

# Tuesday Afternoon Poster Sessions, December 4, 2018

## Energy Harvesting & Storage

### Room Naupaka Salon 1-3 - Session EH-TuP

#### Energy Harvesting and Storage Poster Session

Moderator: Satoshi Ishii, National Institute for Materials Science

**EH-TuP-1 Oxygen Vacancies Boost  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> as High-Performance Electrode for Rechargeable Aqueous Batteries,** *TingTing Qin, W Zhang*, State Key Laboratory of Automotive Simulation and Control, and School of Materials Science & Engineering, and Electron Microscopy Center, and International Center of Future Science, Jilin University, Changchun 130012, China

Metal oxides as electrode materials are of great potential for rechargeable aqueous batteries. However, they suffer from inferior cycle stability and rate capability because of poor electronic and ionic conductivities. Herein, taking vertically-orientated Bi<sub>2</sub>O<sub>3</sub> nanoflakes on Ti substrates as examples, we found that  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> electrode with plenty of intrinsic positively-charged oxygen defects have shown remarkably higher specific capacity (264 mAh g<sup>-1</sup>) and far superior rate capability than that of  $\alpha$ -Bi<sub>2</sub>O<sub>3</sub> with less oxygen vacancies. Through pinpointing the existence form and the role of oxygen vacancies within the electrochemical processes, we demonstrate that oxygen vacancies in  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> serve as central entrapments collecting OH<sup>-</sup> groups via electrostatic force effect, which has boosted the oxidation reaction and enhanced the electrochemical properties. Besides, oxygen vacancies can largely facilitate electronic conductivity. Our work merited an excellent Bi<sub>2</sub>O<sub>3</sub> negative electrode material via giving full play to the role of oxygen vacancies in electrochemical energy storage.

**EH-TuP-3 Novel Cathode Nanomaterials and Electrolytes for Al-ion Batteries,** *Nicolò Canever*, Victoria University of Wellington, New Zealand; *N Bertrand*, Ecole Nationale Supérieure de Chimie de Clermont-Ferrand, SIGMA Clermont, Aubière, France; *T Nann*, Victoria University of Wellington, New Zealand

Battery-based energy storage could be a useful tool for transitioning to a fully renewable-based energy economy. Current battery technologies, however, often lack the cost-effectiveness [1] and safety [2] requirements necessary for large-scale grid energy storage applications. Aluminium-ion batteries (AIBs) are a very promising alternative to Lithium-based systems, thanks to the low cost, non-flammability, and three-electron redox chemistry of aluminium. [3] AIBs could, in principle, offer better cost-effectiveness, energy density [4] and safety, [5] than currently available energy storage technologies. This poster deals with the investigation of new electrode nanomaterials and electrolyte systems for Al-ion batteries, with the aim of improving the performance and cost-effectiveness of AIBs, and facilitate their commercial feasibility.

#### REFERENCES:

- [1] Delucchi, M. A.; Jacobson, M. Z. *Energy Policy* 2011, 39 (3), 1170.
- [2] Barnes, F. S.; Levine, J. G. *Large energy storage systems handbook*; CRC press, 2011.
- [3] K. Das, S.; Mahapatra, S.; Lahan, H. J. *Mater. Chem. A* 2017, 5 (14), 6347.
- [4] Jayaprakash, N.; Das, S. K.; Archer, L. A. *Chem. Commun.* 2011, 47 (47), 12610.
- [5] Lin, M.-C.; Gong, M.; Lu, B.; Wu, Y.; Wang, D.-Y.; Guan, M.; Angell, M.; Chen, C.; Yang, J.; Hwang, B.-J.; Dai, H. *Nature* 2015, 520 (7547), 324.

**EH-TuP-4 Study of Charge Transfer across C<sub>60</sub>/BCP and BCP/Ag Interfaces Using Core-Hole Clock Spectroscopy,** *Tetsuya Miyazawa*, SOKENDAI, Japan; *K Ozawa*, Tokyo Institute of Technology, Japan; *K Kanai*, Tokyo University of Science, Japan; *T Sakurai*, Tsukuba University, Japan; *K Mase*, KEK, Japan

Electronic properties at organic/metal and organic/organic interfaces affect the efficiencies of organic electronic devices such as organic solar cells, perovskite solar cells, and organic field effect transistors. Peuman *et al.* have found that the conversion efficiency of the organic solar cell is improved when bathocuproine (BCP) is inserted as buffer layer between the organic molecule of acceptor and negative electrode [P. Peuman *et al.*, *Appl. Phys. Lett.* **76**, 2650 (2000)]. In order to reveal the role of buffer layers, we investigated C<sub>60</sub>/BCP and BCP/Ag layered systems by resonant photoelectron spectroscopy and X-ray absorption spectroscopy. A core-hole clock analysis was carried out to examine transfer times of an electron from C<sub>60</sub> to BCP and that from BCP to Ag. The sample was prepared by the procedure that monolayer of BCP was deposited on Ag thin film and then monolayer of C<sub>60</sub> was deposited on the BCP. The charge transfer times from

LUMO+1 of BCP to Ag and C<sub>60</sub> to BCP were calculated to be 2.5 fs and less than 60 fs, respectively. In the photoelectric conversion of organic solar cells, electrons generated by exciton separation transfer from organic molecule of acceptor to negative electrode. These results suggest that ultrafast charge transfers across C<sub>60</sub> to BCP and BCP to Ag are one of the role of buffer layers to improve conversion efficiency of organic solar cells.

**EH-TuP-6 Structure and Optical Properties of HfO<sub>2</sub>-based Thermal Emitter Films for Thermophotovoltaic Energy Conversion Devices,** *Gregory Abadias, Y Metayrek, A Michel, J Drevillon*, Institut Pprime, CNRS-Université de Poitiers, France

One of the key points for designing high-efficiency thermophotovoltaic (TPV) systems is to match the spectral emission of the radiator with the spectral range where photons are converted into electron-hole pairs inside the photovoltaic device. Recent studies have shown the potential offered by photonic crystals made of metal/dielectric stack of layers acting as Fabry-Pérot cavity, ensuring spectral selectivity to the emitter. Another material requirement is thermal stability in order to keep the same spectral emission at the operating temperature of the radiator. The Mo/HfO<sub>2</sub> system is a promising candidate material in this respect, as recently reported by Blandre *et al.* [1].

In this work we investigate the synthesis by magnetron sputtering of W/HfO<sub>2</sub> four-layer films for TPV applications. The individual layer thicknesses were optimized based on fluctuational electrodynamics calculations of thermal emissivity of one-dimensional layered media. Prior to the fabrication of the multilayer stack, the structure and optical properties of the transparent HfO<sub>2</sub> layer were investigated as a function of process parameters: substrate temperature  $T_s$  and O<sub>2</sub> flow rate.

Films were characterized by X-ray reflectivity, X-ray diffraction and wavelength dispersive spectroscopy. The optical indices ( $n$  and  $k$ ) were measured experimentally from variable angle spectroscopic ellipsometry in the visible and mid-infrared (MIR) range (up to 35  $\mu$ m). Results show that dense, crystalline HfO<sub>2</sub> layers with monoclinic structure can be formed by reactive magnetron sputtering at room temperature with optical index  $n$  close to 2.1 at 550 nm; however, crystallinity was improved by increasing  $T_s$  up to 500°C, with little variation on  $n$  and  $k$ . In the MIR, the optical properties of HfO<sub>2</sub> were consistent with the data reported by Bright *et al.* [2]. The optical reflectance of the W/HfO<sub>2</sub> stack was measured using spectrophotometer and a good agreement with theoretical predictions was found, attesting of the potential of this system for TPV emitters.

**EH-TuP-7 Bimetallic Cobalt-Iron Hydroxide Encapsulated in Organic Ligand Derived Carbon Layers as an Efficient Electrocatalyst for Oxygen Evolution Reaction,** *Jian Du, F Li*, Dalian University of Technology, China

Water electrolysis as one of the prospective approach to produce hydrogen is limited by the anodic oxygen evolution reaction (OER) due to its sluggish kinetics. Considering the practical application, the development of highly efficient non-noble OER catalysts is essential. Among the reported low-cost electrocatalysts, CoFe-based oxides or hydroxides are intriguing owing to the rich redox chemistry. However, the severe aggregation and intrinsically poor electronic conductivity hinder their electrocatalytic performance. Hybridizing cobalt-iron oxides or hydroxides with carbon materials can not only enhance the conductivity of the catalyst, but also facilitate the uniform distribution of metal species within carbon matrix, thus improving the electrochemical performance towards OER. In view of this, we report here the bimetallic cobalt-iron hydroxide encapsulated in carbon layers derived from organic ligand (Schiff base) via hydrothermal carbonization. In alkaline media, Co Fe/C loaded on GC electrode delivers a current density of 10 mA cm<sup>-2</sup> at an overpotential of 260 mV and exhibits a low Tafel slope of 45.2 mV dec<sup>-1</sup> as well as excellent durability. The remarkable OER performance outperforms those of CoFe-based electrocatalyst in the literature.

**Keywords:** Oxygen evolution reaction, cobalt-iron hydroxide, organic ligand, electrocatalyst

#### Results

As shown in Figure 1, the Co<sub>1.2</sub>Fe/C delivers a current density of 10 mA cm<sup>-2</sup> at an overpotential of 260 mV and exhibits a low Tafel slope of 45.2 mV dec<sup>-1</sup> as well as excellent durability in 1M KOH solution.

Figure 1 (a) LSV curves of GC, Co<sub>1.2</sub>Fe and Co<sub>1.2</sub>Fe/C; (b) Tafel plots of Co<sub>1.2</sub>Fe and Co<sub>1.2</sub>Fe/C; (c) Chronopotentiometric measurement of Co<sub>1.2</sub>Fe/C at 10 mA cm<sup>-2</sup>. All tests were carried out in 1 M KOH.

#### Conclusions

# Tuesday Afternoon Poster Sessions, December 4, 2018

The Co<sub>1.2</sub>Fe/C exhibits excellent OER performance in alkaline media, which can be ascribed to the following factors: 1) the homogenous distribution of metal hydroxide within carbon matrix inhibits the aggregation of the active nanoparticles; 2) the excellent electronic conductivity enables fast electron transport during the OER process; 3) the synergetic effect between the Co<sub>1.2</sub>Fe hydroxide and carbon species also contributes to the improvement of the electrochemical performance.

## Reference

- [1] S. Yin, W. Tu, Y. Sheng, Y. Du, M. Kraft, A. Borgna, R. Xu, *Adv. Mater.* 2017, 1705106.
- [2] F. Li, J. Du, X. Li, J. Shen, Y. Wang, Y. Zhu, L. Sun, *Adv. Energy Mater.* 2018, 1702598.

## **EH-TuP-8 Anchoring Water Oxidation Catalysts on a DS-PEC via Pyridine Group for Light-Driven Water Splitting, Yong Zhu, F Li**, Dalian University of Technology, China; *L Sun*, KTH Royal Institute of Technology, Sweden

Dye-sensitized photoelectrochemical cell (DS-PEC) water splitting into hydrogen and oxygen is a potential approach to realize the conversion solar energy to chemical energy efficiently. Ru(bda) (bda is 2,2'-bipyridine-6,6'-dicarboxylate) is one of the most efficient water oxidation catalysts in DS-PEC. Traditionally, Ru(bda) have been anchored onto the dye-sensitized photoanode by modifying phosphoric acid or carboxylic acid groups. These complexes can reduce the overpotentials of water oxidation and exhibit highest turnover. However, the efficiency of the entire system is inhibited due to the strong recombination effect of electrons injected into the TiO<sub>2</sub> bulk on the photosensitizer and catalyst in the oxidized state. Herein, we have replaced the anchor group of the water oxidation catalysts Ru(bda) (bda is 2,2'-bipyridine-6,6'-dicarboxylate) from phosphoric acid to pyridine. Time-resolved transient absorption spectroscopy demonstrates that the pyridine anchor group have effect of inhibiting electron recombination. The photocurrent densities of 1.5-1.8 mA/cm<sup>2</sup> were achieved and produced an incident photon to current efficiency (IPCE) of 25.5% at 450 nm. Under pH=5.8 under 100mW/cm<sup>2</sup> (>400nm) illumination.

## **EH-TuP-9 On the Thermal Characterization of Heptane-Isooctane Mixtures, Adrian Bedoya, E Marin, S Alvarado**, Cicata Legaria, Mexico

The thermal transport properties of heptane-isooctane mixtures in the liquid phase at room temperature and atmospheric pressure were measured and calculated. The thermal conductivity,  $k$ , was measured using the transient hot-wire (HW) method, and the thermal effusivity,  $e$ , was determined by the front photopyroelectric (FPPE) technique. Then, the thermal diffusivity,  $\alpha$ , and the volume specific heat capacity (heat capacity per unit volume),  $C$ , were calculated using the well-known relationships  $\alpha = (k/e)^2$  and  $C = e^2/k$ , respectively. We show that a correlation between these parameters and octane number exists, and that the obtained thermal parameters proved to be sensitive to detect molecular associations in binary hydrocarbon liquid mixtures. We also report about the thermal conductivity of mixtures of n-alkanes vapors and air showing that almost similar values are obtained for heptane and isooctane, so that octane number rating using the well-established binary mixtures of these substances becomes impossible with thermal properties measurements in the gas phase.

## **EH-TuP-10 A steady-state thermoreflectance method to measure thermal conductivity, Jeffrey Braun, D Olson, J Gaskins, P Hopkins**, University of Virginia

We demonstrate a steady-state thermoreflectance based optical pump-probe technique to measure the thermal conductivity of materials using a continuous wave laser heat source. The technique works in principle on leaving a pump laser on long enough to induce a steady-state temperature rise in a material. A probe beam is then used to detect the resulting change in reflectance, which is proportional to the change in temperature of the sample. Varying the power of the pump beam to induce larger temperature rises, Fourier's law is used to determine the thermal conductivity. We show that this technique is capable of measuring the thermal conductivity of a wide range of materials having thermal conductivities ranging from 1 to > 2000 W m<sup>-1</sup>K<sup>-1</sup>, in excellent agreement to literature values. With a measurement length scale capable of reaching <10 microns, this techniques is capable of measuring both bulk material and films.

## Author Index

**Bold page numbers indicate presenter**

— A —

Abadias, G: EH-TuP-6, **1**  
Alvarado, S: EH-TuP-9, **2**

— B —

Bedoya, A: EH-TuP-9, **2**  
Bertrand, N: EH-TuP-3, **1**  
Braun, J: EH-TuP-10, **2**

— C —

Canever, N: EH-TuP-3, **1**

— D —

Drevillon, J: EH-TuP-6, **1**  
Du, J: EH-TuP-7, **1**

— G —

Gaskins, J: EH-TuP-10, **2**

— H —

Hopkins, P: EH-TuP-10, **2**

— K —

Kanai, K: EH-TuP-4, **1**

— L —

Li, F: EH-TuP-7, **1**; EH-TuP-8, **2**

— M —

Marin, E: EH-TuP-9, **2**

Mase, K: EH-TuP-4, **1**

Metayrek, Y: EH-TuP-6, **1**

Michel, A: EH-TuP-6, **1**

Miyazawa, T: EH-TuP-4, **1**

— N —

Nann, T: EH-TuP-3, **1**

— O —

Olson, D: EH-TuP-10, **2**

Ozawa, K: EH-TuP-4, **1**

— Q —

Qin, T: EH-TuP-1, **1**

— S —

Sakurai, T: EH-TuP-4, **1**

Sun, L: EH-TuP-8, **2**

— Z —

Zhang, W: EH-TuP-1, **1**

Zhu, Y: EH-TuP-8, **2**