International Institute for Carbon-Neutral Energy Research



Powering the Future Internationalizing Research – PART IV of V

P. Sofronis

Kyushu University University of Illinois at Urbana-Champaign

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











Research, continued





The first elucidation of the H₂-activation mechanism using synthetic [NiFe]hydrogenase

Seiji Ogo et al., Science 339, 682-684 (2013)



Crystal structure of [NiFe]complex

Heterolytic activation of H₂ by [NiFe]complex

Synthetic analog of the active site of the [NiFe] hydrogenase that oxidizes hydrogen

Catalytic Materials Transformations

5

PR Hydrogen Embrittlement & Mitigation Strategies

Roadblock: Absorbed hydrogen accelerates material fatigue. Need to understand fracture mechanism to develop predictive models for structural prognosis to ensure safety and reliability of H₂ components

 Discovered new mechanism that controls plasticity and hydrogen-induced degradation

Acta Materialia, Vol. 60, 2739, 2012

A few ppm of oxygen displace hydrogenaccelerated fatigue to higher stresses and even suppress the hydrogen effect altogether

DFT Reveals new insight : Surface-adsorbed O leads to repulsion between $\rm H_2$ and Fe

Somerday, Kirchheim, Staykov, Sofronis, Robertson, Ritchie

CO₂ Capture and Utilization

Reorganization and New Research Focus

Creation of innovative technologies and exploration of the underlying science in CO₂ capture and utilization

CINER Kyushu/Illinois Synergism: Catalysis and Fuel Cells

Electrochemical Conversion of CO₂ to CO for synthetic fuels

Roadblock: Need <u>Catalysts</u> & <u>Electrodes</u> for efficient conversion of CO₂ to CO

Approach: Leverage Kyushu expertise in fuel cell catalysis with Illinois expertise in CO₂ conversion (*Now: world leaders*!)

Catalysts

(previously used for PEMFCs) Nakashima Fujigaya – Kyushu 1. Metal Free: Carbonitrides Supported Kenis, Gewirth – Illinois **CO** evolution Partial CD of CO (mA/cm²) MWNT/Polymer/Au (previously used for SOFCs) - CB/Polvmer/Au 160 CB/Au No precious metals and robust! Unsupported 120 — Au - Aa Lyth, Staykov – Control 80 MWNT/Polymer Kyushu **Current density** CB/Polymer 40 Kenis – Illinois >160 mA/cm² Current density ~100 mA/cm² Best performance -18 -1.6 -1.2 -14 -10 -0 Similar to state-of-the-art (Ag) ever reported! Cathode Potential (V) vs. Aq/AqCI Sequential development

Electrodes

- Same performance with <u>low precious metal loading</u> (0.17 mg/cm²)
- Better selectivity for CO

Automated Airbrush Deposition Method:

Smooth and thin catalyst layers

2. Nanotube based: Poly/MWCNT/Au

Advanced Energy Materials, 2013, 5, 589-599 (Featured in Cover!)

Efficient and Durable Polymer Electrolyte Fuel Cells

40000

2000

- **Target: Raise the temperature**
- **Roadblock: Low durability**

Accomplishment

- High durability (stable against >400,000 voltage cycles)
- High power density at 120°C (currently 80°C)
- Hon-humidified conditions

High Temperature PEFC 100 times more durable than conventional PEFC 0.8 Cell voltage / V Start-up/shut-down 0.6 cycles 80000 Novel electrolyte 120000 0.4 without Acid Leaching 160000 200000 0.2 240000 0 Carbon Nanotube-Based Fuel Cell with 400 800 1200 1600 0 **High Durability** Current density / mAcm⁻²

M. R. Berber, T. Fujigaya, K. Sasaki, and N. Nakashima, Scientific Reports 3, 2013.

Fuel Cell Roadmap

Boxed research targets are high priority

11 Kysuhu/Illinois Synergism on Modeling and 1²CNER **Monitoring CO**, Migration in Complex Environments **CO₂ Storage Research Targets**

Illinois experiments (Christensen) provide validation for computations at Kyushu (Tsuji) Advancing capabilities for reservoir prediction Schematic of proposed monitoring for leaked CO_2

Modeling of droplet dynamics and hydrate film formation and evolution

Reservoir

Injected CO₂.

Cable ŔΟV or

Observation ship

Automatic elevator oustic tomography

Illinois modeling (Pearlstein) provides coupling to monitoring at **Kyushu (Shitashima)** Advancing capabilities for dispersion prediction

Monitoring of CO₂ Leakage from Sub-seabed CCS

Roadblock: Lack of understanding of diffusive behavior and environmental impact of leaked CO₂ from seafloor into the ocean

A pH/ORP sensor was set at 60cm depth into sediment near the leakage point. The result of low pH in sediment suggests that the CO_2 was trapped in pore water during CO_2 release.

- Field Experiments
 - Controlled CO₂ gas release beneath seabed at water depth of 20m
 - Monitored diffusion of leaked CO₂ from seafloor

 Observation of leaked CO₂ in seawater by AUV equipped with pH/pCO₂ sensor and atmospheric mapping survey of CO₂ with CO₂ analyzer

Diffusion of leaked CO₂ around the leakage point and dispersion of CO₂ into atmosphere were detected

Natural Environment Research Council of UK (Shitashima)

K. Shitashima et al., Applied Geochemistry, 30, 114-124, 2013

Journal Front/Back Covers

S. R. Bishop et al., *Energy and Environmental Science*, 6, 1142-1146, 2013

T. Fujigaya et al., *Polymer Journal,* 45, 326-330, 2013

I²CNER-WPI Affiliated Publications

FY	Archival Journals	Confer	Other	Total
2011	53	10	2	65
2012	150	49	16	215
2013	182	10	12	204

2013 numbers are as of Oct. 10

K. Tanaka et al., *Soft Matter*, 9, 5166-5172, 2013

H. R. Jhong et al., *Advanced Energy Materials*, 3, 589-599, 2013

- Editor-chosen focus PRL article: Designing better materials for LEDs Physics 6, 66 (2013)
- Editor-selected article for promising reliability for OLEDs

Scientific Reports, 3, 2127 (2013)

The 2012 SOMIYA Award

Award Project Title

"Design of ionic and mixed conducting ceramics for fuel cell application"

Winners

Prof. John A. Kilner (I²CNER PI, Imperial College London, UK)
Prof. Harry L. Tuller (I²CNER PI, MIT, USA)
Prof. Tatsumi Ishihara (I²CNER Lead-PI, Kyushu University, Japan)
Assist Prof. Bilge Yildiz (MIT, USA)
Dr. José Santiso (CIN2, Spain)

Description

The Sômiya award is named in honor of Dr. Shigeyuki Sômiya, Emeritus Professor of the Tokyo Institute of Technology, and later Dean at Teikyo University of Science and Engineering. Dr. Sômiya is a winner of the MRS Medal and the Japanese Scientific Academic Award.

Award is given biennially

• The team to be honored must have collaborated across at <u>least two continents</u> during the last decade.

•The collaborative work must be of the highest quality and well recognized by the international materials community.

•The impact on technology or society is also a major factor

SOMIYA Award 2012 Winners

Oniversity	- Awara	30010	Design	
Kyushu University	Grand Prize	85%	6.1MB PDF	(
University of Birmingham	Honorable Mention	85%	4.6MB PDF	•
Mingdao University	Top Five Finisher	73%	1.7MB PDF	
Missouri University of Science and Technology	Top Five Finisher	72%	2.2MB PDF	
UCT Bulgaria	Top Five Finisher	71%	5.7MB PDF	

I²CNER winning team members