Energy Harvesting & Storage

Room Naupaka Salon 5-7 - Session EH-MoM2

Surfaces and Interfaces for Efficient Power Conversion and Batteries

Moderator: David Ginger, University of Washington

10:20am **EH-MoM2-8 Fabrication of Proton-conductive BaCeZrYO$_{3-d}$ Coatings by Solution Precursor Plasma Spray (SPPS) Method***, **Yen-Yu Chen**, W. Zeng, C. Liu, G. Yao,* Chinese Culture University, Taiwan

Pervoskite-type proton-conductive ceramic materials have high potentials for the application of sustainable energy fields, such as protonic ceramic fuel cell (PCFC), carbon dioxide conversion, ammonia fuel synthesis, etc. In this study, perovskite-type proton-conductive coatings, BaCeZrYO$_{3-\delta}$ (BCZY), were deposited on NiO/BaZrYO$_{3-\delta}$ (BZY) substrates by a solution precursor plasma spray (SPPS) method. The precursors were consisted the BCZY species of the nitrate salts and dissolved into de-ionic water. The NiO/BZY substrates were prepared by a die-pressing method. Several properties of the coatings were analyzed, including crystal phases by X-ray diffraction (XRD), microstructures by scanning electron microscope (SEM), electrical properties by electrochemical impedance spectroscopy (EIS), etc. The results of XRD show the coatings after post-coating annealing over 600^{o}C are mainly consisted of perovskite phases. The microstructure analysis of the BCZY coatings characterized by SEM show the coatings are mainly consisted of overlapped splats of BCZY materials and a few of surface pores can be found from the coating layers. The average thickness of the coating layers are about several microns. The formation mechanism of the BCZY coatings can be purposed as the BCZY precursor droplet breakup, liquid-phase evaporation, thermal pyrolysis of precursors, solid particles melting, and then the melting particles splatted and overlapped on the substrate to form the BCZY coatings. The details electrical property analysis of the BCZY coating samples are as mentioned in the following report.

10:40am **EH-MoM2-9 Metal Exsolution and Nanoparticle Self-Assembly Dynamics at Complex Oxide Surfaces***, **Moritz Lukas Weber**,* Forschungszentrum Juelich GmbH, Lawrence Berkeley National Laboratory, RWTH Aachen University, Juelich-Aachen Research Alliance*; B. Šmíd,* Charles University, Czech Republic*; H. Kersell,* Lawrence Berkeley National Laboratory (LBNL)*; U. Breuer,* Forschungszentrum Jülich GmbH, Germany*; M. Rose,* Forschungszentrum Jülich GmbH, RWTH Aachen University, Juelich-Aachen Research Alliance (JARA-FIT, Germany*; N. Menzler,* Forschungszentrum Jülich GmbH, RWTH Aachen University, Germany*; R. Dittmann,* Forschungszentrum Jülich GmbH, Juelich-Aachen Research Alliance (JARA-FIT, Germany*; R. Waser,* Forschungszentrum Jülich GmbH, RWTH Aachen University, Juelich-Aachen Research Alliance (JARA-FIT), Germany*; O. Guillon,* Forschungszentrum Jülich GmbH, RWTH Aachen University, Juelich-Aachen Research Alliance (JARA-Energy), Germany*; C. Lenser,* Forschungszentrum Jülich GmbH, Germany*; S. Nemšák,* Lawrence Berkeley National Laboratory (LBNL)*; F. Gunkel,* Forschungszentrum Jülich GmbH, Juelich-Aachen Research Alliance (JARA-FIT), Germany

Metal exsolution attracts much attention for the synthesis of nanostructured catalysts. Thermal reduction of doped perovskite parent oxides induces the migration of reducible cations from the oxide bulk to the surface and results in the self-assembly of metallic nanoparticles that serve as catalytic centers. Ideal exsolution-type catalysts therefore dynamically adapt with respect to the oxygen chemical potential. The parameters that influence the kinetics of nanoparticle exsolution, however remain an open question in the scientific community. Furthermore, little is known about the origin of stability limitations of exsolved nanoparticles that are typically anchored at the oxide support.

We employ epitaxial thin films model systems with atomically defined surfaces to investigate the exsolution response of Ni in SrTi$_{0.9}$Nb$_{0.05}$Ni$_{0.05}$O$_{3-\delta}$ and SrTi$_{0.95}$Ni$_{0.05}$O$_{3-\delta}$ of respective *n*–type and *p*-type defect chemistry. Here, we study the mass transfer of dopants towards the surface as well as the morphological evolution of the nanostructured catalysts. Our thin film approach enables to study differences in the exsolution behavior on the basis of well-defined (001) surfaces, eliminating uncertainties regarding the complex microstructure and anisotropy of ceramic oxides and the presence of secondary surface phases.

In order to assess the dynamic changes at the catalyst surface during metal exsolution, we conduct advanced *in-situ* spectroscopy and scattering analyses. In particular, we employ a recently developed technique that allows for the simultaneous analysis of the chemical and structural evolution of the solid-gas interface based on coupled *in-situ* ambient pressure X-ray photoelectron spectroscopy (AP-XPS) and *in-situ*ambient pressure grazing incidence X-ray scattering (AP-GIXS). Our investigations show that the defect chemistry of the near-surface region determines the dynamics of the exsolution response, where the formation of space charge regions at the perovskite surface plays a major role for the process.

We conclude that the mass transfer during metal exsolution and therefore the nanoparticle self-assembly at the perovskite surface is surface-controlled by interaction with the energy landscape of the complex oxide surface. Derived from our investigations, we propose a mechanistic model that describes how metal exsolution is mediated by the surface defect chemistry and we demonstrate surface engineering of the topmost atomic layers can be utilized as a novel strategy for the active control of the exsolution behavior. Moreover, our observations indicate that the different nature of the surface potential may influence the stability of exsolved nanoparticles.

11:00am **EH-MoM2-10 Characterization of Surfaces and Interfaces in Polymer Electrolyte Membrane Electrolyzers***, **Svitlana Pylypenko**,* Colorado School of Mines

Polymer electrolyte membrane water electrolyzers (PEMWEs) are of significant importance towards enabling the large-scale utilization of renewable hydrogen. Fabrication and integration of components, advancement of scalable manufacturing techniques, elucidation of degradation mechanisms, and development of degradation mitigation strategies all require extensive characterization of materials, components, and devices. The complexity of the systems and problems combined with the multitude of relevant scales require multi-technique characterization and motivate further developments of characterization methods and novel approaches. This talk will discuss some of our recent studies on both catalyst layers (CLs) and porous transport layers (PTLs) for application in PEMWEs. Specifically, this presentation will highlight the complementary nature of electron and X-ray microscopy and spectroscopy methods for the investigation of surfaces, interfaces, and interactions within the CLs comparing results for Ir and IrO$_2$-based CLs, and fresh and aged or tested CLs. Similarly, the characterization of PTLs requires advanced characterization to properly assess the elemental distribution and chemical speciation of PTLs and protective coatings.

11:20am **EH-MoM2-11 Design and Manufacture of Air-Silicon Batteries and the Impact of Plasma-Processed Silicon on the Efficiency of These Batteries***, **Marziyeh Gholami**,* Shahid Beheshti University, Iran (Islamic Republic of)

Silicon, as the second most abundant material on earth, is a significant option as an anode material in air metal batteries, so the theoretical energy density is very high at about 8470 Wh kg^{-1}. The discharge products of this battery are non-toxic and environmentally friendly. The final battery is light in weight and will be used in wet or very dry areas. Also, due to the lack of cathode in these batteries, less space will be occupied and the weight of the battery will be light. These advantages, along with the low cost, have made this battery one of the brightest prospects in the field of energy storage devices.In this primary battery, porous carbon, a catalyst, and a polymer as a cathode play an important role in the structure of the battery.An alkaline solution is used as the electrolyte. If plasma-untreated silicon is used in this battery, it has a lower OCV and a short discharge cycle.so, The research carried out in this project was the processing of silicon surface with plasma in order to increase the effective cross-section of silicon in contact with the electrolyte and increase the open-circuit voltage of the batterydue to the increase in voltage that we will have at the sharp points. Surface roughness is also guaranteed by plasma etching.

11:40am **EH-MoM2-12 Insights into the Interfacial Reactions of High Voltage MgV$_2$O$_4$ Cathodes for Rechargeable Magnesium Batteries***, D. Nguyen, V. Prabhakaran,* Pacific Northwest National Laboratory, Joint Center for Energy Storage Research (JCESR)*; V. Shutthanandan,* Pacific Northwest National Laboratory*; J. Hu,* Pacific Northwest National Laboratory, Joint Center for Energy Storage Research*; G. Alexander, J. Cabana-Jimenez,* University of Illinois at Chicago, Joint Center for Energy Storage Research*; K. Mueller,* Pacific Northwest National Laboratory, Joint Center for Energy Storage Research*; **Vijayakumar Murugesan**,* Pacific Northwest National Laboratory, Joint Center for Energy Storage Research

Interfacial reactions driven by charge transfer occurring at the electrode – electrolyte interface contribute to the formation of complex interphasial layers that govern the performance of energy storage devices. These interfacial reactions are influenced by various factors such as surface chemistry of electrode, electrochemical properties of the electrolyte solution, and the working potential of the device. Precise capturing of critical interfacial reactions and subsequent evolution of solid-electrolyte interphase components is extremely challenging due to the complexity and heterogeneity of the interphasial reactive components, the reaction dynamics under variable potentials, and the smaller dimensions of interphase region. Probing complex interfacial processes requires the integration of advanced spectroscopies within an electrochemical device to monitor interfacial reactions and structural changes during operation. In this study, we investigated the interphasial evolution of MgV_2O_4 cathodes for rechargeable magnesium batteries using both *in situ* and *ex situ* X-ray photoelectron spectroscopy while also probing structural transformation of interphasial chemical species using *operando* Raman spectroscopy. Our study revealed that the solid electrolyte interphase layer on MgV_2O_4 was formed mainly by the decomposition of electrolyte anions that occurred at a very early stage of the initial charging process. The interphase layer also thickened with increased cell potential as well as repeated cycling. Post surface analysis of the MgV_2O_4 cathode after 20 cycles also confirmed surface conditioning processes that is well supported by its electrochemical performance in early cycles. Our study revealed insights into the surface evolution of MgV_2O_4, which provides crucial information for development of an oxide cathode for rechargeable magnesium batteries as well as other battery chemistries that involve sodium and lithium ions.

Energy Harvesting & Storage
Room Naupaka Salon 5-7 - Session EH-WeM1

Surfaces and Interfaces for Solar Cells and Solar Fuels

Moderator: Svitlana Pylypenko, Colorado School of Mines

8:40am **EH-WeM1-3 Surface Recombination and Surface Passivation in Halide Perovskite Semiconductors***, **David Ginger,*** University of Washington **INVITED**

Halide perovskite semiconductors are being aggressively commercialized in solar photovoltaics, and are being explored in the lab as high-performance emitters of both classical and quantum light. While halide perovskites are often hailed as remarkably defect-tolerant semiconductors, they still possess surface defects that limit their performance, both as sources of non-radiative recombination, as well as mobile defects that contribute to mixed ionic/electronic conduction.This talk will describe our work to characterize, and passivate, surface defects in halide perovskite solar cells, beginning with the archetypal halide perovskite, methylammonium lead triiodide (MAPI), and extending to complex mixed-cation and mixed-halide perovskites currently being explored for multijunction tandem cells.We relate surface defects to specific vacancies, correlate their appearance with local strain and chemical defects, and demonstrate robust chemical passivation strategies that allow for increases in device performance and stability.

9:20am **EH-WeM1-5 Passivating Interfaces in Thin Film Photovoltaics***, **Craig Perkins,** D. McGott,* NREL*; E. Colegrove,* NREL, United States Minor Outlying Islands (the)*; A. Hattori,* UC Santa Barbara*; M. Reese,* NREL **INVITED**

Economic considerations, climate change, and concerns over fossil fuel pollution have all contributed to the rise of solar photovoltaics (PV) as a major power source for humankind. As an example, solar PV is forecast to be ~60% of the 85 GW of new generation capacity to be added to US markets in 2022 and 2023. Although silicon-based PV currently dominates the market, this relatively mature technology is being challenged by several newer technologies based on thin films of compound semiconductors. In this talk, I will touch on some of the scientific advances that have driven down costs of PV power, giving particular emphasis to interfaces in PV cells comprised of polycrystalline thin films. Interfaces are of increasing importance in polycrystalline thin film PV devices because the quality of the bulk semiconductors has been improved to the point where minority carrier lifetimes are in many cases limited by carrier interaction with defective interfaces. This in turn limits the device power conversion efficiency (PCE). The analysis of interfaces in thin film PV devices usually presents complications not typically encountered in the study of “free” surfaces, and we review some of the methods used in our lab to characterize buried interfaces. Among these methods is a thermomechanical technique for cleaving CdTe-based solar cells at the interface between CdTe and the transparent conducting oxide located at the front of superstrate architecture cells. This buried interface is the first active junction that is formed in this technology, is one that changes throughout several high temperature processing steps, and its study remains an active research area even after decades of work. We show how combining thermomechanical cleaving with electron spectroscopy can tease out the details of structure, electronic properties, and passivation mechanisms in CdTe. We highlight a common structural feature found in several very different well-passivated PV materials including CdTe, the halide perovskites, and Cu(In,Ga)Se2. I will also describe a recently developed method for room temperature temporary passivation of CdTe thin film surfaces. This passivation strategy, adopted from silicon PV, allows us to measure properties of as-grown absorbers, unlike the previous best known method involving alumina deposition and high temperature processing, both of which affect a film’s bulk properties. Finally, I will review a number of ongoing challenges faced by researchers interested in characterizing interfaces of energy materials with electron spectroscopic methods.

Energy Harvesting & Storage
Room Naupaka Salon 5-7 - Session EH-WeM2

Surfaces and Interfaces for Environmental Processes

Moderator: Craig Perkins, National Renewable Energy Laboratory

10:20am **EH-WeM2-8 Effect of Carbon Support Structures on Electrode Reaction Activity of Catalyst Layer in Polymer Electrolyte Fuel Cell: Large-scale Reactive Molecular Dynamics Simulations***, **Tetsuya Nakamura,** R. Otsuki, Y. Asano, Q. Chen, Y. Ootani, N. Ozawa, M. Kubo,* Tohoku University, Japan

For large output of polymer electrolyte fuel cell, the electrode reaction activity in the catalyst layer (CL) consisting of carbon support with meso pores, Pt nanoparticles (Pt NPs), Nafion chains, and water should be improved. Conventionally, to realize high electrode reaction activity, catalyst elements have been designed by first-principle calculation. However, first-principle calculation does not take into the meso-scale CL structures, such as carbon support, a distribution of the Nafion chains, and water content. Thus, we have constructed meso-scale CL structures and successfully clarified the effect of the pore size of the carbon support on the electrode reaction activity by large-scale reactive molecular dynamics simulation [1]. In addition, to design higher-performance CL structures, we consider it important to control the distribution of water on the carbon support and to improve the coverage states of Pt NPs with the Nafion chains. In this study, the hydrophilic group is introduced on the surface of carbon support to form a water film and we investigated coverage states of the Nafion chains over Pt NPs on the carbon support with different water film thicknesses.

The catalyst particle (CP) model was constructed by coating the Nafion chains and water on the carbon support surface. Six pores were created in an amorphous carbon sphere. In addition, the water film whose thickness is 0.7 and 1.0 nm were formed on the carbon support surface.

To clarify the effect of the thickness of water film on the coverage states of the Nafion chains over Pt NPs, we compared two CP models with different water film thicknesses of 0.7 and 1.0 nm. Here, for high electrode reaction activity, the Nafion chains should cover over Pt NPs partially to allow both high oxygen diffusion and high proton conduction. Figs. 2 (a) and (b) shows the coverage states of the Pt NPs interior of the pore after the calculations when the thickness of water film was 0.7 and 1.0 nm, respectively. Consequently, when the film thickness was 0.7 nm, the Nafion chains penetrated the pore and partially covered the Pt NPs. On the other hand, when the film thickness was 1.0 nm, the Nafion chains did not penetrate the pore. These results suggest that when the thickness of the water film is 0.7 nm, both high oxygen transport and high proton conduction to the Pt NPs in the interior of the pore of carbon support are realized.

[1] Tetsuya Nakamura, Riku Otsuki, Shuichi Uehara, Yuta Asano, Qian Chen, Yusuke Ootani, Nobuki Ozawa, Momoji Kubo, J. Comput. Chem. Jpn., 20, 4, 150-154 (2021)

10:40am **EH-WeM2-9 Large Scale Molecular Dynamics Simulation Study on Ionomer Coating of Pt Nanoparticles of Polymer Electrolyte Fuel Cells***, **Riku Otsuki,** T. Nakamura,* Institute for Materials Research, Tohoku University, Japan*; Q. Chen,* New Industry Creation Hatchery Center, Tohoku University, Japan*; Y. Asano, Y. Ootani,* Institute for Materials Research, Tohoku University, Japan*; N. Ozawa,* New Industry Creation Hatchery Center, Tohoku University, Japan*; M. Kubo,* Institute for Materials Research, Tohoku University, Japan

Polymer electrolyte fuel cells (PEFCs) are widely used for automobiles because it does not emit CO_2 during operation. For more popularization of a fuel cell vehicle, its higher output is required. The output of PEFC depends on a catalyst layer (CL) at the electrode composing of carbon supports, Pt nanoparticles (Pt NPs), ionomers and water molecules. Ionomers play an important role in proton conduction and oxygen gas diffusion. Especially, if Pt NPs and ionomer are not connected via water, proton transport is impossible. However, if the coverage of ionomer on Pt NPs is too high, oxygen gas diffusion is obstructed.Then, to reveal the CL structure with high electrode reaction activity, the coverage states of ionomer on Pt NPs have been earnestly studied by molecular dynamics (MD) method. For example, W. Wang et al. investigated the ionomer distribution over the Pt NPs and carbon particles in the CL model composed of about one hundred thousand atoms[1]. However, such a small model cannot handle the actual agglomerated structure of carbon support, and discussion about an optimal CL structure with high electrode reaction activity is impossible. In this study, we constructed 3 million atoms CL model with the agglomerated structure of the 15 carbon supports (Fig. 1) and analyzed the coverage of Nafion as ionomer over the Pt NPs by MD method to discuss the electrode reaction activity.

Coverage is defined as ratio of number of covered Pt atoms to the number of the Pt atoms on the Pt NPs surface. The distribution of Nafion coverage on each Pt NPs is shown in Fig. 2. The averaged coverage is 69.5%. Coverage of most Pt NPs, which placed on surface of a carbon support or between two carbon supports, ranges from 60 to 90%. On the other hand, it was found that the ionomer coverage of Pt NPs surrounded by three carbon supports is lower than another Pt NPs as shown in Fig. 3. Here, the Pt NPs and Nafion are connected via water clusters, indicating high oxygen gas diffusion and proton conduction. Therefore, we proposed that the Pt NPs surrounded by three carbon supports exhibit high electrode reaction activity. Finally, we conclude Large-scale MD is very effective to reveal how CL structure affect output characteristics of PEFCs

11:00am **EH-WeM2-10 Studying Corrosion Processes of Aluminum Alloys in Diverse Aqueous Environments***, **Micha Ben-Naim**, A. Ivanovskaya , S. Cho, C. Orme, M. Bagge-Hansen,* Lawrence Livermore National Laboratory

Corrosion modes and rates have a strong dependence on environmental conditions. During certain corrosion processes like stress corrosion cracking (SCC) and crevice corrosion, the local chemical environment, including pH and concentration of dissolved ions and gases, can vary dramatically from bulk solution conditions, motivating the study of corrosion properties under a wider range of aqueous environments than would typically be encountered in environmental corrosion. 7000 series aluminum alloys are a class of high-strength alloys used for structural and aerospace applicationsthat are susceptible to corrosion, particularly SCC, but work to date has largely focused on corrosion in aqueous chloride salts.

In this work, we study the corrosion properties of these Al alloys under a wide range of aqueous conditions. We explore new chemical environments that could lead to corrosion in Al alloys while probing the wide pH ranges that can arise in cracks and crevices. We use polished films to both measure bulk corrosion rates and enable the use of surface science techniques. Nondestructive electrochemical techniques enable high measurement throughput while measuring across pH and salt concentration ranges, so we measure corrosion potentials, corrosion rates, and electrochemical impedance spectra in a nondestructive manner. We also use surface characterization techniques (SEM, EDS, EBSD, XPS) to identify changes in surface chemistry and morphology. By combining electrochemical methods with surface science, we seek to gain a fundamental understanding of the corrosive regimes for these alloys.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Energy Harvesting & Storage
Room Naupaka Salon 1-3 - Session EH-WeP
Energy Harvesting and Storage Poster Session

EH-WeP-1 Spintronic Diode as a Signal Detector and RF Energy Harvester*, **Andrei Slavin**,* Oakland University

The spin-torque magnetic diode (STMD) effect [1] is a quadratic rectification effect of the input microwave current $I_{RF}(t)$ in a magneto-resistive nano-junction, which is commonly observed in a traditional regime of operation of an STMD, when the magnetization of the "free" layer lies *in-plane*, and when the frequency $f_s$of the current $I_{RF}(t)$ is close to the ferromagnetic resonance (FMR) frequency f_0 of the junction. It was demonstrated theoretically in [2] that in an STMD, biased by an *out-of-plane* static magnetic field, a novel dynamical regime of STMD operation characterized by large-angle out-of-plane magnetization precession can be realized.

It was demonstrated experimentally in [3] that the out-of-plane magnetization precession regime in an STMD predicted in [2] can be realized without *any bias magnetic field*, if an STMD "free" layerhas a *perpendicular magnetic anisotropy*.It was further shown in [3] that the developed bias-free STMD provides sufficient dc voltage to power a practical nanodevice − a black phosphorus photosensor.

Here we present an analytical and numerical theory explaining the performance of such a bias-free STMD with perpendicular magnetic anisotropy [4].We show that such a device can operate as a broadband energy harvester capable of converting incident RF power into a DC power with a conversion efficiency of ~5%.

References

[1] A. Tulapurkar, Y. Suzuki, A. Fukushima et al., Nature., Vol.438, p.339 (2005).

[2] V. Prokopenko, I. N. Krivorotov, E. Bankowski et al., J. Appl. Phys., Vol. 111, p.123904 (2012).

[3] B. Fang, M. Carpentieri, S. Louis et al., Phys. Rev. Appl., Vol. 11, p.014022 (2019).

[4] P. Yu. Artemchuk, O. V. Prokopenko, E. N. Bankowski *et al*., AIP Advances., Vol. 11, p. 025234 (2021).

EH-WeP-2 Strain Imaging of a $LiTi_2O_4$ Anode in a Li-Ion Battery*, **Keiji Takata**,* Kansai University, Japan

Li-ion batteries have advantages including high energy density, high output voltage, and the absence of the memory effect, and so they are recognized as promising candidates for energy storage. These advantages are mainly provided by the lowest electrode potential of Li^+/Li and low density of Li, which are −3.04 V and 0.534 g/cm^3, respectively. Li-ion batteries have advanced a great deal through the use of intercalation and have been applied in portable electronic devices and electric vehicles.

Li-ion batteries operate through the migration of Li ions between the electrodes. Therefore, non-destructive observation of the migration with high spatial resolution is important.

When charging and discharging, Li-ions are extracted or inserted into electrode materials, which generally causes changes in volume. An atomic force microscope (AFM) can detect and image these volume changes through current collectors with high spatial resolution, which enables us to investigate Li-ion migration without destruction.

Here, we present our results of $LiTi_2O_4$. $LiTi_2O_4$ is an anode material with high safety having a theoretical capacity of 160 mA h g^{-1} (from $LiTi_2O_4$ to $Li_2Ti_2O_4$). The phase change from spinel to rock-salt lead to very small volume changes. Therefore, it might be difficult to observe the Li migration by this method. Cathode of observed samples was layered $LiCoO_2$, and electrolyte and separator are commonly used materials. AFM detects surface displacements synchronizing the charging/discharging cycle, and provides strain images along with topography.

The strain images consist of dark regions that any strain was not detected and bright regions that relatively constant strains were detected. We considered these images together with the frequency dependence of the images and impedance spectroscopy, and concluded that the dark regions were $LiTi_2O_4$ particles and the bright regions resulted from electrolyte flux induced by the gradient of Li-ion concentration in the interspace of the particles. The gradient of Li-ion concentration and electrolyte flux in the interspace were generated by the charging/discharging. Electric fields, the electrolyte flux, and diffusion move Li ions from one electrode to another electrode. This electrolyte flux is one of the most important issues for increasing the energy density of lithium ion batteries.

Reference s :

[1] Keiji Takata, Mitsuhiro Okuda, Nobuki Yura, and Ryota Tamura, Applied Physics Express 5 (2012) 047101, DOI: 10.1143/APEX.5.047101.

[2] Yuki Matsushita, Ryuma Osaka, Kenta Butsugan, and Keiji Takata, J. Chem. Phys. **145**, 114201 (2016). [http: // dx.doi.org / 10.1063 / 1.4962833]

EH-WeP-3 A Novel Doping Strategy of PTAA for High-Performance Inverted Perovskite Solar Cell*, **Jihyeon Heo**, H. Park, H. Park,* Hanyang University, Korea

Organic-inorganic hybrid halide perovskite solar cells (PSCs) have achieved great developments with their high-power conversion efficiency (PCE) surpassing 25.8%. Among various research to maximize the performance of PSCs, a modification of charge transport materials plays an important role to attain such a high-performance of PSC. Particularly, doping engineering can enhance the charge extraction/transport capability of the charge transport layer. Although organic hole transport materials (HTM) including small molecules such as 2,2′,7,7′-tetrakis(N,N-di-p-methoxyphenylamine)-9,9′-spirobifluorene (spiro-OMeTAD) and conducting polymers such as poly(3-hexylthiophene-2,5-diyl) (P3HT) and Poly[bis(4-phenyl)(2, 4, 6-trimethylphenyl)amine] (PTAA) are advantageous with high-quality thin films by a simple solution process, an additional doping process is necessary due to their inherent low hole mobility. Therefore, a search for suitable p-type dopants and their fabrication methods for organic HTM should be further studied. In this work, we propose a simple interfacial doping (ID) strategy of PTAA/F4-TCNQ double layer structure with the application of a new solvent 2-butanone. Through this approach, the optoelectrical performance with high power conversion efficiency of 20.67% (p-i-n structure) is achieved and the reproducibility of PTAA-based PSCs is improved with significantly reduced process time compared to the existing solution blend doping (SBD) method. To compare the SBD and ID strategies, both doping methods are analyzed from an electrochemical and morphological viewpoint. As a result, it is confirmed that the ID method improves the thin film properties of PTAA, and the maximized dispersion of F4-TCNQ by 2-butanone achieves effective doping of PTAA, enabling the realization of high-performance PSCs.

EH-WeP-4 The Role of Artificial Intelligence in Minimizing Analysis Errors, Illustrated with EXAFS, Nanoindentation, and Core Level Photoemission*, **Jeff Terry**,* Illinois Institute of Technology

We have developed artificial intelligence based methodology that can be utilized to reliably analyze experimental results from Extended X-ray Absorption Fine Structure (EXAFS) measurements. This development will help to address the reproducibility problems that slow research progress and inhibit effective tech transfer and manufacturing innovation in these scientific disciplines. A machine learning approach was applied to the analysis of extended X- ray absorption fine structure (EXAFS) spectroscopy measurements collected using a synchrotron radiation facility. Specifically, a genetic algorithm was developed for fitting of the measured spectra to extract the relevant structural parameters. The current approach relies on a human analyst to suggest a potential set of chemical compounds in the form of feff.inp input files that may be present. The algorithm then attempts to determine the best structural paths from these compounds that are present in the experimental measurement. The automated analysis looks for the primary EXAFS path contributors from the potential compounds. It calculates a goodness of fit value that can be used to identify the chemical moieties present. The analysis package is called EXAFS Neo and is open source written in Python. It requires the use of Larch and Feff for calculating the initial EXAFS paths. We have recently extended the code to make use of Feff8.5lite so it can calculate the paths needed for populating the analysis from within the EXAFS Neo package. We have expanded the use of the base genetic algorithm software to fitting of Nanoindentation, X-ray astronomy data, and to the analysis of core level photoemission. The publication describing the analysis package and where to obtain the software can be downloaded at: https://doi.org/10.1016/j.apsusc.2021.149059 or by contacting the speaker.

**EH-WeP-5 In Situ Cryo-Xps Analysis of Intercalation Mechanism in Aqueous Zn-MnO₂ Batteries*, Bhuvana M. Sivakumar,* ***H. Chang, K. Hankins, M. Fayette, V. Shutthanandan, V. Murugesan, D. Choi, X. Li, D. Reed,* Pacific Northwest National Lab

Aqueous Zinc ion batteries (ZIB) based on Zn^{2+} intercalation chemistry is gaining attention as large scale energy storage system due to zinc's high capacity (820 mA h g^{-1}), high abundance and stability along with lower material costs.However, a comprehensive understanding of the principles governing Zn-MnO_2 electrochemistry has not yet been achieved. In particular, the identity of intercalating cationic species (i.e. Zn^{2+} and/or H^+) and subsequent redox evolution in MnO_2 cathode material is still not clear. Towards understanding the electrochemical changes in the MnO_2 cathode (such as oxidation changes at metal centers) during the battery cycling process, we employed *in situ* cryogenic x-ray photoelectron spectroscopy (cryo-XPS) technique. Our unique *in situ* coin cell setup coupled with cryo-XPS characterization uniquely reveals the chemical identity and distribution of active participants in MnO_2 cathode under various charge and discharge conditions without the need for disruptive sample preparations such as solvent washing or Ar sputtering.By preserving the interface, we observed the broadening of Zn 2p core spectra indicating the evolution of Zn-O and Zn-SO_4 bonding environment during long term cycling process (up to 200 cycles).Similarly, the Mn 2p core spectra reveal the emergence of Mn^{3+} from parent Mn^{4+} indicating the Zn intercalation induced redox reactions within cathode material.These new molecular-level insights about the intercalation mechanism and subsequent redox state changes will be discussed based on electronic states evolutions within MnO_2 cathodes.

EH-WeP-6 High-Generating Electrical Power of Chemo-Mechanical Energy Harvesters from Carbon Nanotube Yarn Twist*, Seongjae Oh,* Department of Energy Science Sungkyunkwan University, Republic of Korea*; S. Kim,* Department of Advanced Textile R&D Korea Institute of Industrial Technology, Republic of Korea

The ocean covers 70% of the Earth, and monitoring the ocean conditions (wave height, wave frequency, temperature, pH, etc.) that play an important role in modern life is emerging as an important technology. In the ocean, it is difficult to use secondary batteries or supercapacitors because the ocean has infinitely wide space and fluidity, so research on energy harvesting for self-powered is required. In this regard, research on chemo-mechanical harvesters that converts mechanical energy in the ocean into electrical energy has been recently conducted, and expectations for the possibility of using an actual self-powered system are growing.

Among chemical mechanical harvesters, a carbon nanotube (CNT) based chemo-mechanical harvester was reported in 2017[1]. The chemo-mechanical harvester showed remarkable harvesting performance of frequency normalized peak power or highest peak power between a few Hz and 600 Hz compared to other types. This harvester used a coiled CNT yarn made by highly twisting a CNT yarn. As stretching the coiled CNT yarn, the density of the coiled CNT yarn increases. When the density of the coiled CNT yarn increases, it is to escape the ions of the electrochemical double layer formed on the surface of the CNT inside the coiled CNT yarn, just like water comes out when a wet towel is pulled out. In this way, the mechanical contraction is converted into electrical energy. In this work, to improve the performance of this harvester, we propose a novel internal structure that can facilitate ion access inside the coiled CNT yarn and maximize the density change when the coiled CNT yarn is stretched[2]. The coiled CNT yarn with a novel internal structure has four times the peark power and more than twice the efficiency compared to the performance reported in 2017[1]. This structure opened up the possibility to further improve the performance of the harvester and it was analyzed by molecular dynamics modeling. Our results are expected to contribute to the implementation of self-powered IoT systems in the ocean.

Ref.

[1] S. H. Kim et. al, "“Harvesting electrical energy from carbon nanotube yarn twist” *Science* 357, 773-778 (2017)

[2] S. Oh et. al, "Chemo-mechanical energy harvesters with enhanced intrinsic electrochemical capacitance in carbon nanotube yarns” *Advanced science* accepted (2022)

EH-WeP-7 TOF-SIMS Analysis for Power Semiconductors*, Jaeyeong Lee,* *Y. Jeong, H. Moon, J. Jin,* Korea Basic Science Institute, Korea (Democratic People's Republic of)

Power semiconductors convert, control, and distribute power in electronic devices, which increases battery life and reduces power usage, which is very important for improving the efficiency of energy harvesting devices. Power semiconductors are being applied in various energy harvesting fields such as batteries for electric vehicles and solar power generation, and the demand is increasing due to the rapid growth of mobile devices such as smartphones. Among them, power semiconductors using Silicon Carbide (SiC) are attracting attention due to their small size and stability against high temperature and high voltage, but they are experiencing difficulties in developing more diverse devices due to the advanced technology required for production. In this study, we have conducted analysis for Power semiconductor using Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS). Using TOF-SIMS, it is possible to check the behavior of component ions by depth of the metal-oxide-semiconductor field-effect transistor (MOSFET) device through depth profile analysis as well as the distribution of ion components on the surface of the device. By comparing the TOF-SIMS data of a device that failed due to exposure to harsh environments such as high temperature and high humidity with that of a normal device, it was possible to check where the change occurred in the case of a failure and the change in components. In Figure 1, the failed device was analyzed using TOF-SIMS. Ti+ and Al+ were mainly detected at the interface of the junction, and Si+ ions, an insulating film component, were observed at the interface of the gate pad. In addition, a lot of Si- and P- ions were detected at the defective site. The distribution of Si+ in the underlying layer of Al+ ions indicates that the wire bonding lift occurred at the junction of the Al metal and the underlying Si layer.

Author Index

Bold page numbers indicate presenter

— A —
Alexander, G.: EH-MoM2-12, 1
Asano, Y.: EH-WeM2-8, 3; EH-WeM2-9, 3
— B —
Bagge-Hansen, M.: EH-WeM2-10, 4
Ben-Naim, M.: EH-WeM2-10, **4**
Breuer, U.: EH-MoM2-9, 1
— C —
Cabana-Jimenez, J.: EH-MoM2-12, 1
Chang, H.: EH-WeP-5, 6
Chen, Q.: EH-WeM2-8, 3; EH-WeM2-9, 3
Chen, Y.: EH-MoM2-8, **1**
Cho, S.: EH-WeM2-10, 4
Choi, D.: EH-WeP-5, 6
Colegrove, E.: EH-WeM1-5, 3
— D —
Dittmann, R.: EH-MoM2-9, 1
— F —
Fayette, M.: EH-WeP-5, 6
— G —
Gholami, M.: EH-MoM2-11, **1**
Ginger, D.: EH-WeM1-3, **3**
Guillon, O.: EH-MoM2-9, 1
Gunkel, F.: EH-MoM2-9, 1
— H —
Hankins, K.: EH-WeP-5, 6
Hattori, A.: EH-WeM1-5, 3
Heo, J.: EH-WeP-3, **5**
Hu, J.: EH-MoM2-12, 1
— I —
Ivanovskaya , A.: EH-WeM2-10, 4
— J —
Jeong, Y.: EH-WeP-7, 6
Jin, J.: EH-WeP-7, 6
— K —
Kersell, H.: EH-MoM2-9, 1
Kim, S.: EH-WeP-6, 6
Kubo, M.: EH-WeM2-8, 3; EH-WeM2-9, 3
— L —
Lee, J.: EH-WeP-7, **6**
Lenser, C.: EH-MoM2-9, 1
Li, X.: EH-WeP-5, 6
Liu, C.: EH-MoM2-8, 1
— M —
McGott, D.: EH-WeM1-5, 3
Menzler, N.: EH-MoM2-9, 1
Moon, H.: EH-WeP-7, 6
Mueller, K.: EH-MoM2-12, 1
Murugesan, V.: EH-MoM2-12, **1**; EH-WeP-5, 6
— N —
Nakamura, T.: EH-WeM2-8, **3**; EH-WeM2-9, 3
Nemšák, S.: EH-MoM2-9, 1
Nguyen, D.: EH-MoM2-12, 1
— O —
Oh, S.: EH-WeP-6, **6**
Ootani, Y.: EH-WeM2-8, 3; EH-WeM2-9, 3
Orme, C.: EH-WeM2-10, 4
Otsuki, R.: EH-WeM2-8, 3; EH-WeM2-9, **3**
Ozawa, N.: EH-WeM2-8, 3; EH-WeM2-9, 3
— P —
Park, H.: EH-WeP-3, 5
Perkins, C.: EH-WeM1-5, **3**
Prabhakaran, V.: EH-MoM2-12, 1
Pylypenko, S.: EH-MoM2-10, **1**
— R —
Reed, D.: EH-WeP-5, 6
Reese, M.: EH-WeM1-5, 3
Rose, M.: EH-MoM2-9, 1
— S —
Shutthanandan, V.: EH-MoM2-12, 1; EH-WeP-5, 6
Sivakumar, B.: EH-WeP-5, **6**
Slavin, A.: EH-WeP-1, **5**
Šmíd, B.: EH-MoM2-9, 1
— T —
Takata, K.: EH-WeP-2, **5**
Terry, J.: EH-WeP-4, **5**
— W —
Waser, R.: EH-MoM2-9, 1
Weber, M.: EH-MoM2-9, **1**
— Y —
Yao, G.: EH-MoM2-8, 1
— Z —
Zeng, W.: EH-MoM2-8, 1