TASK 26

ADVANCED MATERIALS FOR WATERPHOTOLYSIS

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PURPOSE

Photoelectrochemical (PEC) hydrogen production using sunlight to directly split water is one of the paramount enabling technologies for a future where hydrogen is widely deployed as an energy carrier. The "traditional" semiconductor-based PEC material systems studied to date, in particular the simple metal oxides such as TiO_2, WO_3, and Fe_2O_3, however, have been unable to meet all the performance, durability, and cost requirements for practical hydrogen production. Technology-enabling advances are needed in the development of new, advanced materials systems. Toward this end, the IEA Hydrogen Implementation Agreement Task-26, working in close conjunction with the U.S. Department of Energy's "Working Group on PEC Hydrogen Production," brought together international experts in analysis, theory, synthesis, and characterization from the academic, industry, and national laboratory research sectors across the world, with exciting and important results on several fronts.

FRAMEWORK SUMMARY

The specific technical goal of this Task is the research and development of new semiconductor materials for stable and efficient PEC hydrogen production systems. In order to meet this goal Task-26 has formulated a comprehensive "Task" structure, as illustrated below in Figure 1, serving as the central organizational framework for Task activities. Task-26 relies heavily on individual Tasks and Task Leaders to coordinate collaborative efforts in international PEC R&D and facilitate the PEC materials breakthrough process.

expansion of original task D

A: PEC R&D Administration	
A1	Research Coordination
A2	Database Development
A3	Reporting

expanded from original task B1

M: Focus Materials	
M1	Modified WO3 Films
M2	Modified Fe2O3 Films
M3	Silicon Alloy Films
M4	Copper Chalcopyrite Films
M5	Nanostructured Sulfides
M6	III-V Semiconductors
M7	Modified TiO2 Films
M8	Vanadate Semiconductor
M9	*others*

expanded from original task C3

S: Standardized Testing/Screening	
S1	Standard Testing Protocols
S2	Standard PEC Screening
S3	Standards Reviewing

expansion of original task C

C: Materials Characterizations	
C1	Standard Measurements
C2	Advanced Solid-State
C3	Advanced In-Situ Methods

original tasks B2 abd B3

D: Materials Discovery	
D1	Combinatorial Discovery
D2	Auxiliary Materials

expanded from original tasks D1 abd A

E: Techo-Economics Analyses	
E1	System Configurations
E2	Baseline TE Analyses

original task A

T: Materials Theory	
T1	Solid-State Calculations
T2	Interface Calculations

Figure 1: Task Force definitions evolved from original IEA HIA Task-26 subtasks

STATUS OF TECHNOLOGY

It is recognized that PEC hydrogen production is at relatively early stage of development. Though it is one of the most promising approaches for practical conversion of sunlight to chemical energy, and much progress has been made in recent years, the technology readiness level (TRL) of various PEC technologies remains at TRL 1 and TRL 2. See Figure 2 to the right.

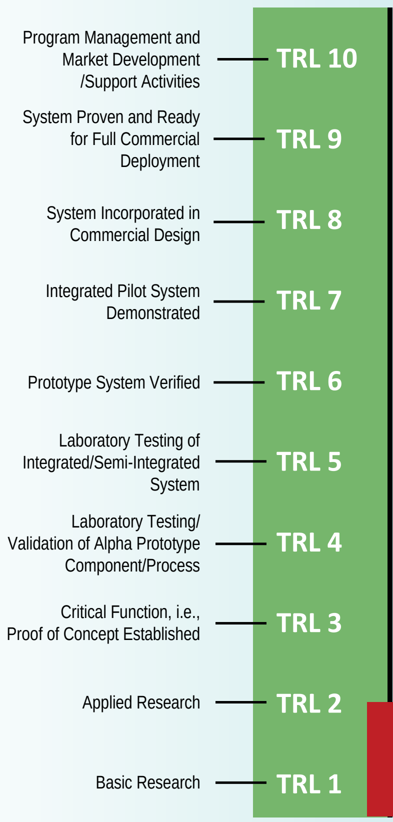

Figure 2: Technology Readiness Level (TRL)

VITAL STATISTICS

Term

2008-2011

Members

USA
EC
Netherlands
Switzerland
Germany
Japan
S. Korea
Australia

Expert Participants (over 50, primary and associate)

Dr. Hironori Arakawa
Dr. Jan Augustinski
Dr. Artur Braun
Dr. Todd Deutsch
Dr. Huyen Dinh
Dr. Kazunari Domen
Dr. Nicolas Gaillard
Dr. Michael Graetzel
Dr. Clemens Heske
Dr. Thomas Jaramillo
Dr. Jae Sung Lee
Dr. Andreas Luzzi
Dr. Bjorn Marsen
Dr. Eric McFarland
Dr. Eric Miller
Dr. Tadashi Ogitsu
Dr. Ian Plumb
Dr. Kazuhiro Sayama
Dr. Kevin Sivula
Dr. John Turner
Dr. Roel van de Kroel
Dr. Lionel Vayssieres
Dr. Heli Wang
Dr. Scott Warren
Dr. Brandon Wood

MEMBERS

TASK 26	COUNTRY	EXPERT NAME (INDICATE IF SUBTASK LEADER)	INSTITUTION NAME
1	USA	John Turner	NREL
2		Tom Jaramillo	Stanford
3		Eric McFarland	UCSB
4		Nico Gaillard	U. Hawaii
5		Tadashi Ogitsu	LLNL
6		Huyen Dinh	NREL
7		Todd Deutsch	NREL
8		Zhebo Chen	Stanford
9		Jess Kaneshiro	U. Hawaii
10		Brandon Wood	LLNL
11		Bill Ingler	U. Toledo
12		Heli Wang	NREL
13		Brian James	SAINC
14		Yanfa Yan	NREL
15		Eric Miller	US DOE
16		OTHERS	various
17	EU: Switzerland	Artur Braun	EMPA
18		Michael Graetzel	EPFL
19		Kevin Sivula	EPFL
20		Scott Warren	EPFL
21	EU: Netherlands	Roel Van de Kroel	U. Delft
22		Yongqi Liang	U. Delft
23	EU: Poland	Jan Augustinski	U. Warsaw
24	EU: Germany	Bjorn Marsen	Helmholtz-Zentrum Berlin
25		Clemens Heske	Solar Energy Helmholtz-Zentrum Berlin
26		Marcus Baer	Helmholtz-Zentrum Berlin
27		Lothar Weinhardt	U Wurzburg, Germany
28		Monika Blum	Solar Energy Helmholtz-Zentrum Berlin
29	EU: OTHER	OTHERS	various
30	JAPAN	Kazuhiro Sayama	AIST
31		Hironori Arakawa	Tokyo U. Science
32		Kazunari Domen	U. Tokyo
33		Akihiko Kudo	Tokyo U. Science
34		Ryu Abe	Hokkaido U.
35		OTHERS	various
36	SOUTH KOREA	Jae Sung Lee	POSTECH
37		Wonyong Choi	POSTECH
38		OTHERS	various
39	AUSTRALIA	Grant Mathieson	ANSTO
40		Ian Plumb	

Central objectives of Task-26 include international outreach and expansion of cooperative and collaborative activities between the US D.O.E. PEC Working Group and the international research community in areas related to PEC materials discovery and development. Combining ever-advancing world-class capabilities in analysis, theory, synthesis, and characterization is the surest path to the needed scientific advances in PEC semiconductor materials. With this in mind, Task-26 has relied on its international base, coordinating numerous international meetings further the cause, as illustrated in example meetings shown in Figure 2. Synergistic activities among the US DOE Working Group projects, European PEC projects such as "NanoPEC," and Asian research projects such as those in Japan and Korea have paid strong dividends, as evidenced in recent progress and results.

2011 Meetings
December 2010, April 2011,
"Hu'a Iki International Experts"
Honolulu, HI, San Francisco, CA

Figure 3:"Hu'a Iki"(Hawaiian for "tiny bubbles") meetings of international Task-26 Experts

ACTIVITIES AND RESULTS IN 2011

As of 2011, the primary task activities have started winding down in preparation for final Task documentation, and in preparation for a proposal for a new approach for integrating ongoing PEC work into a future IEA HIA Task framework. Over the past three years, the research methodology of Task-26 integrating collaborative tasks in PEC materials theory, synthesis, characterization and analysis has paid dividends in terms of technical achievements in PEC materials research and development. The tools in Task-26 research arsenal have been in Task A, C, S, and T activities. The most productive and significant activities have been the successful utilization of these tools in effecting advances in PEC materials systems (Task M). Major accomplishments resulting from these activities have been documented in previous reports, and will be further organized and documented in a series of updated Materials White Pape currently in preparation by the Task Experts for incorporation into the Task-26 Final Report.

Broadly speaking, over the course of Task-26, renewable solar hydrogen production via PEC water splitting has been successfully demonstrated on the laboratory scale using current materials systems, but challenges remain in meeting all targets in solar-to-hydrogen (STH) conversion efficiency, durability, and cost. The research methodology of Task-26, integrating collaborative tasks in PEC materials theory, synthesis, characterization, and analysis, has led to some significant advances in the PEC state of the art over the course of the Task. Important accomplishments have been achieved over a broad spectrum of PEC materials R&D through the duration of Task-26, which are being thoroughly documented in the White Paper updates. Some of the notable achievements have included:

Achievement of new benchmark performance in oxide-based materials, specifically in iron-oxide based material systems as a result of the EU NanoPEC Project [1].

Achievement of new benchmark performance levels in III-V materials multi-junction photoelectrodes at NREL as a result of the US PEC Working Group efforts, shown in Figure 2 [2,3].

Achievement of new benchmark performance levels in copper-chalcopyrite thin film materials in multi-junction photoelectrode configurations at UH/MVSystems as a result of the US PEC Working Group efforts [4].

Successful demonstration of Z-scheme photocatalyst systems and screening of numerous photocatalyst materials in research institutes in Japan, including AIST and TUS [5,6,7,8].

Successful demonstration of enhanced performance heterojunction thin film material systems in South Korea at POSTECH [9].

Development of new MoS_2 nano-particle catalysts and concurrent development of novel macro-structures for integration into practical photoelectrochemical hydrogen production devices (Figure 5); including macroporous scaffold consisting of a transparent conducting oxide (TCO) upon which the MoS_2 nanoparticles can be vertically integrated for support, confinement and electronic contact [10,11]. (Stanford)

Continued work on the refinement of the "Standardized Methodologies for PEC Measurements and Reporting" effort. Agreements are being negotiated with Springer to publish the documents in book form with assigned editors (Huyen Dinh of NREL, Eric Miller of DOE, and Zhebo Chen of Stanford University) [*www2.eere.energy.gov/hydrogenandfuelcells/pec_standards_review.html#standards*].

Publication of hundreds of PEC articles in scientific journals and in conference proceedings by Task-26 Experts and associated research groups.

Publication of two important books on PEC Hydrogen Production with major contributions from the Task-26 Experts [12,13].

Although the Task-26 is winding down, technical advances continue to be realized through implementation of the Task's R&D methodologies, and these advances will be incorporated into the Task Final Report. Up-to-date PEC Materials White Papers are under preparation by Task Experts which will be integrated as the primary content of the Final Report; specific topics include: (2) III-V semiconductors; (2) Fe_2O_3 based materials; (3) WO_3 based materials; (4) I-III-VI_2 materials; (5) MoS_2 nanostructured materials; (6) $BiVO_4$ materials; (7) TaON materials; (8) PEC Materials Theory Updates; and (9) New oxide materials.

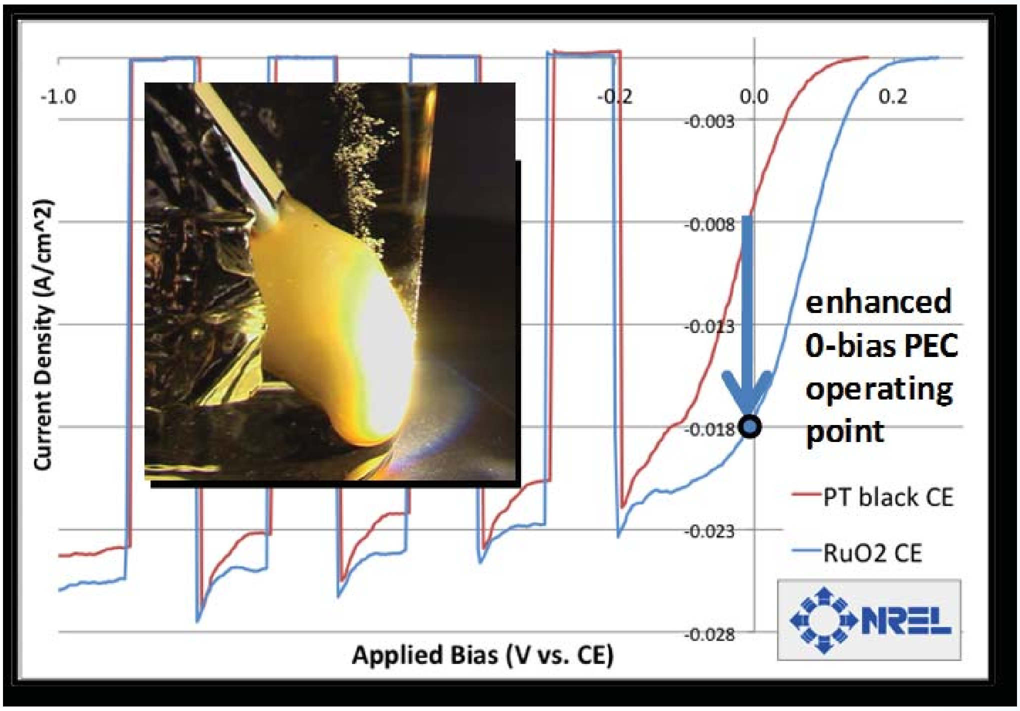

Figure 4: New benchmark performance in PEC solar water-splitting from NREL GaAs/GaInP$_2$ devices

FUTURE WORK

Continued work on documentation and on information management is the current priority as Task-26 winds down. Efforts are focused on the completion of the updated series of PEC Materials White Papers for integration into the Task-26 Final Report. Potential follow-up PEC work in a future IEA HIA Task structure has been discussed with Task Experts, and a conceptual approach integrating PEC into a broader Task focused on "Renewable Hydrogen" (along with Bio-Hydrogen, Solar-Thermochemical Hydrogen, and others) is being considered with support from Experts.

END NOTES

1] NanoPEC Project Publications website: http://nanopec.epfl.ch/publications

2] T. Deutsch, Semiconductor Photoelectrodes for Direct Water Splitting, Pacifichem 2010 Congress, Honolulu, HI. December 15-20, 2010.

3] J. A. Turner and T. Deutsch, US D.O.E. Hydrogen Program Annual Merit Review Meeting 2011, Arlington, VA, May 9-13, 2011: http://www.hydrogen.energy.gov/pdfs/review11/pd035_turner_2011_o.pdf

4] A. Madan, J. Kaneshiro, et al., US D.O.E. Hydrogen Program Annual Merit Review Meeting 2011, Arlington, VA, May 9-13, 2011: http://www.hydrogen.energy.gov/pdfs/review11/pd053_madan_2011_o.pdf

5] Arai, T., Konishi, Y., Iwasaki, Y., Sugihara, H., and Sayama, K.: High-Throughput Screening Using Porous Photoelectrode for the Development of Visible-Light-Responsive Semiconductors J. Comb. Chem. 9, 574–581 (2007)

6] Kusama, H., Wang, N., Miseki, Y., and Sayama, K.: Combinatorial Search for Iron/Titanium-Based Ternary Oxides with a Visible-Light Response. J. Comb. Chem. 12, 356–362 (2010)

7] Higashi, M., Abe, R., Ishikawa, A., Takata, T., Ohtani, B., and Domen, K.: Z-scheme Overall Water Splitting on Modified-TaON Photocatalysts under Visible Light (l < 500 nm). Chem. Lett. 37, 138-139 (2008)

8] Arakawa, H., Zou, Z., Sayama, K., and Abe, R.: Direct Water Splitting By New Oxide Semiconductor Photocatalysts Under Visible Light Irradiation. Pure Appl. Chem. 79, 1917–1927 (2007)

9] POSTECH PEC Group website: http://ecocat.postech.ac.kr/

10] T. F. Jaramillo, 2009 American Institute of Chemical Engineers Annual Meeting, Nashville, TN. Nanostructured MoS2 for the Photoelectrochemical (PEC) Production of Hydrogen, November, 2009.

11] T. F. Jaramillo, et al., US D.O.E. Hydrogen Program Annual Merit Review Meeting 2011, Arlington, VA, May 9-13, 2011: http://www.hydrogen.energy.gov/pdfs/review11/pd033_jaramillo_2011_o.pdf

12] BOOK: Photoelectrochemical Hydrogen Production, R. Van de Kroel, M. Gratzel editors, Springer, 2011.

13] BOOK: On Solar Hydrogen & Nanotechnology, L.Vayssieres editor, Wiley, 2010.