IEA Hydrogen Implementation Agreement
Semi-Annual Progress Report
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Task 26: Advanced Materials for Waterphotolysis

Dr. Eric L. Miller, Operating Agent

SUMMARY

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 breakthroughs are needed in the development of new, advanced materials systems. Toward this end, the IEA Hydrogen Implementation Agreement Annex-26, working in close conjunction with the U.S. Department of Energy's "Working Group on PEC Hydrogen Production", is bringing 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.

TASK DESCRIPTIONS

The four overarching objectives of the Annex-26 program comprise:

- Intensification of international collaboration, making use of extended fields of expertise in areas of materials theory, synthesis and characterization, as well as data and data-base management;
- Advancement of photoelectrode materials science, particularly addressing the discovery of new practical materials, with bulk and surface properties specifically engineered to meet the requirements for efficient and stable PEC water splitting;
- Demonstration of stable and efficient water splitting in the leading materials systems, using standardized performance characterizations and round-robin testing procedures;
- Promotion of photolysis of water through publications, education and outreach program.

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

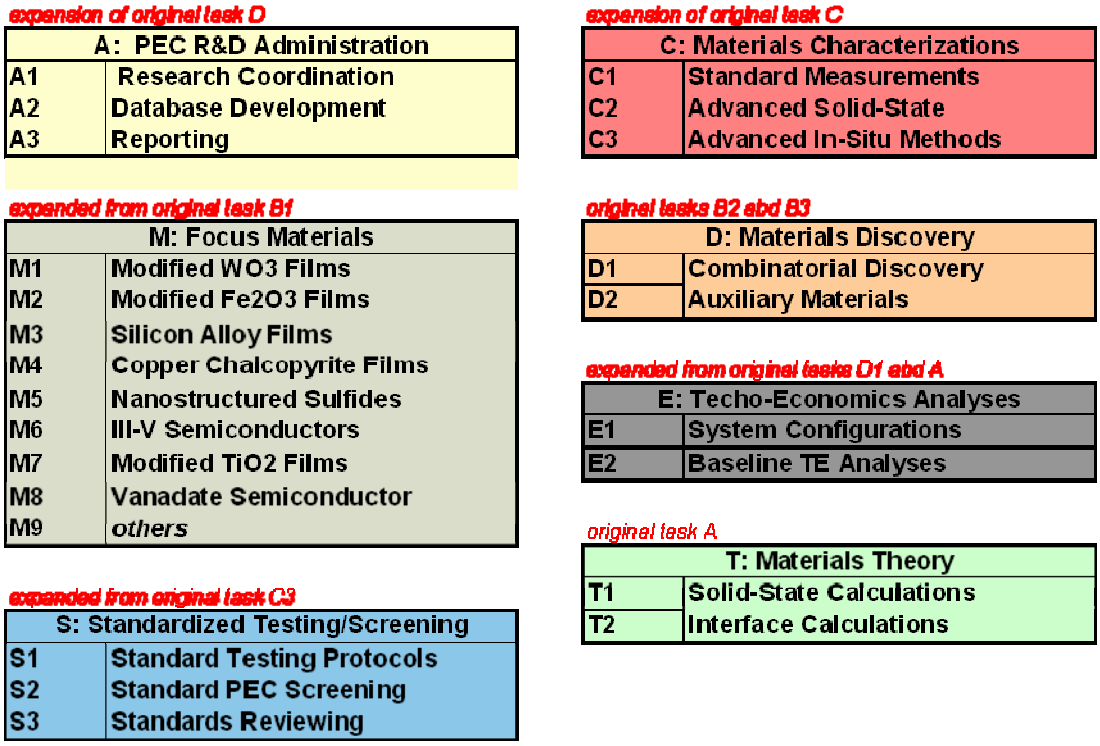

Figure 1: Task Force definitions evolved from original IEA-HIA Annex-26 tasks.

PRIMARY ACTIVITIES

Primary task activities during the past six months have made significant strides toward the Annex-26 objectives and goals. These activities have included: (1) Successful international meetings centered on advancing the state-of-the-art in PEC research and development; (2) continued expansion and organization of the Annex-26 Experts base, focusing particularly on refining membership in the various Task Forces; (3) Numerous collaborative publications among the Annex-26 Experts; (4) Continued progress in the efforts to establish 'standardized" PEC methods and testing protocols; (5) Continued progress in Techno-Economics analysis of PEC systems; (6) New progress in developing theoretical models for PEC materials and interfaces; (7) Continued progress in advancing techniques to characterize PEC materials and interfaces; (8) Continued progress in the development of specific PEC materials classes; and (9) Design and deployment an Annex-26 "Sharepoint" website to be hosted in conjunction with the US Department of Energy's PEC Working Group. Major accomplishments resulting from these activities are enumerated by task below.

MAJOR ACCOMPISHMENTS

There have been numerous accomplishments over the spectrum of Annex-26 Task Force activities. These are summarized below by task:

- **TASK C: Further Deployment of PEC Materials Characterization "Tool Chest" to Facilitate Technical Breakthroughs:**
  - UV/Soft X-ray/electron spectroscopic tools for evaluating optoelectronic and chemical properties of PEC materials' surfaces, near-surfaces and bulk fully operational
  - Significant analytical results obtained in R&D of important PEC materials classes, including complex metal oxides, chalcopyrites and silicon alloys
  - Future tests planned in evaluation of III-V as well as metal sulfide nano-structured semiconductors
  - SALSA "Solid and Liquid Spectroscopic Analysis" characterization facility installed at the LBNL Beamline 8.0 Advanced Light Source for the in-situ evaluation of PEC semiconductor/electrolyte interfaces, as shown in Figure 2. [Heske group at UNLV: http://faculty.unlv.edu/heske/]

- **TASK T: New Additions to the PEC Materials Theory "Tool Chest" to Facilitate Technical Breakthroughs:**
  - First principle models of the PEC interface constructed based on III-V semiconductor systems [Al-Jassim group at NREL: http://www.nrel.gov/pv/measurements/research_staff.html]
  - Effects of O, H and OH termination modeled for a III-V model material system, and important correlations established between surface morphology and interaction with interfacial water molecules, is illustrated in Figure 3. [Ogitsu group at LLNL: https://www-pls.llnl.gov/?url=about_pls-scientific_staff-ogitsu_t

- **TASK S: Significant Progress in Establishing Standards for PEC Testing Protocols:**
  - First revision of 16 protocol documents completed [Dinh, et al. at DOE PEC WG: http://www1.eere.energy.gov/hydrogenandfuelcells/production/photoelectrochemical.html]
  - Summary paper published in Journal of Materials Science: http://www.mrs.org/s_mrs/sec_subscribe.asp?CID=18419&DID=243524&action=detail
  - Website set up to facilitate review/revision process: http://www2.eere.energy.gov/hydrogenandfuelcells/pec_standards_review.html#standards
  - International review process underway for current document set; numerous international reviews being processed

- **TASK E: Completion of Initial PEC H_2 Production Technoeconomic Analysis**
  - Designed conceptual systems to produce H_2 using PEC processes
  - Calculated capital costs and operating costs for conceptual designs
  - Performed boundary level analysis to predict levelized hydrogen costs
  - Identified necessary systems improvements and future work. [James group at DTI: http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/pec_technoeconomic_analysis.pdf

- **TASK M: Significant Progress in the Development of PEC Materials, Interfaces and Water-Splitting Devices Toward Annex Performance Milestones:**
  - Successful demonstration of bandgap tailoring in photoactive MoS_2 nanoparticles, as illustrated in Figure 4 [Jaramillo Group at Stanford: http://soe.stanford.edu/research/layout.php?sunetid=jaramillo]
  - Identification of crystalline semiconductor device configurations based on current III-V materials with >15% STH conversion efficiency [Deutsch group at NREL: http://www.nrel.gov/hydrogen/proj_production_delivery.html#split]

- Identification of thin-film device configurations based on current chalcopyrite and silicon compound materials with >5% STH conversion efficiency [Madan atMVSystems Inc. http://mvsystemsinc.com/ and Gaillard at UH http://www.hnei.hawaii.edu/hydro.photo.asp]
- Successful first year of the EU-funded NanoPEC project (lead by Dr. Michael Graetzel of EPFL) with significant initial progress in the development of nanostructured oxide based material systems: http://nanopec.epfl.ch/**.**
- Successful demonstration by at the Tokyo University of Science of robust 3% STH multi-junction device configurations comprising WO_3 PEC cells boosted by two dye-sensitized solar cells (DSSC) [Arakawa Group at TUS http://www.tus.ac.jp/en/] and successful demonstrate of robust high-efficiency DSSC configurations [Sayama group at AIST http://www.aist.go.jp/NIMC/english/authors/personnel/Sayama_K_.html]

- **TASK A: Significant Progress in Annex Organizational and Promotional Efforts:**
  - Book Chapter "On Solar Hydrogen and Nanotechnology" published featuring numerous chapters authored by IEA-Annex-26 Experts: http://www.wiley.com/WileyCDA/WileyTitle/productCd-0470823976.html
  - MRS Special Issue on Photocatalysis for Energy and Environmental Sustainability Published featuring contributions from over a dozen IEA-Annex-26 PEC Experts: http://www.mrs.org/s_mrs/sec_subscribe.asp?CID=17951&DID=23156
  - Experts Briefing held in Tokyo, Japan in December 2009; held in conjunction with the 4th International Collaboration Workshop at the Tokyo University of Science, including Japanese PEC Experts Drs. Arakawa and Sayama.
  - Design and initial deployment of organization "Sharepoint" web site, (co-sponsored by the US Department of Energy's PEC Working Group) to facilitate Annex R&D tasks and activities, shown if Figure 5: https://photoelectrochemical.sharepointsite.net/default.aspx

STATUS OF MILESTONES

The major milestone for the past six months of Annex-26 was the initial design and deployment of the annex "Sharepoint" website to facilitate international PEC activities and collaborations. This milestone was met, though much work is still needed in the refinement, population and promotion of this website.

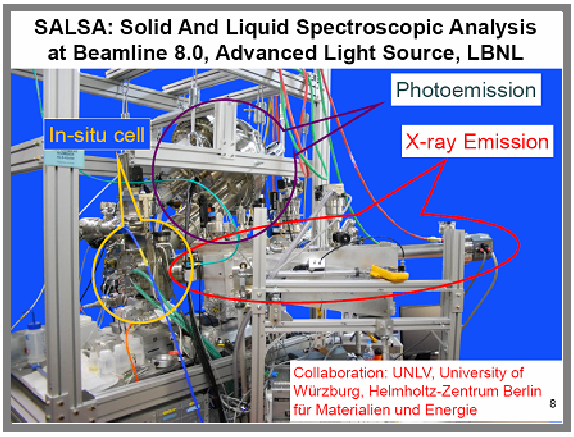

Figure 2: Advanced PEC Characterization Tool [Heske: UNLV]

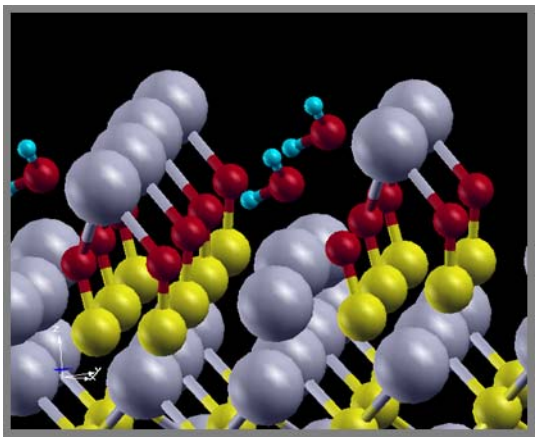

Figure. 3: Advanced PEC Interface Theory [Ogitsu: LLNL]

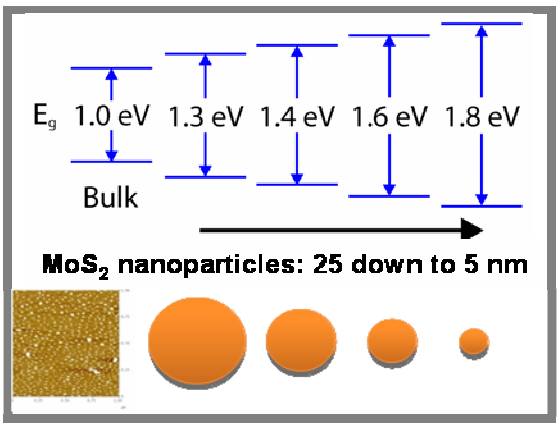

Figure 4: New Nanoparticle Photocatalyst [Jaramillo: Stanford]

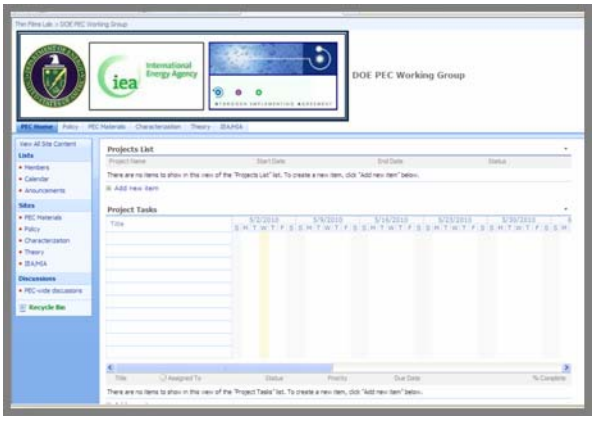

Figure. 5: New DOE / IEA-HIA PEC Website

WORK PLAN FOR NEXT SIX MONTHS

Full deployment and promotion of the PEC Sharepoint site is being planned for the next six months. In addition, several important meetings are being planned for 2010 and 2011 to bring together the Annex-26 Experts, including:

- European Experts Briefing Meeting to be held in conjunction with the WHEC conference in Essen, Germany in May 2010.
- Asian Experts Briefing Meeting to be held in conjunction with the IPS conference in Seoul Korea in July 2010.
- *Hu'a Iki Honolulu 2010*, the third Joint Meeting of the U.S. Department of Energy's PEC Working Group and the IEA-HIA Annex-26 Experts (the initial Hu'a Iki event is being held in December 2010 in conjunction with the Pacifichem conference: http://manoa.hawaii.edu/pechp/2010/
- *Hu'a Iki San Francisco 2011*, the fourth Joint Meeting of the U.S. Department of Energy's PEC Working Group and the IEA-HIA Annex-26 Experts is being planned for April 2011 to be held in conjunction with the MRS 2011 Spring Meeting: http://manoa.hawaii.edu/pechp/2011/

EFFECTIVENESS OF TASK PARTICIPATION

International outreach and expansion of US D.O.E. PEC Working Group activities related to PEC materials discovery and development to international collaborators is one of the central objectives of the IEA-HIA Annex-26. Combining ever-advancing world-class capabilities in analysis, theory, synthesis and characterization is the surest path to the needed scientific breakthroughs in PEC semiconductor materials. With this in mind, Annex-26 will continue to expand its international base, and to schedule as many of these international meetings as possible to further the cause. 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 are already paying dividends, and will be expanded through Annex-26 efforts.

EXECUTIVE COMMITTEE ITEMS

- Use of appropriate IEA-HIA graphics and logos in the new Annex-26 Sharepoint website
- Approval of hosting the Annex-26 Sharepoint website in conjunction with the US DOE PEC Working Group site
- Approval to use IEA-HIA website link in the Annex-26 Sharepoint website