International Institute for Carbon-Neutral Energy Research

I²CNER

Powering the Future
Internationalizing Research – PART III of V

P. Sofronis
Kyushu University
University of Illinois at Urbana-Champaign

November 7, 2013

New Value Chains and the Rise of Open Innovation in Asia
Stanford University

KYUSHU UNIVERSITY

wpi World Premier International Research Center Initiative

ILLINOIS 1867 UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

I^2CNER Structure

I²CNER's Organizational Structure

Director accessed directly

PRESIDENT OF KYUSHU UNIVERSITY: President Arikawa

I²CNER DIRECTOR: Prof. Sofronis
- Administers the affairs of the Institute. ~ *KU Regulations*
- Sets the research directions, promotes research quality, and provides overall management of I²CNER and Satellite. ~*Agreement*
- Decides any necessary matters concerning the Members at the Institute.

~ *Governing Document* (*Divisional and Personnel Structure for the Thematic Research Areas of I²CNER*)

ILLINOIS SATELLITE INSTITUTE

ASSOCIATE DIRECTOR: Prof. Christensen
- Research administration and contacts with KU

EXECUTIVE ADVISOR: Mr. Dick
- Budget issues

EXTERNAL ADVISORY COMMITTEE (EAC)

INTERNAL PROGRAMS REVIEW COMMITTEE (IPRC)

SRA SELECTION COMMITTEE

FACULTY RECRUITING COMMITTEE (FRC)

SCIENCE STEERING COMMITTEE (SSC)

SRA: Super Research Assistant

ASSOCIATE DIRECTOR: Prof. Ishihara
- Serves in the promotions committee.
- Is in charge of I²CNER workshop organizations.
- Administers seminar series.
- Oversees facilities and equipment.
- Provides input and advice to Director.

ASSOCIATE DIRECTOR: Prof. Takata
- Serves at the FRC
- Promotes international and industrial collaborations.
- Handles graduate student research matters.
- Serves on the SRA Selection Committee.

ADMINISTRATIVE OFFICE

ADMINISTRATIVE DIRECTOR: Prof. Funaki
- Administers the affairs of the office to facilitate the operations of the Institute. ~ *KU Regulations*
- Provides administrative support to the research personnel of I²CNER. ~ *Agreement*

RESEARCH DIVISIONS (Thematic clusters)

Hydrogen Production	Thermal Science and Engineering	CO_2 Capture and Utilization
Hydrogen Materials Compatibility	Hydrogen Storage	CO_2 Storage
Fuel Cells	Catalytic Materials Transformations	Energy Analysis

I²CNER COUNCIL

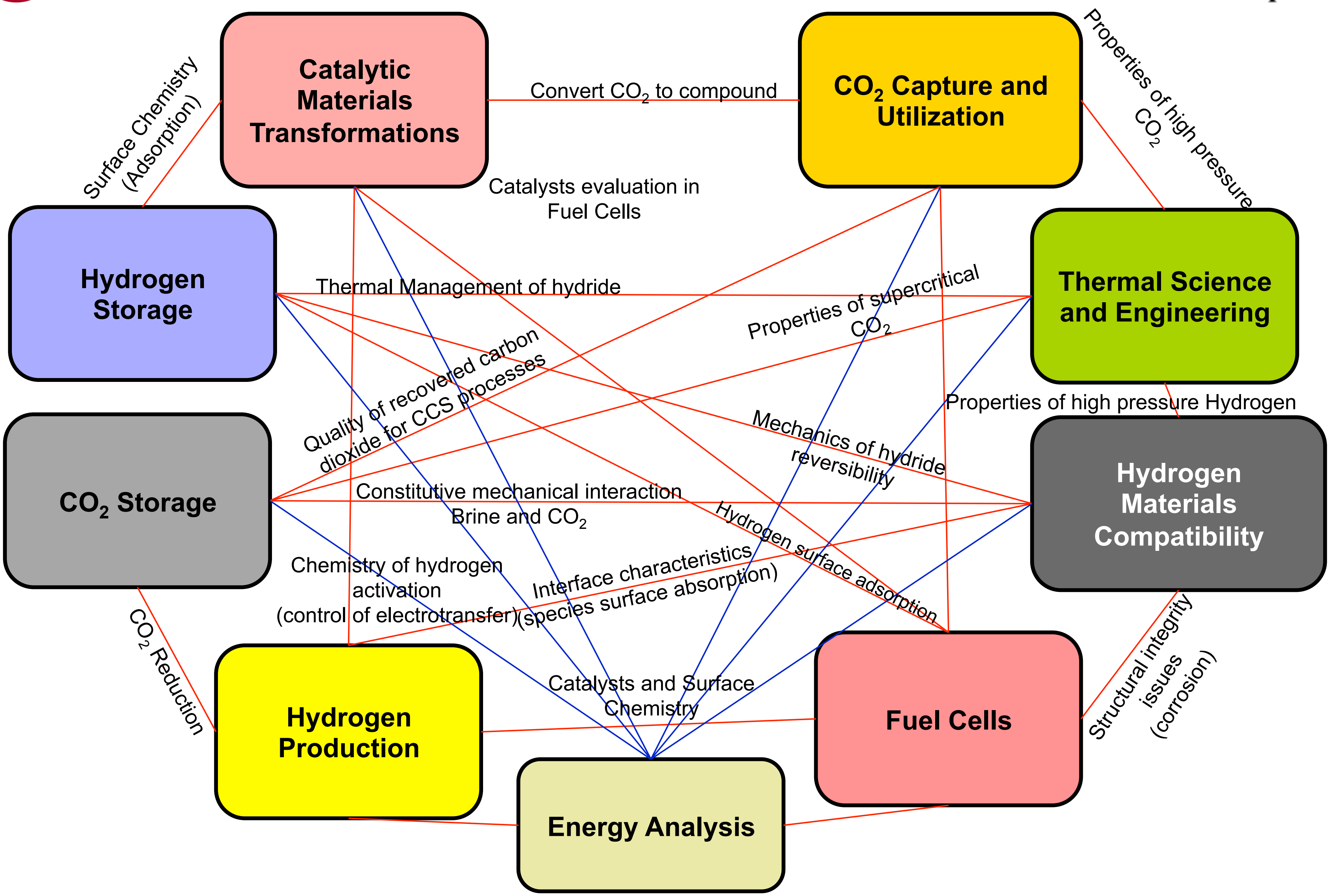
External Advisory Committee

- **Members**
  - Prof. Ronald Adrian, Arizona State University, USA (Chair)
  - Dr. Deborah Myers, Argonne National Laboratory, USA (Vice-Chair)
  - Dr. Robert Finley, Illinois State Geological Survey, USA
  - Prof. Reiner Kirchheim, University of Gottingen, Germany
  - Prof. Robert McMeeking, University of California, USA
  - Dr. Kevin Ott, Los Alamos National Laboratory
  - Prof. Tetsuo Shoji, Tohoku University , JAPAN
  - Dr. George Thomas, Sandia National Laboratories/EERE Office of US DOE, USA

- **Institute was reviewed on February 1, 2012 and May 30, 31, 2013**
- **Implementation of recommendations**



Research Teams—Fusion of Disciplines



Division interactions and interdisciplinary fusion research

26 Principal Investigators

(as of October 1, 2013)

Hydrogen Production


ISHIHARA Tatsumi


ADACHI Chihaya


TAKAHARA Atsushi


SAKAI Ken


KILNER John

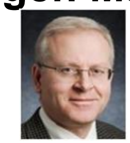
Hydrogen Storage


AKIBA Etsuo


HORITA Zenji

Hydrogen Materials Compatibility


SOMERDAY Brian


SOFRONIS Petros


SUGIMURA Joichi


TAKAKI Setsuo


KIRCHHEIM Reiner


ROBERTSON Ian

Catalytic Materials Transformations


OGO Seiji


YAMAUCHI Miho


KATSUKI Tsutomu

Fuel Cells


SASAKI Kazunari


NAKASHIMA Naotoshi


TULLER Harry


GEWIRTH Andrew

CO_2 Capture and Utilization


FUJIKAWA Shigenori


KUSAKABE Katsuki

Thermal Science and Engineering


TAKATA Yasuyuki


ZHANG Xing

CO_2 Storage


TSUJI Takeshi

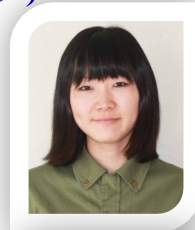

CHRISTENSEN Ken

I²CNER Female Researchers

(as of October 1, 2013)

Miho Yamauchi
Catalytic Materials Transfor
WPI Principal Investigator
Kyushu University

Chao-Nan Xu
Hydrogen Materials Compatibility
WPI Visiting Professor
National Institute of Advanced Industrial Science and Technology

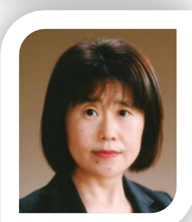


Maki Matsuka
Hydrogen Production
WPI Associate Professor
Kyushu University

Ping Chen
Hydrogen Storage
WPI Professor
Dalian Institute of Chemical Physics(China)

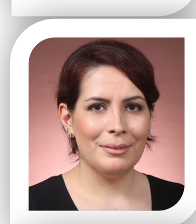
Akari Hayashi
Fuel Cells
WPI Associate Professor
Kyushu University

Nicola Perry
Fuel Cells
WPI Postdoc
Kyushu University



Junko Matsuda
Hydrogen Storage
WPI Assistant Professor
Kyushu University

Jennifer Rupp
Fuel Cells
WPI Associate Professor
Federal Institute of Technology, Zurich



Hoda Emami
Hydrogen Storage
WPI Postdoc
Kyushu University

Helena Tellez Lozano
Hydrogen Production
JSPS Postdoctoral Fellow
Imperial College London

Visiting Female Students from Illinois

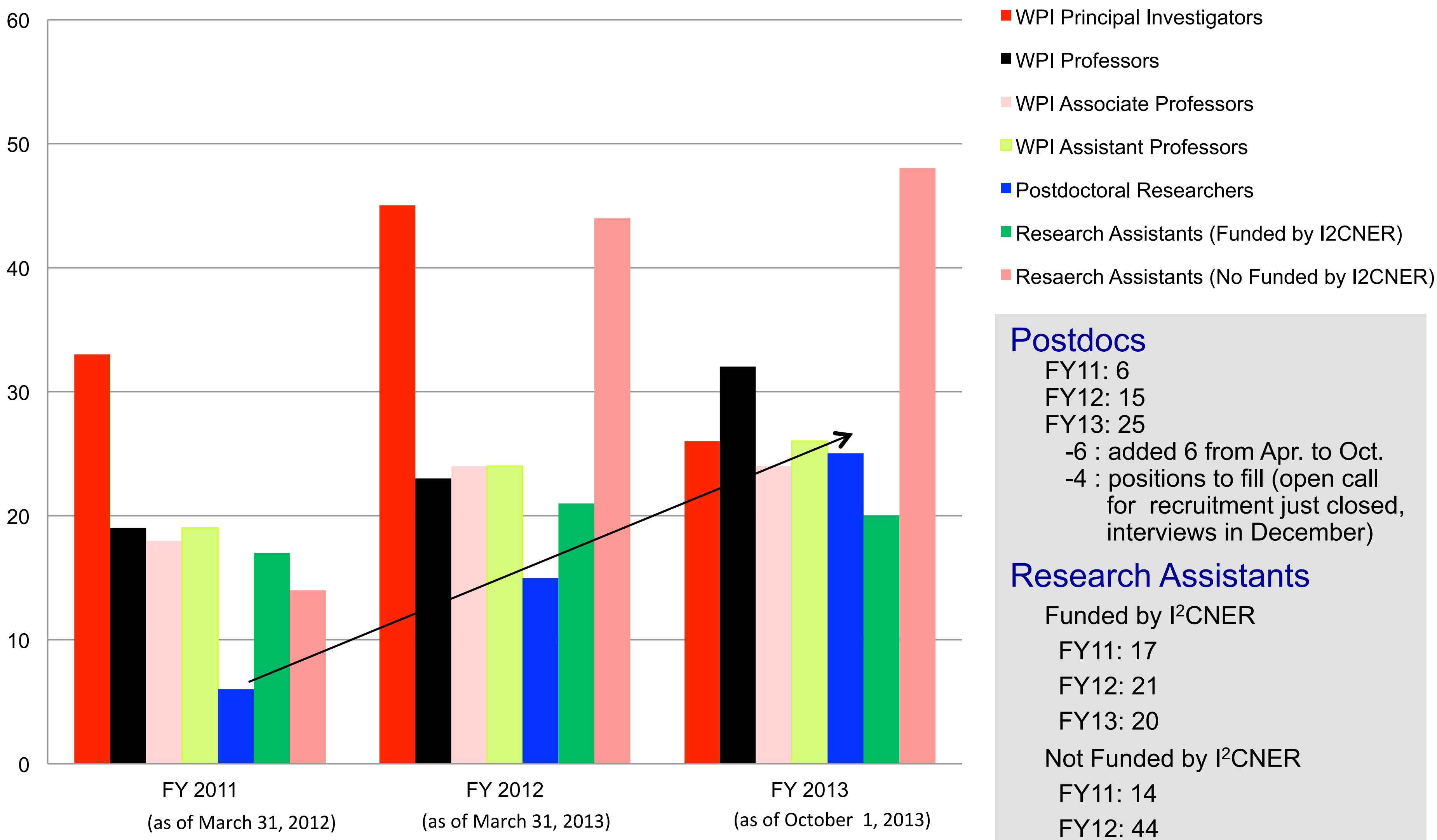
● **Kelly Nygren & May Martin**
June - August 2011
Visited Hydrogen Structural Materials Div.

● **Molly Jhong**
January & June 2012
Visited CO_2 Separation & Concentration Div. and Fuel Cells Div.

● **Kelly Nygren & Megan Emigh**
June - August 2013
Visited Hydrogen Materials Compatibility Div.

18/152 =11.6%

I²CNER Personnel Summary



- Total number of researchers: 155 (128 Kyushu, 27 Illinois)
- Non-Japanese: 72 or 46%

Postdocs

FY11: 6
FY12: 15
FY13: 25
-6 : added 6 from Apr. to Oct.
-4 : positions to fill (open call for recruitment just closed, interviews in December)

Research Assistants

Funded by I²CNER
FY11: 17
FY12: 21
FY13: 20

Not Funded by I²CNER
FY11: 14
FY12: 44
FY13: 48

I²CNER Researchers ~ Breakdown

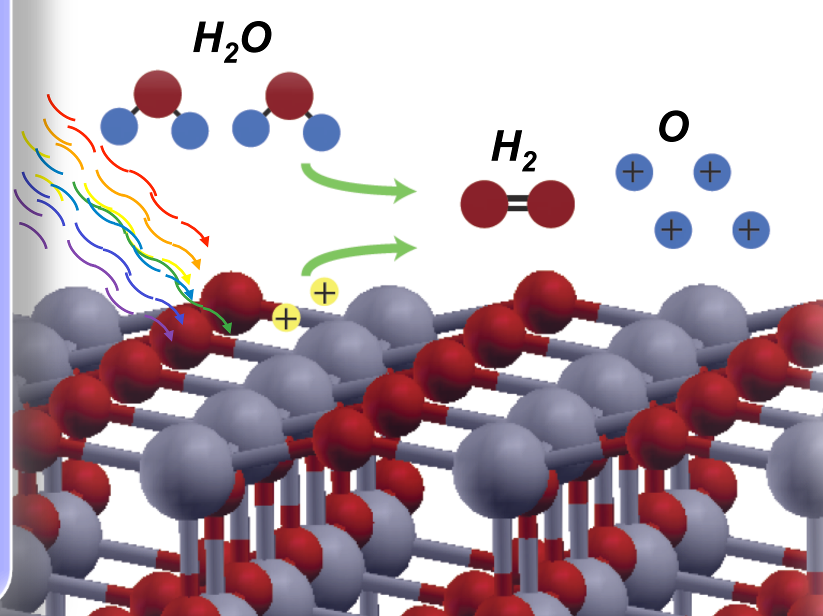
(as of October 1, 2013)

WPI Title	Total (*Non-Japanese)	Kyushu	Illinois
PI	26 (9)	24	2
Prof	32 (14)	26	6
Assoc Prof	24 (5)	23	1
Asst Prof	26 (8)	24	2
Other (faculty)	2 (1)	1	1
Post doc	25 (20)	23	2
RA	20 (15)	7	13
Total	**155 (72)**	**128**	**27**

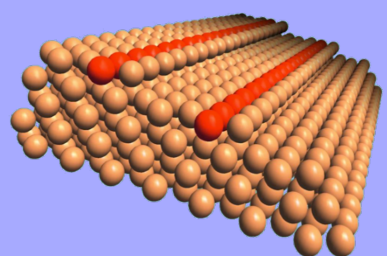
- **Non-Japanese : 72/155 = 0.464 (46%)**
- **Female researchers: 18/155= 11.6%**

Research

Photocatalytic Hydrogen Production International Approach



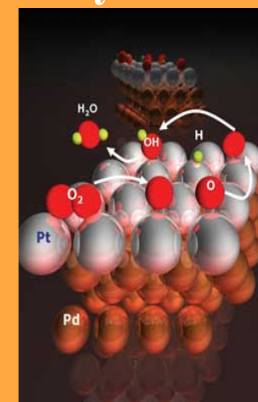
Understanding Surfaces & Interfaces in Photocatalysis



Takahara, Staykov, Ertekin, Hagiwara, Martin, Rockett



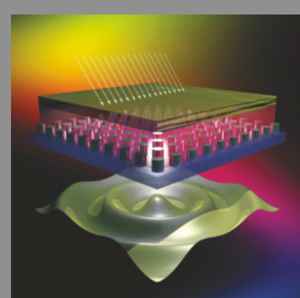

Probing Catalytic Activity in Devices



Ishihara, Sasaki, Gewirth, Hagiwara, Takahara, Hayashi, Ogo, Rauchfuss




New Materials for Light Absorption and Charge Separation



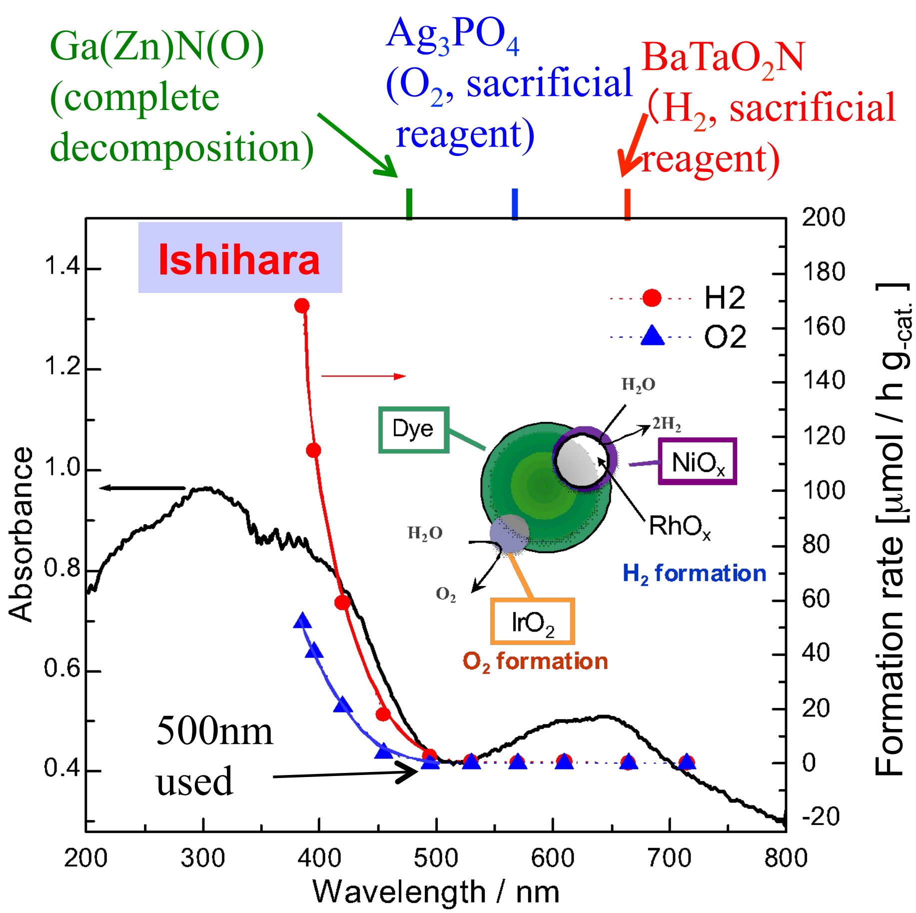
Ishihara, Adachi, Hayashi, Hagiwara, Martin, Ertekin, Gewirth

Roadblock: H_2 production efficiency using visible light is less than 0.1%

Photocatalytic Water Splitting with Visible Light

Roadblock: H_2 production efficiency using visible light is less than 0.1%

- Achieved promising 2.7% efficiency at 420nm with combination of organic dye and GaN (ZnO)

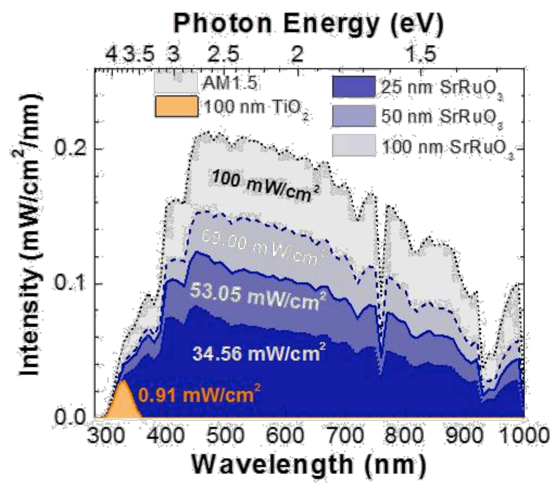


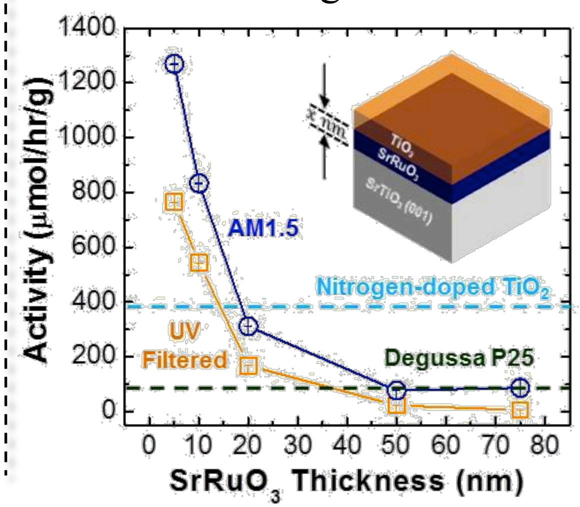
Phys. Chem. Chem. Phys.,13, 18031 (2011)

- Novel oxide heterostructures enable efficient absorption of 75X more sunlight than TiO_2 → higher efficiency

$SrRuO_3$ absorbs strongly across the visible regime → better utilization of sunlight

Hot-carrier injection into TiO_2 give rise to strong catalysis under AM1.5 light





Martin

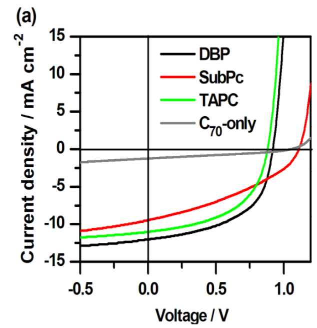
Under review at *Nature Materials*

Highly Efficient Organic Solar Cells (PCE>15%)

Our Goal
Solar cell (ex.11%)
X
Steam electrolyzer (90%)
=10%

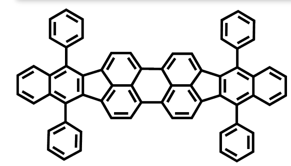
-Low-cost: Organic materials
-Large area and flexibility
-Energy savings for production
-Large absorption coefficient
-Unlimited molecular design

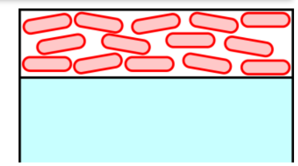
Highly efficient bulk heterojunction photovoltaic cells based on C_{70} and tetraphenyldibenzoperiflanthene
Yan-qiong Zheng; William J Potscavage Jr.; Takeshi Komino; Masaya Hirade; Junji Adachi; Chihaya Adachi
Appl. Phys. Lett., 102, 143304, (2013)



IV) Bulk hetero-junction with high purity materials (PCE=7.0%)

III) Control of Molecular Orientation (PCE=6.3%, V_{oc}=5.89 V)

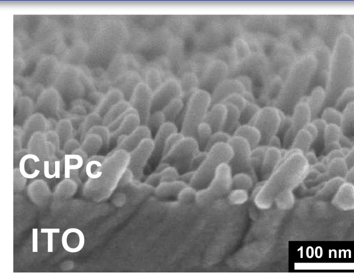




Very high open-circuit voltage of 5.89 V in organic solar cells with 10-fold-tandem structure
Appl. Phys. Lett. 100, 243302 (2012)

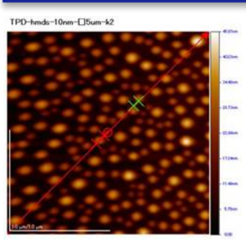
Small molecular organic photovoltaic cells with exciton blocking layer at anode interface for improved device performance
Appl. Phys. Lett., 99, 153302 (2011)
Top 20 Most Downloaded Articles

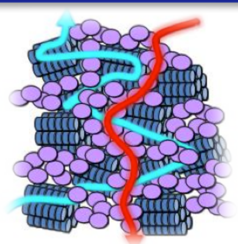
II) Preparation of Nano-pillars (PCE=1.2%)



Formation of Organic Crystalline Nanopillar Arrays and Their Application to Organic Photovoltaic Cells
Appl. Mat. Int. 3, 80-83, (2011)
Top 10 Most Read Articles

I) Control of Nano-sized Grain Morphology (PCE=4.1%)





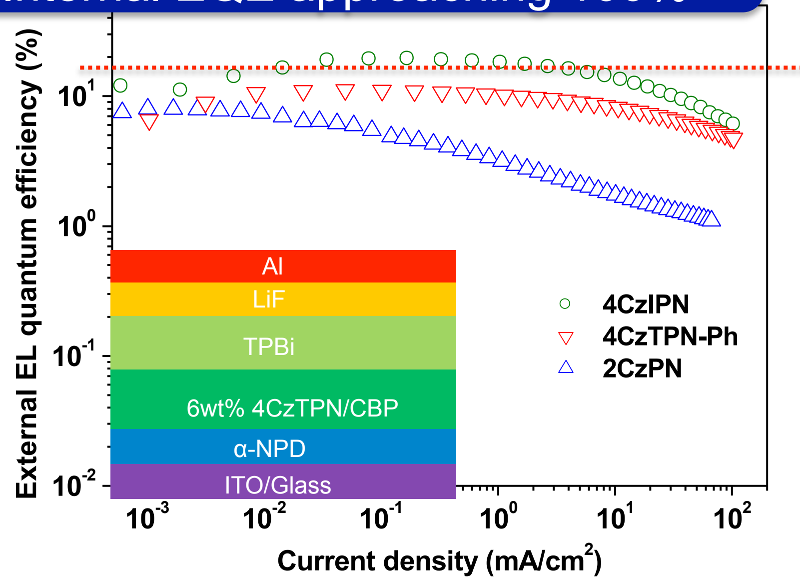
Nanocrystal growth and improved performance of small molecule bulk heterojunction solar cells composed of a blend of chloroaluminum phthalocyanine and C70
Appl. Phys. Exp. 3, 121602 (2010)

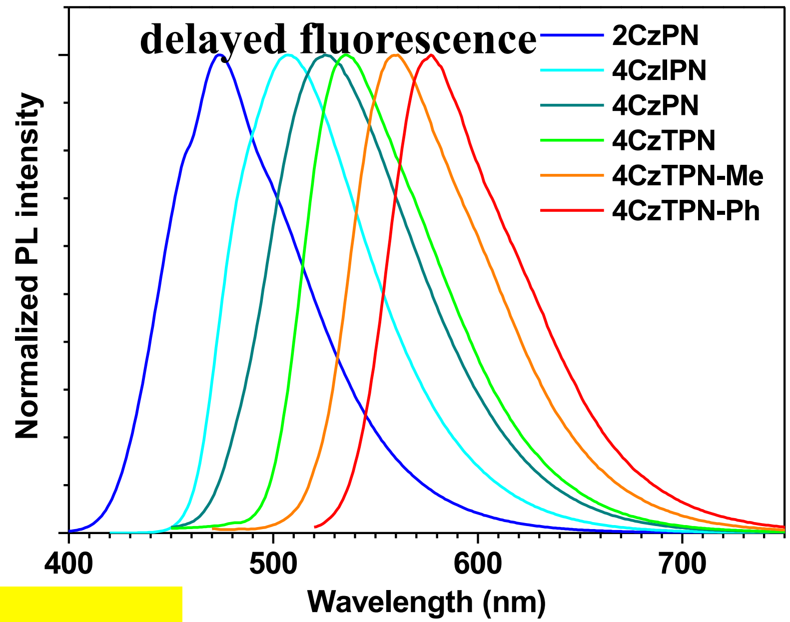
Using photovoltaics to push hydrogen production from water to higher efficiencies

Third Generation Organic Light Emitting Materials for OLEDs

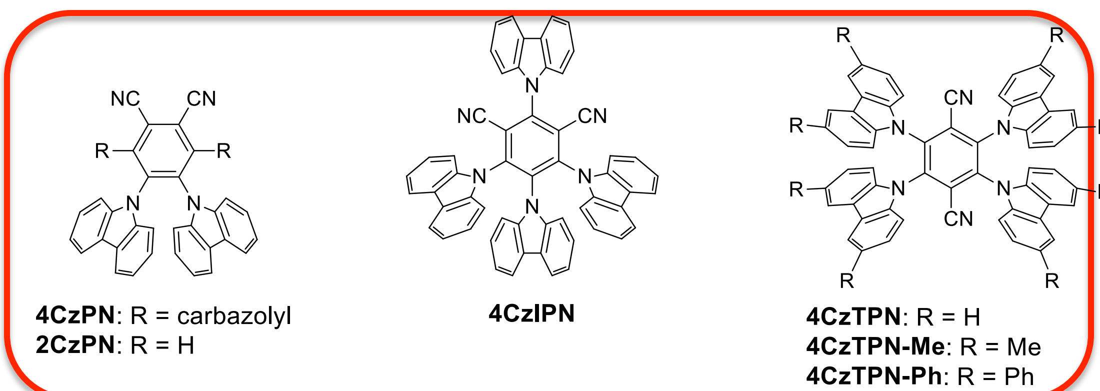
Achieved: External EQE~20%, Internal EQE approaching 100%

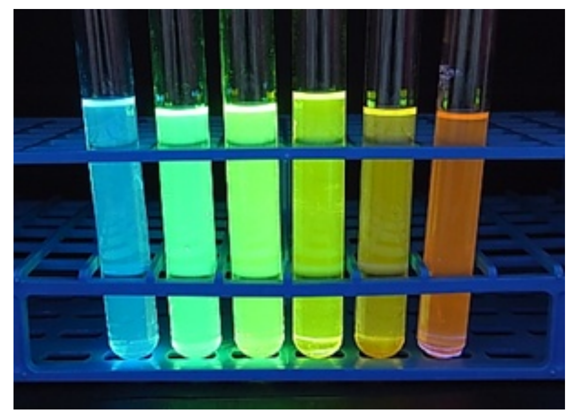
"Excellent demonstration of fusion research"
"Technological developments in energy conservation areas"





A new class of organic electroluminescent molecules in which the energy gap between singlet and triplet excited states is minimized by design

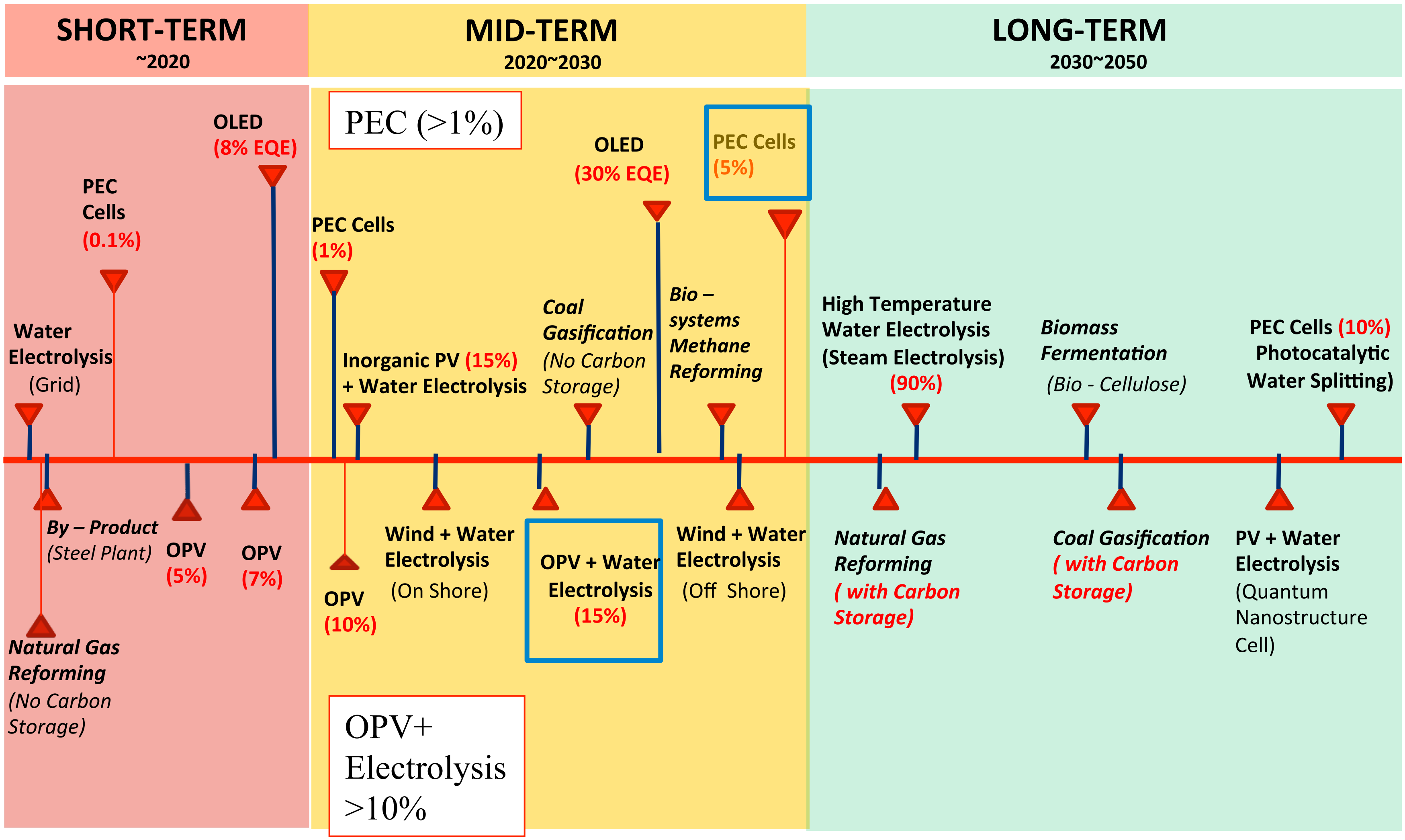




Dicyanobenzene derivatives

H. Uoyama et al., Nature 492, 234-238 (2012)

Hydrogen Production Roadmap



Boxed research targets are high priority

Italics indicate a non-I²CNER research theme

Electrochemomechanics: Reducing the Chemical Expansion Coefficient in Ceria by Addition of Zirconia

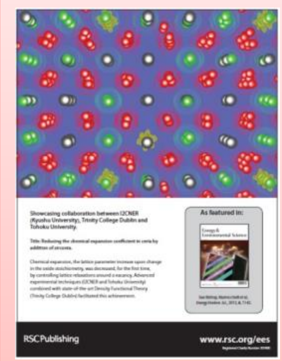
Advanced electrode materials for SOFCs exhibit **large changes in oxygen content** (“*breathing*” of O_2)

➡ This ***deleterious chemical expansion*** results in **poor SOFC durability!!** *←Roadmap target*

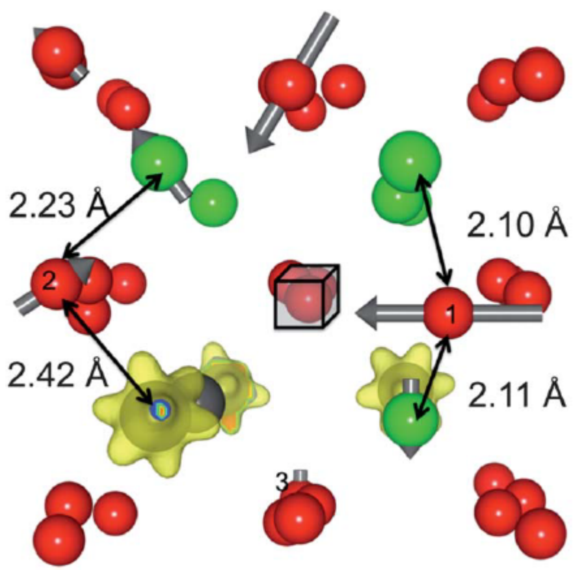
Bottleneck: Poor understanding of atomistic mechanism = lack of guidance to ↓ chemical expansion

Discovery: Expansion from the larger size of the reduced cation after an oxide ion is removed from the lattice vs contraction by the oxygen vacancy left behind

Back cover highlight!

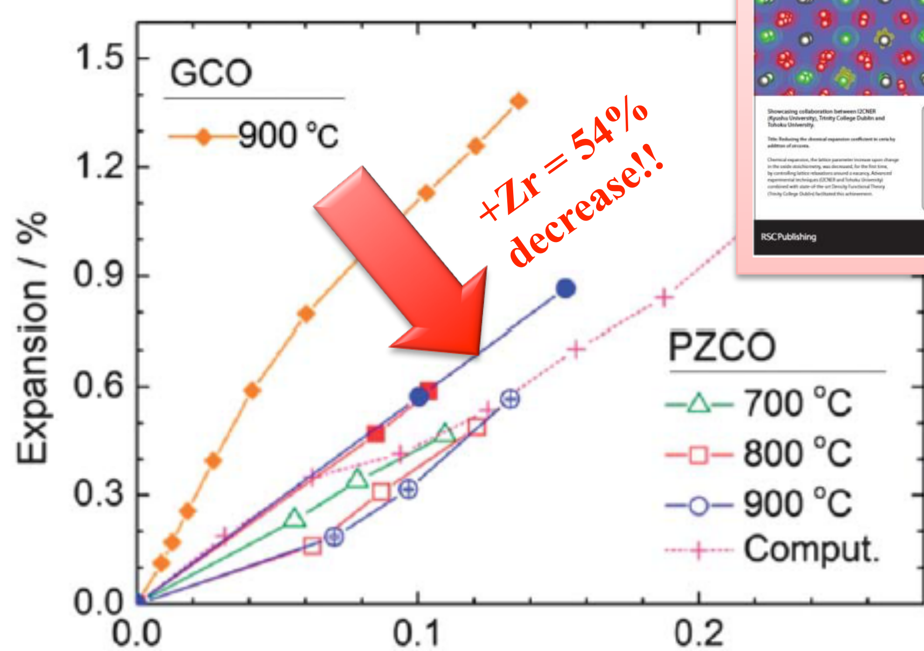


Computational Insight



S. R. Bishop et al., ***Energy and Environmental Science***, 6 (2013) 1142

Experimental Validation



Change in oxygen content of electrode

Discovery: smaller cations allow larger relaxations around the O vacancy