.01

**In Situ and Operando Characterization of CO<sub>2</sub> Reduction Reaction Catalysts Using Soft and Hard X-Ray Spectroscopy** [Junko Yano](#)<sup>1,2</sup>; <sup>1</sup>Lawrence Berkeley National Lab, United States; <sup>2</sup>Lawrence Berkeley National Lab, United States.

11:00 AM ES7.4.02

**Corrosion Behavior of p-GaInP<sub>2</sub> Thin Films for Photoelectrochemical Water Splitting Studied by Ambient Pressure X-Ray Photoelectron Spectroscopy** Monika Blum; University of Nevada, Las Vegas, United States.

11:15 AM ES7.4.03

**X-Ray Characterization of Solar Fuels Catalysts under Operation** Walter Drisdell; Lawrence Berkeley National Laboratory, United States.

11:30 AM ES7.4.04

**Soft X-Ray Spectroscopic Investigation of the CdS/Cu(In,Ga)<sub>2</sub>S<sub>2</sub> Interface in Thin Films for Photoelectrochemical Water Splitting** James C. Carter; University of Nevada, Las Vegas, United States.

11:45 AM ES7.4.05

**Characterization of BiVO<sub>4</sub> Powders and Thin Films by Electron Microscopy** Hector A. Calderon; Instituto Politecnico Nacional - ESFM, Mexico.

SESSION ES7.5: Understanding Interfaces  
Session Chairs: Lianzhou Wang and Junko Yano  
Tuesday Afternoon, April 18, 2017  
PCC North, 200 Level, Room 222 BC

1:30 PM \*ES7.5.01

**Charge Transfer Processes in Catalyzed Semiconductor Photoelectrodes** Shannon W. Boettcher; University of Oregon, United States.

2:00 PM \*ES7.5.02

**Probing Energetics and Kinetics at the Interface of the Photoelectrode and Water** Dunwei Wang; Boston College, United States.

2:30 PM ES7.5.03

**Direct Observation of Photoelectrochemical Water Oxidation Intermediates on  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Electrode Surfaces Employing Operando ATR-IR Spectroscopy** Omid Zandi; University of Texas at Austin, United States.

2:45 PM ES7.5.04

**Amorphous Molybdenum Sulphide—Surface Water Dependent Properties, Humidity Sensing and Electrolyte Free Water Splitting** Torben Daeneke; RMIT University, Australia.

3:00 PM BREAK

SESSION ES7.6: Protection Layers  
Session Chairs: Shannon Boettcher and Lianzhou Wang  
Tuesday Afternoon, April 18, 2017  
PCC North, 200 Level, Room 222 BC

3:30 PM ES7.6.01

**Atomic Layer Deposited Transition Metal Oxide-Titania Alloys as Corrosion Resistant Schottky Contacts for Silicon Photoanodes** Olivia Hendricks; Stanford University, United States.

3:45 PM ES7.6.02

**Controlling the “Leakiness” of TiO<sub>2</sub> Protection Layers** Aafke C. Bronneberg; Helmholtz-Zentrum Berlin für Materialien und Energie, Germany.

4:00 PM ES7.6.03

**Charge Transfer Characterization on Atomic Layer Deposited TiO<sub>2</sub> Protective and Conductive Layers for Photoelectrochemical Solar Fuels** Carles Ros Figueras; IREC, Catalonia Institute for Energy Research, Spain.

4:15 PM ES7.6.04

**Enhanced Photoelectrochemical Efficiency and Stability Using A Conformal TiO<sub>2</sub> Film on A Black Silicon Photoanode** Yanhao Yu; University of Wisconsin-Madison, United States.

4:30 PM ES7.6.05

**Passivating Silicon Photocathodes by Solution-Deposited Ni-Fe Layered Double Hydroxide for Efficient H<sub>2</sub> Evolution in Alkaline Media** Jiheng Zhao; Stanford University, United States.

SESSION ES7.7: Poster Session  
Tuesday Afternoon, April 18, 2017  
8:00 PM - 10:00 PM  
Sheraton, Third Level, Phoenix Ballroom

ES7.7.01

**Phase Transition-Induced Band Edge Engineering of BiVO<sub>4</sub> to Split Pure Water under Visible Light** Won Jun Jo; Massachusetts Institute of Technology, United States.

ES7.7.02

**Cu<sub>2</sub>O Based Photostable Photoanodes by the Au Passivation for High-Efficiency Photoelectrochemical Applications** Hee Jun Kim; UNIST, Korea (the Republic of).

ES7.7.03

**Photoelectrochemical Hydrogen Production by Water Splitting over Dual-Functionally Modified Oxide—P-Type N-Doped Ta<sub>2</sub>O<sub>5</sub> Photocathode Active under Visible Light Irradiation** Tomiko M. Suzuki; Toyota Central R&D Labs Inc, Japan.

ES7.7.04

**Enhanced Visible Light Photocatalytic Water Reduction of a g-C<sub>3</sub>N<sub>4</sub>/SrTa<sub>2</sub>O<sub>6</sub> Heterojunction** Shiba P. Adhikari<sup>1, 2</sup>; <sup>1</sup>Wake Forest University, United States; <sup>2</sup>Centre for Energy Studies, United States.

ES7.7.05

**Interface Engineering of Colloidal CdSe Thin Film Photocathodes for Solar-Driven Hydrogen Evolution** Hui Li; Wake Forest University, United States.

ES7.7.06

**Unique Role of Metal Oxide 2D Nanosheet in Optimizing Catalyst Performance of Graphene for Oxygen Reduction Reaction** Xiaoyan Jin; Ewha Womans University, Korea (the Republic of).

ES7.7.07

**Direct Fabrication of BaNbO<sub>2</sub>N Crystals on Niobium Substrates for Visible-Light-Responsive Photoanode by Flux Coating under Ammonia Flow** Sayaka Suzuki; Shinshu University, Japan.

SESSION ES7.8: Oxygen Evolution Catalysts  
Session Chairs: Artur Braun and Francesca Maria Tora  
Wednesday Morning, April 19, 2017  
PCC North, 200 Level, Room 222 BC

9:00 AM ES7.8.01

**The Reaction Mechanism with Free Energy Barriers at Constant Potentials for the Oxygen Evolution Reaction at the IrO<sub>2</sub> (110) Surface** Yuan Ping; University of California, Santa Cruz, United States.

9:15 AM ES7.8.02

**Electronic Structure of Manganese Based Oxides under OER** Katarzyna Skorupska<sup>1, 2</sup>; <sup>2</sup>Max-Planck-Institut für Chemische Energiekonversion, Germany; <sup>3</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany.

9:30 AM ES7.8.03

**Elucidating the Role of the Mn Oxidation State in Thin Film MnO<sub>x</sub> Oxygen Evolution Catalysts** Paul Plate; Helmholtz-Zentrum Berlin, Germany.

9:45 AM ES7.8.04

**Development of Solar Fuels Photoanodes through Combinatorial Integration of Ni-La-Co-Ce and Ni-Fe-Co-Ce Oxide Catalysts on BiVO<sub>4</sub>** Aniketa Shinde; California Institute of Technology, United States.

10:00 AM BREAK

SESSION ES7.9: III-V Semiconductors  
Session Chairs: Roel Van de Krol and Lydia Wong  
Wednesday Morning, April 19, 2017  
PCC North, 200 Level, Room 222 BC

SESSION ES7.12: Towards Practical Systems  
Session Chairs: Katherine Ayers, Miguel Modestino, Francesca Maria Toma  
and Roel Van de Krol  
Thursday Morning, April 20, 2017  
PCC North, 200 Level, Room 222 BC

**10:30 AM \*ES7.9.01**

**Recent Advances in III-V Multijunction Semiconductor Photo-Electrochemical Water Splitting** Todd G. Deutsch; National Renewable Energy Laboratory, United States.

**11:00 AM ES7.9.02**

**Solar-to-Hydrogen Efficiency—Shining Light on Photoelectrochemical Device Performance** James L. Young; National Renewable Energy Laboratory, United States.

**11:15 AM ES7.9.03**

**Photo-Induced Gain of Open-Circuit-Potential (OCP) in GaN Photoelectrodes for Characterizing Defects and Photoelectrochemical Activity** Yuuki Imazeki; University of Tokyo, Japan.

**11:30 AM ES7.9.04**

**GaN-Based Nanopillars for Solar Water Splitting** Siva Karuturi; Australia National University, Australia.

**11:45 AM ES7.9.05**

**Self-Oriented Sb<sub>2</sub>Se<sub>3</sub> Nanoneedle Arrays on a Conductive Substrate for Photoelectrochemical Water Splitting Prepared by Simple Spin-Coating Method** Wooseok Yang; Yonsei University, Korea (the Republic of).

SESSION ES7.10: Understanding and Improving Hematite  
Session Chairs: Giulia Galli and Akihiko Kudo  
Wednesday Afternoon, April 19, 2017  
PCC North, 200 Level, Room 222 BC

**1:30 PM \*ES7.10.01**

**Intermediates in PEC Water Oxidation—How They Come and How They Go** Artur Braun; Empa, Switzerland.

**2:00 PM \*ES7.10.02**

**Strategies to Improve the Performance of Semiconductor Photoelectrodes for Photoelectrochemical Water Splitting** Lydia Wong; Nanyang Technological University, Singapore.

**2:30 PM BREAK**

SESSION ES7.11: Theory and Modeling  
Session Chairs: Todd Deutsch and Roel Van de Krol  
Wednesday Afternoon, April 19, 2017  
PCC North, 200 Level, Room 222 BC

**3:30 PM \*ES7.11.01**

**Optimizing Solar Interfaces from First Principles—In Search for Descriptors** Giulia Galli; University of Chicago, United States.

**4:00 PM ES7.11.02**

**Modelling the Electrochemical Interface—Applications to CO<sub>2</sub> Reduction** Michal Bajdich; Stanford, SLAC, United States.

**4:15 PM ES7.11.03**

**Understanding CO<sub>2</sub> Reduction on Transition Metals** Karen Chan; SLAC National Accelerator Laboratory, United States.

**4:30 PM \*ES7.11.04**

**Catalysis on Nanoparticle Derived Aerogels** Alexander Eychmueller; TU Dresden, Germany.

**8:30 AM \*ES7.12.01**

**An Integrated Inorganic-Biological Hybrid System for a Complete Artificial Photosynthesis** Daniel G. Nocera; Harvard University, United States.

**9:00 AM \*ES7.12.02**

**Electrochemical Carbon Dioxide Reduction as an Alternative Source of Fuels and Chemicals** Sichao Ma; Opus 12, United States.

**9:30 AM ES7.12.03**

**A Monolithic and Scalable Device Based on Adapted Silicon HIT Photovoltaic Structures Enabling Bias-Free CO<sub>2</sub> Conversion to Syngas** Felix Urbain; IREC, Catalonia Institute for Energy Research, Spain.

**9:45 AM ES7.12.04**

**Design, Analysis and Optimization of High Voltage Photovoltaic Electrolysis System for Solar Fuel Production from CO<sub>2</sub>** Gowri M. Sriramagiri<sup>1,2</sup>; <sup>1</sup>University of Delaware, United States; <sup>2</sup>Institute of Energy Conversion, United States.

**10:00 AM BREAK**

**10:30 AM \*ES7.12.05**

**Working Together to Enable Gigawatt Scale Renewable Hydrogen Production—Solar Fuels and Large Scale Electrolysis** Katherine Ayers; Proton OnSite, United States.

**11:00 AM ES7.12.06**

**User-on-Demand Power Supply System Operation Using the Concept of High Performance Solar to Hydrogen Conversion Device** Masakazu Sugiyama; The University of Tokyo, Japan.

**11:15 AM ES7.12.07**

**A Durable and Efficient Solar Hydrogen Generator** Karl A. Walczak; Lawrence Berkeley National Laboratory, United States.

**11:30 AM ES7.12.08**

**Developing Microfluidic Air-Based Solar-Hydrogen Generators** Miguel A. Modestino; New York University, United States.

**11:45 AM ES7.12.09**

**Tandem Cell Approach for Artificial Photosynthesis** Gurudayal Gurudayal; Lawrence Berkeley National Laboratory, United States.

SESSION ES7.13: BiVO<sub>4</sub> Photoelectrodes  
Session Chairs: Akihiko Kudo and Lianzhou Wang  
Thursday Afternoon, April 20, 2017  
PCC North, 200 Level, Room 222 BC

**1:30 PM \*ES7.13.01**

**Elucidating Excited State Processes in Transition Metal Oxide Photoelectrodes** Ian D. Sharp; Lawrence Berkeley National Lab, United States.

**2:00 PM ES7.13.02**

**Time-Resolved Terahertz Study of Carrier Trapping and Polaron Formation in BiVO<sub>4</sub>** Rainer Eichberger; Helmholtz-Zentrum Berlin für Materialien und Energie, Germany.

**2:15 PM ES7.13.03**

**Nanoscale Imaging of Charge Carrier Transport in Monoclinic Bismuth Vanadate Photoanodes via Atomic Force Microscopy** Johanna Eichhorn; Lawrence Berkeley National Laboratory, United States.

**2:30 PM ES7.13.04**

**Photoelectrochemical Water Oxidation of BiVO<sub>4</sub> Photoanodes with 50 cm<sup>2</sup> Active Area** Yimeng Ma; Helmholtz-Zentrum Berlin, Germany.

2:45 PM ES7.13.05

**Pulsed Laser Deposition of Ternary Oxide Photoelectrodes—BiVO<sub>4</sub> as a Model Material** Moritz Koelbach; Helmholtz-Zentrum Berlin für Materialien und Energie, Germany.

3:00 PM BREAK

SESSION ES7.14: Nitride and Oxynitride Absorbers

Session Chairs: Akihiko Kudo and Ian Sharp

Thursday Afternoon, April 20, 2017

PCC North, 200 Level, Room 222 BC

3:30 PM \*ES7.14.01

**Improvement of Water Oxidation Ability of Oxynitrides Aiming at Application to Photoanodes** Hideki Kato; Tohoku University, Japan.

4:00 PM ES7.14.02

**Fabrication of Ta<sub>3</sub>N<sub>5</sub> Crystal Layers on Tantalum Substrate Using NaCl-Na<sub>2</sub>CO<sub>3</sub> Flux Evaporation and Their Photoelectrochemical Properties** Minori Yanai; Shinshu University, Japan.

4:15 PM ES7.14.03

**Enhanced Water-Splitting Performance of Granular Oxynitride Photoanode Films through Improving Inter-Particle Charge Transport** Zhaosheng Li; Nanjing University, China.

SESSION ES7.15: 2D Materials

Session Chairs: Gang Liu and Kazuhiro Takanabe

Friday Morning, April 21, 2017

PCC North, 200 Level, Room 222 B

8:30 AM \*ES7.15.01

**Direct Observation of Single-Atom Photocatalytic Reaction Centers for Hydrogen Production Using Two-Dimensional Oxide Nanosheet** Shintaro Ida; Kyushu University, Japan.

9:00 AM \*ES7.15.02

**2D Inorganic Nanosheets for Solar Fuel Production** Seong-Ju Hwang; Ewha Womans University, Korea (the Republic of).

9:30 AM ES7.15.03

**Two-Dimensional g-C<sub>3</sub>N<sub>4</sub>/Ca<sub>2</sub>Nb<sub>2</sub>TaO<sub>10</sub> for Efficient Visible Light Photocatalytic Hydrogen Evolution** Supphasin Thaweesak; Nanomaterials Centre, School of Chemical Engineering and AIBN, The University of Queensland, Australia.

9:45 AM ES7.15.04

**Efficient Photoelectrochemical Hydrogen Production Using Wafer-Scale, Defect-Engineered Transition Metal Disulfide Thin Film Catalysts** Ki Chang Kwon; Seoul National University, Korea (the Republic of).

10:00 AM BREAK

SESSION ES7.16: Chalcogenide Photoelectrodes

Session Chairs: Seong-Ju Hwang and Shintaro Ida

Friday Morning, April 21, 2017

PCC North, 200 Level, Room 222 B

10:30 AM \*ES7.16.01

**Surface-Modified Chalcogenide Thin Films as Efficient Photocathodes for Water Reduction** Shigeru Ikeda; Konan University, Japan.

11:00 AM ES7.16.02

**Photoelectrochemical and Solid-State Properties of Wide Bandgap Copper Chalcopyrites for Renewable Hydrogen Generation** Nicolas Gaillard; University of Hawaii, United States.

11:15 AM ES7.16.03

**Cd-Doped CZTS Photocathode for Enhanced Photoelectrochemical Water Splitting** Ying Fan Tay; Nanyang Technological University, Singapore.

11:30 AM ES7.16.04

**Feasible and Non-Expensive Photocathodes Based on Kesterites for Water Splitting** Carles Ros Figueras; IREC, Catalonia Institute for Energy Research, Spain.

11:45 AM ES7.16.05

**Growth of P-Type CdS<sub>y</sub>Se<sub>1-x</sub>:Cu Absorber Layer for Overall Water Splitting in PEC Cells** Zi Ye; The Chinese University of Hong Kong, Hong Kong.

SESSION ES7.17: Particle-Based Systems

Session Chairs: Francesca Maria Toma and Roel Van de Krol

Friday Afternoon, April 21, 2017

PCC North, 200 Level, Room 222 B

1:30 PM \*ES7.17.01

**Quantitative Identification of Limitations in Semiconductor Particulate System for Photocatalytic Water Splitting** Kazuhiro Takanabe; King Abdullah University of Science and Technology (KAUST), Saudi Arabia.

2:00 PM \*ES7.17.02

**Solar-Driven Photocatalysts with Wide Spectrum Absorption and High Charge Separation Ability** Gang Liu; Institute of Metal Research, CAS, China.

2:30 PM ES7.17.03

**Modelling Photocatalytic, Particle-Based Water Splitting** Marc Schiffler; EPFL, Switzerland.

2:45 PM BREAK

SESSION ES7.18: Novel Oxide Absorbers

Session Chairs: Akihiko Kudo and Roel Van de Krol

Friday Afternoon, April 21, 2017

PCC North, 200 Level, Room 222 B

3:15 PM ES7.18.01

**Discovery of Solar Fuels Photoanode Materials by Integrating High-Throughput Theory and Experiment** Santosh K. Suram; California Inst of Technology, United States.

3:30 PM ES7.18.02

**Electronic and Photoelectrochemical Characterization of Oxygen Deficient Fe<sub>2</sub>TiO<sub>5</sub> Photoanodes for Application in Solar Water Splitting** Prince S. Bassi; Nanyang Technological University, Singapore.

3:45 PM ES7.18.03

**Fabrication of Fe<sub>2</sub>TiO<sub>5</sub> Epitaxial Thin Films for Photoelectrochemical Applications** Motoki Osada; Stanford University, United States.

4:00 PM ES7.18.04

**Solar Water Oxidation on a Tri-Layered Bi<sub>2</sub>MoO<sub>6</sub> / MoO<sub>3</sub> Heterojunction Photoanode Prepared by an Anodization-Hydrothermal Intercalation Route** Shi Nee Lou; University of New South Wales, Australia.

4:15 PM ES7.18.05

**A Novel Perovskite Oxides for Visible Light Photocatalytic Hydrogen Production** Zaicheng Sun; Beijing University of Technology, China.