

Anode Support Proton Conducting Fuel Cell with Air Spray Coated Thin Film Electrolyte

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Keywords: Solid Oxide Fuel Cell, air spray coating, ceramic

Solid oxide fuel cells with proton conducting ceramic electrolyte can operate at intermediate temperature (400-600 °C). Fabricate the electrolyte into thin film is a strategy to enhance the performance as well as reduce the operation temperature. However, the poor sinterability of the proton conducting ceramic make it a challenge to fabricate the thin film proton conducting fuel cell. Most of the thin film proton conducting fuel cell with the electrolyte at micron scale are usually fabricated by high-vacuum deposition technique, such as pulsed laser deposition (PLD)[1], or atomic layer deposition (ALD)[2] which is costly and time consuming.

We here report a fabrication process of the thin film proton conducting fuel cell. The NiO-BaCe_{0.7}Zr_{0.1}Y_{0.1}Yb_{0.1}O₃-□□BZCYYb□ anode substrate was fabricated by co-pressing the supporting layer and anode function layer and sintering at 1100°C. The BZCYYb electrolyte powder was mixed with ethanol following by roll milling for 24 hours and deposited on the anode substrate. A thin electrolyte with the thickness of 2 μm was achieved by spray coating the 1 wt.% slurry.

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[2] J.H. Shim, J. Park, J. An, T.M. Gür, S. Kang, F.B. Prinz, Intermediate- temperature ceramic fuel cells with thin-film yttrium-doped barium zirconate electrolytes, *Chem. Mater.* 21 (2009) 3290-3296.

Atomic Layer Deposited Ru Nanoparticles on SFMO Electrode for Enhancing Electrochemical Kinetics

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Keywords: Atomic Layer Deposition, Catalysts, Electrochemistry, Electrode, Solid Oxide Fuel Cells

Solid oxide fuel cells (SOFCs), which operate at high temperatures (typically >800 °C), are regarded as the next generation of power applications due to their high energy efficiency and fuel flexibility. However, several challenges must be considered because of their elevated operating temperatures, including high maintenance costs, limited material selection, and degradation during long-term operation. Therefore, to address these issues, efforts have been focused on lowering temperatures to the intermediate range (500-800 °C). However, a significant hurdle arises as the reactions in SOFCs are mainly thermally activated, posing a problem with the electrochemical kinetics, particularly in the cathode part. Thus, a substantial enhancement of electrochemical kinetics in the cathode becomes imperative.

Perovskite and its derivatives have been investigated as one of the most promising SOFC cathode materials due to their considerable catalytic activity and stability. Nevertheless, the use of perovskite materials at intermediate temperatures remains challenging due to their relatively high activation barrier for the oxygen reduction reaction (ORR). Additionally, the chemical degradation of Sr-containing perovskite materials during long-term operation, known as Sr-segregation, is considered one of the limitations. An effective strategy involves the application of surface modification or the introduction of nanoparticles containing highly catalytically active species onto a perovskite electrode surface. This approach offers flexibility in material selection and inherent simplicity, making it a promising technique for enhancing electrochemical kinetics as well as chemical stability.

In this study, we applied plasma-enhanced atomic layer-deposited (PE-ALD) Ru nanoparticles on the SFMO cathode surface to demonstrate the enhancement of electrochemical kinetics in the cathode. Because ALD ensures excellent uniformity and conformality, it is ideal for depositing nanoparticles uniformly on the surface of a highly porous perovskite cathode. Furthermore, Ru can be considered an effective catalyst for ORR, offering the possibility of preventing Sr segregation.

Carbon-Based Optoelectronic Conversion Towards High Performance and Intelligence

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Keywords: Graphene, Intelligence, Optoelectric logic operations, Optoelectronic Conversion

In this talk, we discuss our attempts to improve the performance and intelligence of carbon-based optoelectronic devices. To begin, we will introduce the strategies for synthesizing wafer-scale single-crystal graphene materials and achieving scalable production. The device fabrication processes compatible with CMOS will also be introduced. Next, we will talk about the construction of graphene-based heterojunction structures and analyze some interesting phenomena such as polarity-tunable and photovoltage-driven effects. The photoelectric conversion with ultrahigh gain, ultrahigh responsivity, rapid response, and broad spectral sensitivity will be discussed. Finally, we will introduce device structures that can exhibit both positive and negative photoresponse, highlighting their self-distinguishable capabilities and their application in optoelectronic logic operations and visual-audio perception.

Characterization of Yb₂SiO₅-based environmental barrier coating prepared by plasma spray-physical vapor deposition

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Keywords: Environmental barrier coating (EBC), Phase evolution, Plasma spray-physical vapor deposition (PS-PVD), Ytterbium silicate

Due to the high-input power compared to atmospheric plasma spraying (APS), plasma spray-physical vapor deposition (PS-PVD) can primarily achieve a splat-like deposition, allowing for the preparation of high-density environmental barrier coatings (EBCs). In this paper, dense Yb₂SiO₅-based coatings are prepared by PS-PVD at different substrate temperatures. It was found that the coating deposited at the substrate temperature of 700 °C contained a large amount of silicon-rich amorphous phase. When the substrate temperature increased to 1100 °C and a slow cooling process after deposition was involved, a coating with high crystallinity of ~77% and low porosity of less than ~2% was achieved. Phase evolution of the coatings was studied by a semi-in-situ hightemperature X-ray diffractometer. During the heating process, metastable phases X1-Yb₂SiO₅ and α-Yb₂Si₂O₇ emerged and transformed into stable phases following high-temperature treatment. Furthermore, the effects of long-term thermal aging at 1300 °C on the microstructure, phase composition, thermal conductivity, and hardness of the coating prepared at the substrate temperature of 1100 °C were found to be limited.

Design and fabrication of biomimetic (Gd_{0.9}Yb_{0.1})₂Zr₂O₇ thermal barrier coatings and their mechanism on molten CMAS resistance

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Keywords: Biomimetic structure, CMAS, Plasma spray-physical vapor deposition (PS-PVD), Thermal barrier coatings (TBCs), Ultrafast laser

The silicate deposits from volcanic ash, desert sand and dust melt at high temperature and adhere to the hot components of turbine engines; whereupon attack the thermal barrier coatings (TBCs), eventually leading to the premature failure of the TBCs, thereby endangering operating safety. The challenge for the high-temperature protective coatings is how to improve CMAS resistance of thermal barrier coatings. Recently, a 10 mol% Yb₂O₃-doped Gd₂Zr₂O₇ (GYbZ) TBC has been developed as one of the most promising candidates of advanced TBC materials. In this paper, we attempt to construct biomimetic microstructure on GYbZ coating surface, providing theoretical and technical support for the development of ultra-high temperature thermal barrier coatings with excellent silicate resistance for the next generation aero-engine.

Development of vertical tissue culture/observation platform with air-liquid interface/tissue separability

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Keywords: Air-Liquid Interface, Cell culture platform, Vertical tissue growth

Superhydrophobic surfaces have the characteristic of forming an air layer between solid and liquid. Using this surface property, a wide Air-Liquid Interface (ALI) can be provided between cells and solid surfaces, dramatically improving cell culture. ALI is an especially important factor in skin cell/tissue culture, and if not properly secured, tissue growth may fail.

In addition, there are several chronic problems in the skin tissue culture field. If the grown skin tissue is removed for observation, the tissue may be damaged or cells may come off. In addition, side observation is important for the growth of skin tissue, and no existing methods have been reported to observe tissue growth in real time.

In this study, a completely new, unprecedented cell culture platform is introduced. This cell culture platform has a shape similar to a picture frame, and cells grow through thin gaps in the body. Thus cells can be observed growing vertically in real time through the window of the transparent body. The key point is that by forming a micro/nano surface structure on the side excluding the window of the vertical culture platform to realize the superhydrophobic properties of the surface, it is possible to secure a stable ALI between the vertical interface of the cell/tissue and the side wall. Lastly, efficient use of culture media can reduce consumption to less than 10% of existing levels. With the development of this cell culture platform, we plan to pioneer a new vertical cell culture market.

Effect of ALD-Derived Oxygen Vacancy Rich Nano-Thin Coatings on Improving Perovskite Air Electrodes in Solid Oxide Cells

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Keywords: Atomic Layer Deposition, Solid Oxide Cells, Surface Coatings

Perovskite-based electrodes consistently encounter challenges associated with the segregation of specific cation species, such as Sr^{2+} , Ba^{2+} , and Pb^{2+} , towards their surfaces. These segregated cation ions react with H_2O and CO_2 in the air/fuel atmosphere, forming the undesired precipitates that passivate electrochemically active sites between the surface and air/fuel. One key factor contributing to the instability of perovskite oxide surfaces is the electrostatic attraction by oxygen vacancy enrichment at perovskite surfaces. This unstable chemical composition severely degrades the performance and durability of solid oxide cell (SOC) electrodes.

$\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\square}$ (SFMO) has emerged as a promising candidate for SOC electrodes owing to exceptional electrical and ionic conductivity in both fuel and air atmosphere. In comparison to bare SFMO, ALD ZrO_2 coated SFMO exhibited a significant enhancement of chemical stability in the long term of 50 hours. This result showed that ALD ZrO_2 nano-thin coatings successfully suppressed surface cation segregation within SFMO perovskite bulks. Furthermore, we observed the promotion of charge transfer reactions on ALD ZrO_2 capped SFMO electrodes. Detailed characterization through HRTEM and XPS analysis revealed the presence of abundant oxygen vacancy rich in ZrO_2 coatings derived by ALD.

In this study, we present the effect of oxygen vacancy in surface coatings containing ZrO_2 , TiO_2 , and HfO_2 derived by ALD on SOC electrode performances of SFMO perovskites. To gain deeper insights, we controlled the oxygen vacancy concentration by changing ALD conditions such as growth temperatures, and additional plasma treatment. This study highlights that oxygen vacancy rich coatings on perovskite-based SOC electrode surfaces provide a pathway to achieve long-term stability and improve performance.

Effective Area of Nano-membrane for improvement of Si-based μ -SOFC

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Keywords: Etching, nano-membrane, μ -SOFC

The global net zero (carbon neutrality) is essential in order to limit global warming to 1.5°C. To achieve global net zero, environmentally friendly fuel cells are an emerging area for their potential of efficient energy conversion. Especially, Solid Oxide Fuel Cell (SOFC) are promising as a next-generation power source due to their efficiency, and high-power density. Its high operating temperature that exceed 700°C, however, causes the degradation of system components, and imposes high cost of materials. To overcome these disadvantages, micro-SOFC (μ -SOFC) has been proposed to achieve nanomembrane structure that composed of nanoscale electrolyte and electrode thickness for electrochemical reactions at low temperatures. Although the nano-membrane structure enables low-temperature operation, the reduction of the effective area with the mechanical and thermal safety of μ -SOFC still remains a challenge. To solve these problems, the design and fabrication of an efficient nano-membrane structure is of the most importance.

In this study, we have demonstrated the fabrication of μ -SOFC membrane, which involves the etching profile using deep reactive ion etching (DRIE) for creating the desired structures and stress dispersion. Through various control of parameters such as working pressure, flow rate, power, cycle time, we were able to fabricate a tapered profile with dispersed stress by deliberately balancing combination of isotropic and anisotropic etching methods.

This work was supported by the Korea Government programs (KCCUS20230001 and Training DX-based carbon supply network environmental experts) and the Training

Gyeonggi-do semiconductor industry experts (GSPEC01A).

High temperature stability and CMAS resistance of (Gd_{0.2}Y_{0.8})₃Al₅O₁₂ (GYAG)/YSZ thermal barrier coatings prepared by PS-PVD

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Keywords: (Gd_{0.2}Y_{0.8})₃Al₅O₁₂, CMAS corrosion, Plasma spray-physical vapor deposition (PS-PVD), Thermal barrier coatings (TBCs), high temperature stability

Environmental deposits with a main component of calcium-magnesium-alumina-silicate (CMAS) threaten aviation safety seriously. The silicate deposits ingested into the engines melt and adhere to the surface of thermal barrier coatings (TBCs) on hot-section components at high operating temperatures, accelerating the failure of coatings. Here, we prepared (Gd_{0.2}Y_{0.8})₃Al₅O₁₂ (GYAG)/YSZ double ceramic layered TBCs, consisting of dense lamellar GYAG top coat and columnar structured YSZ coating, by plasma spray-physical vapor deposition (PS-PVD) to mitigate degradation induced by CMAS. Characterization results of GYAG/YSZ coatings before and after thermal exposure at 1250 °C reveal excellent high temperature stability. Interaction between molten CMAS and GYAG/YSZ coating at 1250 °C was investigated. The results show that the infiltration of molten CMAS was effectively inhibited. Due to the reaction between GYAG and molten CMAS, crystalline products (anorthite, garnet and apatite) with high melting point precipitated, reducing the volume of CMAS melt and impeding the further infiltration of molten CMAS. GYAG/YSZ TBC is proved to be a promising coating to against CMAS attack.

High throughput advanced materials design for the energy transition

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Keywords: Digital material foundry, combinatorial synthesis, computational

The development of advanced materials has traditionally been a slow process, often taking decades from initial research to commercialization. However, two major paradigm shifts are underway in materials science that promise to significantly accelerate this process: firstly, the emergence of truly predictive Computational Materials Design based on advanced and efficient quantum mechanical methods like Density Functional Theory (DFT). DFT has matured into a highly predictive theory that can accurately gauge a wide range of materials properties, such as phase stability, electronic structure, and thermochemistry, through automated calculations.

Secondly, the development of Combinatorial Materials Science (CMS) allows for the synthesis of materials libraries with varying compositions across a substrate using techniques like the wedge-type multilayer approach. This enables rapid synthesis and screening of a vast number of material compositions.

The Digital Materials Foundry integrates these two paradigm shifts by combining advanced computational modeling with automated combinatorial synthesis and characterization techniques. Our approach involves:

1. Synthesizing thin-film material libraries using Physical Vapor Deposition, which enables rapid and reliable synthesis of a broad spectrum of materials.
2. Characterizing the synthesized films with Angle-resolved Photoemission Spectroscopy (ARPES) for electronic structure determination and X-ray diffraction for crystal structure analysis, in a single integrated Ultra-High Vacuum system.
3. Leveraging advanced computational methods like DFT to guide and accelerate the optimization of materials for various energy applications, such as hydrogen storage, metamaterials, magnesium batteries, and magneto-electrocatalysis.

By co-developing combinatorial synthesis and computational techniques, we significantly accelerate and dramatically reduce the time from initial research to commercialization.

Highly efficient and stable inverted perovskite solar cells enabled by homogenized fullerene with enhanced electron transport

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Keywords: Perovskite solar cells ; efficiency; stability

Fullerene derivatives are extensively employed in inverted perovskite solar cells due to their excellent electron extraction capabilities. However, [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) agglomerates easily in solution and exhibits a relatively low ionization barrier, limiting its hole-blocking capabilities and increasing charge recombination losses. Here, tetramethylthiuram disulfide (TMDS) is introduced into the PCBM solution to induce the formation of reducing sulfur radicals through UV light irradiation, allowing for n doping of the PCBM material. The resulting modified PCBM layer exhibits enhanced conductivity and electron mobility, greatly restricting hole injection into the cathode and significantly suppressing charge recombination. As a result, the resulting devices incorporating TMDS achieve a champion efficiency of 25.25% (0.1 cm²) and 23.63% at a larger area (1.0 cm²) with negligible hysteresis. More importantly, the optimized devices retain 95% and 94.6% of their initial efficiency after 1090 h under damp heat testing (85 °C and 85% relative humidity) and after 1271 h under maximum power point-tracking conditions, respectively.

In situ growth of copper-iron bimetallic nanoparticles in A-site deficient $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\delta}$ as an active anode material for solid oxide fuel cells

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Keywords: Solid oxide fuel cells; Synergistic effect; Copper-iron bimetallic nanoparticles; Exsolution

The metallic exsolved ceramic anode materials for Solid oxide fuel cells (SOFCs) have garnered immense attention owing to the abundant active sites and high catalytic efficacy. However, the performance and durability of nanoparticle decorated ceramic anodes are still hindered by the morphology and size of exsolved nanoparticles, but there are few studies on the specific dissolution rules and conditions. Here, the Cu element is doped into high-performance $\text{Sr}_{1.9}\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6.6}$ materials to study the exsolution rule of nanoparticles and the change of nanomorphology in the reduced state. According to the results of the study, the reduction in H_2O environment and the low temperature is an effective method to control the whisker-like Fe nanoparticles to improve the catalytic performance, and the doping of Cu can ensure the formation of Cu-coated core-shell structure to inhibit the agglomeration of nanoparticles.

Influence of Operational Conditions on the Crystallographic Behavior of Iridium-Based Catalysts in Proton Exchange Membrane Water Electrolysis

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Keywords: Iridium-based catalyst, Lattice structure, Oxygen evolution reaction, PEMWE

The global drive to reduce carbon emissions positions hydrogen as a key alternative energy source, particularly when produced by carbon neutral methods such as Proton Exchange Membrane Water Electrolyzer (PEMWE). Given its potential for integrating with renewable energy sources to produce hydrogen without carbon emissions, PEMWE's efficiency and durability are of major importance. This requires a thorough understanding of the operating conditions that influence the performance and stability of critical components such as iridium-based catalysts.

This study focuses on understanding the effect of operating conditions on the crystal structure of iridium-based catalysts used in PEMWE. Specifically, it investigates the crystallographic changes of these catalysts under varying voltage conditions, including the transition to metallic Ir observed during abrupt voltage drops to open circuit voltage (OCV). Through comprehensive analyses using transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDS) and X-ray diffraction (XRD), the study identifies key operational thresholds that trigger these structural changes. The results show that operating conditions have a significant impact on the crystallographic integrity and consequently the catalytic performance of iridium-based catalysts in PEMWE. These findings will contribute to the design of operating protocols aimed at maximizing catalyst lifetime and efficiency.

Investigating the Efficiency of Vanadium Redox Flow Battery Electrodes with VNbMoTaWO Films by HiPIMS Technology: Effect of W Contents

by KRISHNAKANT TIWARI | CHEN HAO WANG | JYH WEI LEE | BIH SHOW LOU* | NATIONAL TAIWAN UNIVERSITY OF SCIENCE AND TECHNOLOGY | NATIONAL TAIWAN UNIVERSITY OF SCIENCE AND TECHNOLOGY | MING CHI UNIVERSITY OF TECHNOLOGY | CHANG GUNG UNIVERSITY

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Keywords: High entropy alloy oxide (HEAO) film, VNbMoTaWO, graphite felt., high power impulse magnetron sputtering, tungsten (W), vanadium redox flow batteries

This study presents an innovative approach for surface modification of graphite felt (GF) electrodes for Vanadium Redox Flow Battery (VRFB) using high power impulse magnetron sputtering (HiPIMS) technology. The research focuses on depositing the VNbMoTaWO high entropy alloy oxide films with various W contents onto GF electrodes to optimize the VRFB's performance. Through systematic variations in tungsten composition via adjustments in deposition time and oxygen flow rate, the study investigates its nuanced effects on electrode efficiency alongside the VNbMoTaW target composition. Rigorous electrochemical analyses and battery tests reveal the intricate interplay between tungsten and high entropy alloy composition for VRFB performance. The findings not only advance our understanding of GF electrode modification but also provide practical insights for enhancing VRFB reliability and applicability in large-scale energy storage systems. The demonstrated improvements in performance and stability underscore the significance of the tungsten content of the VNbMoTaWO film in advancing the feasibility of VRFB technology.

Machine learning-assisted CMAS viscosity prediction and its application in the infiltration dynamics analysis of CMAS into TBCs

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Keywords: Machine learning; CMAS; viscosity prediction; infiltration; TBCs

The corrosion of vulnerable thermal barrier coatings (TBCs) by silicate melts (SMs) is severely detrimental to the service life of aero-turbine. The SMs damage the TBCs through the process of wetting, spreading and especially infiltration. The viscosity of SMs, which determines the infiltration speed, has a critical effect on the severity of the destruction of TBCs. In this work, the quantitative relationship between the SMs viscosity and infiltration speed in EB-PVD prepared columnar YSZ coatings is mathematically investigated by a series of experiments. In the meantime, in order to obtain more accurate and real-time viscosity of SMs, 3021 CMAS viscosities and 3212 viscosities of multi-component silicate melts (Multi-Melts) were collected from experiments and published literature for training machine learning models to predict viscosity of SMs. The behavior of well-tuned neural networks on test datasets can reach 0.958 and 0.98 in predicting the viscosity of Multi-Melts and CMAS. Compared to previous models based on physical formulas, machine learning provides more approaches to overcome overfit and exhibit better behavior. On the basis of the well-trained models, a function is developed to recommend substitute CMAS components to simulate the viscosity of a given Multi-Melts.

Mechanical and Thermal Stability of Si-Based μ -SOFC

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Keywords: COMSOL Multiphysics, Stability, μ -SOFC

In recent years, the requirement for carbon neutrality and reduction of greenhouse gases is emerging in consideration of global warming. Thus, interest in renewable energy is increasing in each country to change the main energy source from fossil fuels to renewable energy. Among renewable energies, hydrogen-based fuel cells, as a next-generation energy source, have gained attention. A fuel cell is an energy conversion device that generates electricity through a reaction between hydrogen and oxygen and produces water as by-products. Among the types of fuel cells, solid oxide fuel cell (SOFC) has the advantage of high-power generation efficiency, but there is a problem that they operate in a high-temperature environment. Therefore, a micro-SOFC (μ -SOFC) was designed because there is a need to reduce the thickness of the electrolyte and electrode of the fuel cell so that the electrochemical reaction actively occurs even at low temperatures. The micro-SOFC (μ -SOFC) is essential to improve the mechanical and thermal stability of an electrolyte thin film in nano-membrane structure.

In this study, to confirm the mechanical and thermal stability of an electrolyte film (100nm thickness), the stress caused by temperature change was measured using COMSOL Multiphysics simulation. In COMSOL program, Modeling, material setting, and domain condition with boundary condition setting were performed to determine the magnitude and location of the maximum stress caused by temperature change.

This work was supported by the Korea Government programs (KCCUS20230001 and Training DX-based carbon supply network environmental experts) and the Training

Gyeonggi-do semiconductor industry experts (GSPEC01A).

MOLECULAR TRANSPORT IN THE LOW-DIMENSIONAL ENVIRONMENT TOWARDS EFFICIENT SEPARATION

by HYUNG GYU PARK | POSTECH

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Keywords: carbon nanotubes, fast mass transport, high-flux membrane, membrane technology, porous graphene, ultimate permeation

Fast mass transport inside and across nanoscale graphitic surfaces such as carbon nanotubes and graphene, respectively, forms the basis of Carbon Nanofluidic phenomena and poses potential applications in energy and clean technologies. This talk will review an existing paradigm of the fast transport in carbon nanotube conduits with a proposal of a new scaling relation to answer a question, "How fast is fast?" Then follows our story of shifting the paradigm with recognition of equivalence between a nearly frictionless channel and no-channel-but-only openings. Synthesis, transfer, perforation, and device integration of graphene enable altogether preparation of an atomically thin, porous membrane for the embodiment of this new concept. Transport physics across the orifice points to an ultimate permeation of fluids (both in molecular and viscous transport regimes), heralding a high-flux membrane. High-flux membranes are in need of proper applications in membrane technology, for which this talk introduces active endeavors of producing porous graphene at large scales, furthering our understanding of transport theories and designing composite membrane materials for enhanced chemical separation.

Morphological evolution of Pt-films on two dielectric materials substrates at various temperatures

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Keywords: Molecular dynamics simulations, Morphological evolution, Pt film

Metal thin films on dielectric materials are thermodynamically unstable and the microstructure evolves at high temperatures, and how to reliably predict the evolution of metal thin films has been a topic of great importance. The temporal structural transitions of Pt films on sapphire and quartz substrates at elevated temperatures have been investigated by combining molecular dynamics simulations and 2D GIWAXS. Upon annealing, the surface morphology of the Pt films changes and the scattering rings become sharp, showing structural evolution and increased crystallinity. During the relaxation of amorphous Pt blocks and Pt films, temperature dominates the nucleation and growth mechanisms of crystallization, with the substrate acting as a template for the arrangement of Pt atoms. At high temperatures, angular grains form in the platinum layer and crystallization starts near the substrate and then spreads to the top layer. At intermediate temperatures, the grains increase but partially retain their initial morphology, and spontaneous and substrate-promoted crystallization occur simultaneously.

Morphology Controlled of NiCo₂O₄ as Superior Bifunctional Oxygen Reduction Reaction/Oxygen Evolution Reaction Electrocatalyst for Zinc-air Battery

by Jyh-Ming Ting | National Cheng Kung University

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Keywords: NiCo₂O₄, hydrothermal, oxygen evolution reaction, oxygen reduction evolution, zinc-air battery

Nickel cobalt spinel oxide has attracted many attentions due to its electrochemical activity. The advantages of NiCo₂O₄ includes the multiple oxidation states of Ni and Co, good chemical and thermal stability, and rich expose octahedral and tetrahedral active sites. These are desirable for using as an oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) bifunctional catalyst. In this work, morphology modification NiCo₂O₄ has been investigated. The morphology has been controlled during the hydrothermal synthesis with the assistance of a surfactant and post heat treatment. X-ray diffractometry, scanning electron microscopy, transition electron microscopy, inductively coupled plasma elemental analysis, and x-ray photoelectron spectroscopy were used to examine the material characteristics, among which the morphology and the oxidation state are addressed. The morphology control allows the transformation of NiCo₂O₄ rods into porous sheets. Thus, electrochemical surface area analysis indicates that the number of active sites is increased and electrochemical impedance spectroscopy analysis shows that the charge transfer resistance decreases. Linear sweep voltammetry shows the significant decreasing of the onset potential, leading to increased ORR half-wave potential and reduced OER overpotential. The use of NiCo₂O₄ as electrocatalyst in Zinc-air battery is also demonstrated and discussed.

Multi-element oxide-sulfide heterostructure for efficient electro-Fenton oxidation

by Yemima Purba | Jyh-Ming Ting | National Cheng Kung University | National Cheng Kung University

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Keywords: *Electrochemical advanced oxidation, ORR selectivity, heterogeneous electro-Fenton, oxide-sulfide heterostructure, tetracycline.*

Electrochemical advanced oxidation processes, such as Fenton process, have attracted a lot of attentions as compared to the conventional degradation process. In this work, we have investigated multi-element oxide-sulfide heterostructures with controlled phase ratios via varying the synthesis condition. The phase, morphology, oxidation state, charge transfer, hydrogen peroxide selectivity, and EF degradation performance are characterized using various characterization techniques, such as X-ray diffractometry, scanning electron microscopy, transmission electron microscopy, x-ray photoelectron spectroscopy, electrochemical impedance spectroscopy, linear sweep voltammetry, and tetracycline degradation, respectively. We demonstrate that under the optimized condition, the material effectively generates hydrogen peroxide and exhibits tetracycline degradation efficiency of 98% within 2-h. The electron transfer and ORR selectivity are discussed experimentally and theoretically.

Nanostructured Carbon Materials as Multifunctional Electrodes for PEM fuel cells

by Daniel Chua | National University of Singapore

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Keywords: Graphene, MoS₂, Nanostructured Carbon, PEM fuel cells

Carbon materials have attracted much attention due to their unique properties, ranging from low

dimensional effects, good structural integrity, high electrical and thermal conductivity, and chemical stability. Increasingly, carbon-based materials have progressed from thin films to the nanoscale dimensioned carbon nanotubes and graphene.

In this talk, we will show that we can engineer various 1D and 2D carbon-based materials and these nanostructured materials have direct applications in PEM fuel cells. These nanostructuring reduces the process steps required to prepare the different layers at each electrode. We will further show that with careful design, these nanostructuring work increases both the performance (power generated) and robustness of the fuel cells. This is supported with a series of in-situ tests which includes accelerated degradation test and electrochemical impedance spectroscopy. We will also mention briefly other benefits in the nanostructuring such as resistance to catalyst poisoning.

N-doped carbon nanocage co-encapsulating WC nanoparticles and NiFe alloy for outstanding bifunctional electrocatalysis in OER and ORR.

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Abstract ID: 10354
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Keywords: Bifunctional electrocatalyst; Prussian Blue Analogue; N-doped carbon; Oxygen evolution reaction; Oxygen reduction reaction; Zn-air battery

Developing electrocatalysts based on earth-abundant materials with optimized intrinsic active sites is essential to enhance the performance of bifunctional oxygen evolution reaction (OER) and oxygen reduction reaction (ORR). In this investigation, we engineered a hollow carbon framework using NiFe Prussian Blue analogs (PBAs) as templates, incorporating polypyrrole (PPy) and phosphotungstic acid (PW12). The pyrrole monomer underwent polymerization on the nanocubic PBA surface in the presence of PW12, resulting in PBA@PPy-PW12. Carbothermal reduction then produced an N-doped carbon shell embedded with NiFe alloy and tungsten carbide (WC) nanoparticles. The polymeric nature of PPy-PW12 not only prevented the aggregation of PBA and WC structures but also enhanced electrical conductivity by connecting neighboring nanospheres. Additionally, the incorporation of WC significantly boosted the bifunctional electrocatalytic activity of the carbon-based catalyst, attributed to the synergistic effects between WC and NiFe materials within the NC layer. As a result, NiFe/W0.3C@NC exhibited outstanding OER (overpotential = 290 mV for 10 mA/cm²; Tafel slope = 57 mV/dec) and ORR (half-wave potential = 0.81 V; Tafel slope = 61 mV/dec) performances. This study provides a promising avenue for the development of high-performance electrocatalysts for energy conversion systems, demonstrating remarkable efficiency, stability, and practical potential.

New aqueous redox flow batteries

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Symposium: 4. Energy & Sustainability (ENS)

Keywords: Aqueous redox flow batteries; Battery performance; Battery stability; Organic active materials; Organometallic active materials

Aqueous Redox flow batteries (ARFBs) are a promising technology for large scale energy storage system. For improving the performance and stability of the ARFBs, the determination of proper active materials is most important. The active materials are immersed into supporting electrolytes, and such produced anolyte and catholyte are stored in tank. They decide cell voltage and maximum solubility, followed by capacity and power density of ARFBs. So far, vanadium was the main host of active material. However, due to its natural limitations, many attempts are made to replace it to other materials that have appropriate redox kinetics. As the alternative, organic and/or organometallic complex materials can be considered because they offer the benefits such as adjustable redox potential and solubility, a low crossover rate, and a relatively cheap cost. In this presentation, of the candidates, special quinone derivatives and iron based complex materials that are dissolved in high pH electrolytes are considered as active materials. Initially, their electrochemical properties and kinetic parameters are evaluated quantitatively to determine their optimal condition. In turn, cycle tests of ARFBs using them are implemented to enhance their performance and stability. Based on that, we corroborate that ARFB using organic and organometallic complex materials as redox couple is viable enough to compete with vanadium RFB and lithium battery.

Overcoming Iodine Film Challenges in the Flow Battery System

by Mingyu Shin | Chanho Noh | Yongchai Kwon | Seoultech | Seoultech | Seoultech

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Keywords: Additive, Aqueous electrolytes, Flow battery, Iodine film

Renewable energy sources like solar and wind are essential for meeting rising energy demands while minimizing environmental impact, despite their unstable and intermittent energy production. Energy storage systems, particularly flow batteries (FBs), play a crucial role in addressing these issues due to their scalability, safety, and long-duration storage capabilities. Among FBs, the all-vanadium FB (VFB) is notable for its ability to reuse electrolytes even after cross-contamination, enhancing system efficiency. However, limitations such as solubility, cell voltage, cost, and operational temperature drive research towards alternative materials like zinc. Zinc-Iodine RFBs (ZIFBs) emerge as a promising alternative with lower toxicity and higher solubility, although challenges like low solubility of iodine and surface film formation need addressing for improved performance. In this study, an additive was used in iodine-based redox flow batteries to prevent the formation of an iodine film on the electrode surface. While one type of additive led to iodine precipitation due to low water solubility, another with higher solubility effectively dissolved iodine back into the electrolyte. Electrochemical evaluations and spectroscopic analyses confirmed the improved solubility and interaction of dissolved I_2 with I^- . Batteries operated with this additive showed stable cycling and performance, even at higher electrolyte concentrations, suggesting a solution to the iodine film issue in iodine-based systems.

Oxidized Nickel to Prepare an Inorganic Hole Transport Layer for Efficient and Stable CH₃NH₃PbI₃ based Perovskite Solar Cells

by Kun-Mu Lee | Seoungjun Ahn | Chang Gung University | Chang Gung University

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Keywords: Nickel oxide, Perovskite, Photovoltaic, Solar Energy, Solar cell

In this study, we report a perovskite solar cell (PSC) can be benefited from the high quality of inorganic nickel oxide (NiO_x) as a hole transport layer (HTL) film fabricated from the physical vapor deposition (PVD) process. The power conversion efficiency (PCE) of PSC is found to depend on the thickness of NiO_x HTL. The NiO_x thickness is optimized via quantitative investigation of the structure, optical and electrical properties. With an active area of 11.25 cm², a PSC module (25 cm²) with a PCE of 15.1% is demonstrated, while statistically averaged PCE = 18.30% with an open voltage (V_{oc}) 1.05 V, short-circuit current density (J_{sc}) 23.89 mA/cm², and fill factor (FF) 72.87% can be achieved from 36 devices with smaller active areas of 0.16 cm². After the stability test at 40% relative humidity (RH) and 25 °C for 1200 h, the highest performance NiO_x-based PSC is shown to be about 1.2-1.8 times superior to PEDOT:PSS organic HTL based PSC at the same environment.

Probing local heat generation within a coin cell

by Soyoung Park | Woosung Park | Sogang University | Sogang University

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Keywords: Heat generation, battery, coin cell, local temperature

Local temperature rise in electrochemical cells dictates its performance, life, and reliability, and internal temperature monitoring carry a key information to improve various aspect of battery operations. However, direct measurements of its local temperature are technically challenging as the systems are thermally and electrically isolated as well as chemically active environment. Here, we fabricate a chemically stable thermometer, combining with a coin cell for *in operando* temperature monitoring. Specifically, we measure the temperature at an interface between a separator and anode. We find that a rapidly increasing temperature while charging with constant current, and exponentially decaying its profile at rest. Based on the exponentially decaying profile, we build a phenomenologically equivalent thermal model with experimentally defined time constant of the system. Using heat equation, we experimentally estimate the local heat generation, and compared it with a summation of both entropic and Joule heating.

Semi-transparent Colored Solar Cells for Agrivoltaics Ecosystem Applications

by Can Sheng | Hunan University

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Keywords: agricultural greenhouses, photosynthetic, power conversion efficiency, semitransparent solar cells

The emergence of agricultural photovoltaic (PV) ecosystems is expected to address the issue of land competition between solar PV panels and crops. Semitransparent color thin-film PV technology, applied in greenhouses, achieves solar energy conversion while meeting the photosynthetic needs of crops, presenting tremendous prospects in significant agricultural applications. This article reviews the recent progress in semi-transparent solar cells (ST-SCs), including cadmium telluride solar cells, copper indium gallium selenide solar cells, organic solar cells, dye-sensitized solar cells and perovskite solar cells. In addition, the strategies to tune film color and enhance both the transparency and power conversion efficiency of ST-SCs are described through optimizing the composition of the active layer, the ratio of donor and acceptor layers, the thickness of the active layer, and device structure. Some perspectives on future opportunities for agricultural greenhouses applications of semitransparent solar cells are also discussed

Structural and Morphological Evolution of High Entropy MOF-Derived Electrocatalyst during Oxygen Evolution using In Situ Transmission Electron Microscopy

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Keywords: High Entropy Material, In Situ TEM, MOF derived, OER

Metal-organic framework (MOF) has been extensively applied for oxygen evolution reaction (OER) due to having adjustable metal active sites and tunable morphology. However, both poor electrical conductivity and limited surface area results in mostly unsatisfactory OER performances. On top of that, it is of importance to understand changes in structure and morphology during OER especially at the nanometer scale. Such understanding may usher new ways to improve activity, selectivity, and stability of OER electrocatalyst in the future. With that in mind, we developed a high entropy MOF derived electrocatalyst and characterized its performances toward OER. Investigation towards structural and morphological evolution were performed using *In Situ* Transmission Electron Microscopy (*In Situ* TEM). In addition, typical materials characterization involving scanning electron microscopy (SEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and inductively coupled plasma (ICP) were also performed.

Study on interfacial band alignment of p-CdTe multiple composite photoelectrode and mechanism of efficient solar water splitting for hydrogen production

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Keywords: Interfacial band alignment, Photoelectrochemical, Solar hydrogen production, Water splitting, p-CdTe composite photoelectrode

Photoelectrochemical (PEC) water splitting is attractive because it harnesses abundant solar energy and enables solar-to-fuel production at scale. An ideal photoelectrode requires strong light absorption, efficient charge separation and transport, and rapid water-oxidation (reduction) reaction kinetics. It has been considered that building the heterostructured photoelectrode with energetics matching at interface could commendably meet these demands. Herein we designed and constructed the p-CdTe/n-CdS/TiO₂/Pt multilayer photocathode. Note the introduction of n-CdS eliminated the large conduction band offset between p-CdS and TiO₂, under which condition the photoelectrons could efficiently transfer from p-CdTe to n-CdS, then to TiO₂, and finally to Pt for water reduction under light illumination. Therefore, the obtained p-CdTe/n-CdS/TiO₂/Pt photocathode yielded significantly improved PEC water splitting performance as compared to the p-CdTe/Pt photocathode. Additionally, we also developed the n-CdS/p-CdTe/TiO₂/Ni/NiO_x photoanode for PEC water oxidation, which showed a light-limited photocurrent density of 24.5 ± 0.5 mA cm⁻² and a photovoltage of 780 ± 20 mV. It has been demonstrated that the TiO₂ coating, with its in-gap charge-transport intermediate band, could facilitate hole transport as light exited the p-CdTe/TiO₂ interface. With proper interfacial chemistry, the electrochemical potential energy of the coating intermediate band matched that of the p-CdTe valence band. Moreover, the stabilized n-CdS/p-CdTe/TiO₂/Ni/NiO_x photoanode showed 100 h stability for water oxidation. The above studies provide insightful guidance for designing stabilization contacts for efficient and stable light-driven water splitting.

Superwetting Surfaces for Energy and Environmental Applications from Capillary Tubes to Micro Channels

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Keywords: Coatings, CuO nanowires, Electrochemical Anodization, Superwettability, TiO₂ nanotubes

Capillarity is a crucial and pervasive phenomenon in nature and has found important applications in wearable electronics, medical devices, miniature energy conversion and storage systems. Superwetting coating plays an essential role in drag reduction, corrosion resistance, heat transfer enhancement, and so on. However, it remains a great challenge to prepare such a coating of superwettability inside capillary tubes, in view of the spatial confinement. This presentation introduces the fabrication of uniform and superhydrophilic nanostructured arrays at capillary tubes and microchannels. Their applications in solar cell, solar-driven water evaporation, oil-water separation, and vanadium redox flow battery are demonstrated and discussed.

Surface Engineering of Solid Oxide Cell Electrodes by Powder Atomic Layer Deposition

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Keywords: Electrode, Powder Atomic Layer Deposition, Solid Oxide Cell, Surface Engineering

Employing porous structures is essential in high-performance electrochemical energy devices. However, obtaining uniform functional coatings on high-tortuosity structures can be challenging, even with specialized processes such as atomic layer deposition (ALD). Herein, we present a novel method for achieving a porous composite electrode for solid oxide fuel cells (SOFCs) by coating $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-6}$ (LSCF) powders with ZrO_2 using a powder ALD process. Unlike conventional ALD, powder ALD can be used to fabricate extremely uniform coatings on porous electrodes with a thickness of tens of micrometers. The powder ALD ZrO_2 coating is found to effectively suppress chemical degradation of the LSCF electrodes. The cell with the powder ALD coated cathode shows a 2.2 times higher maximum power density and 60 % lower thermal degradation in activation resistance than the bare LSCF cathode cell at 700-750 °C. The result demonstrated in this study is expected to have significant implications for high-performance and durable electrodes in energy conversion/storage devices.

Synchrotron X-ray study of electromigration in eutectic Bi-Sn micro joints

by Yi-An Wu | Zhao-Yu Yang | Wan-Zhen Hsieh | Pei-Tzu Lee | Chang-Meng Wang | Hung-Cheng Liu | Cheng-En Ho | Yuan Ze University, Taoyuan 320, Taiwan, R.O.C. | Yuan Ze University, Taoyuan 320, Taiwan, R.O.C. | National Synchrotron Radiation Research Center (NSRRC), Hsinchu 300, Taiwan, R.O.C. | X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, USA. | Shenmao Technology Inc., Taoyuan 328, Taiwan, R.O.C. | Kinsus Interconnect Technology Corp., Taoyuan 328, Taiwan, R.O.C. | Yuan Ze University, Taoyuan 320, Taiwan, R.O.C.

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Keywords: Environmental sustainability; net-zero emissions; low-melting temperature; eutectic Bi-Sn; electromigration; Synchrotron X-ray

Continuous pursuits of environmental sustainability and advanced electronics manufacturing have pushed the utilization of low-melting-temperature solder alloys in the consumer electronic products and the internet of things (IoT) markets. Among the potential low-melting-temperature candidates, eutectic Bi-Sn alloy is gaining increased attention owing to its favorable eutectic temperature (138 °C) and cost effectiveness. The reduced melting point facilitates a diminished temperature difference between soldering and ambient temperatures, thereby decreasing PCB warpage and enhancing joint reliability. Moreover, the utilization of low-melting-temperature Bi-Sn enables to decrease the soldering temperature that is beneficial to lower current load and align with the target of net-zero emissions. In this study, we conducted an *in-situ*, non-destructive analysis on the electromigration of eutectic Bi-Sn micro joints via Synchrotron X-ray Laue diffraction mappings and nanobeam X-ray fluorescence spectroscopy measurements at the beamline 21A, Taiwan Photon Source (TPS). Failure of micro joints might be caused with remarkable segregation of Bi-rich and Sn-rich phases as a result of electromigration. The underlying mechanisms associated with electromigration-induced phase segregation of an eutectic alloy and the resulting joint failure will be discussed in this paper.

Systematic investigations on the microstructural evolution and degradation mechanism of Cr₃Si-coated Zry-4 under DBA and BDBA conditions

by Haiyan Liao | Haibo Ruan | Weijiu Huang | Jin Hu | Xiangkong Xu | Xiaohan Deng | Junjun Wang | Kunming University of Science and Technology | Chongqing University of Arts and Sciences | Chongqing University of Arts and Sciences | Kunming University of Science and Technology | Chongqing University | Chongqing University of Technology | Chongqing University of Technology

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Keywords: Cr₃Si coating; High-temperature steam oxidation; Zry-4; Accident tolerant fuels

Cr₃Si and Cr coatings were deposited on Zry-4 substrates via magnetron sputtering to examine their oxidation behavior under high-temperature steam conditions. At 1200°C, a dense Cr₂O₃ formed on the surface of the Cr₃Si coating surface, exhibiting a parabolic growth law that effectively prevented the internal diffusion of oxygen. Additionally, an in-situ Zr₂Si layer, developed between the Cr₃Si coating and Zry-4 substrate, significantly mitigated the outward diffusion of Zr. However, at 1350°C in steam, the continuity of the Zr₂Si layer was disrupted due to the formation of ZrCr₂, which facilitated the outward diffusion of Zr to the interface between the remaining Cr₃Si layer and the outer Cr₂O₃ layer. Despite the reaction between the Cr₂O₃ layer thickness caused by redox reactions between Cr₂O₃ and Zr, the Cr₃Si coating still managed to delay the steam oxidation of the Zry-4 substrate for over 60 min at 1350°C. On the uncoated side, the thickness of the formed ZrO₂ reached 186 μm. For the Cr coating, after 30 min of oxidation in steam at 1350°C, a significantly liquid eutectic formed between the Cr coating and the Zry-4 substrate, compromising the coating's overall structural stability. These findings suggest that the Cr₃Si coatings hold promise for robustly protecting zirconium alloy cladding in scenarios involving design basis accidents (DBA) and beyond design basic accidents (BDBA).

Visible transparent radiative cooling coating for building thermal management and energy saving

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Keywords: Passive radiative cooling; Transparent coating; Energy saving

Passive radiative cooling technology can reduce the surface temperature without any energy input, thus has attracted significant attention recently. Incorporating passive radiative cooling into building energy saving can effectively mitigate the massive building energy consumption. Among all kinds of emerging radiative cooling materials, radiative cooling coating has been identified to possess superiority in both cooling capability and scalability. Herein, to deal with the window energy consumption in buildings, a superhydrophobic inorganic transparent coating with high visible transparency, near-infrared reflectivity, and min-infrared emissivity was proposed. The coating shows excellent super-hydrophobicity, wear-resistance, and self-cleaning property. The cooling ability is confirmed by outdoor measurement. It is believed that the transparent radiative cooling coating holds great potential for energy saving buildings and other facilities.