Topical Symposium on Sustainable Surface Engineering Room Town & Country B - Session TS1-1-MoM

Coatings for Batteries and Hydrogen Applications I

Moderators: Martin Welters, KCS Europe GmbH, Germany, **Chen-Hao Wang**, National Taiwan University of Science and Technology, Taiwan , **Fan-Bean Wu**, National United University, Taiwan

10:00am **TS1-1-MoM-1 Coating Innovations for Green Energy: Enabling Hydrogen Technologies***, **Mehmet Öte [oetemhm@schaeffler.com]**,* Schaeffler Technologies AG & Co. KG, Germany **INVITED**

In light of urgent climate challenges, the transition from fossil fuels to green energy sources necessitates significant advancements in hydrogen technologies. This keynote presentation will emphasize the crucial role of innovative coatings across all components of electrolyzers and fuel cells, including bipolar plate coatings, transport layer coatings, and catalyst-coated membranes. We will provide a comprehensive review of the evolving requirements for these coatings, assessing their impact on both performance and sustainability.

Key focus areas will include advancements in anti-corrosion and electrically conductive coatings designed to enhance the efficiency and lifespan of components within hydrogen systems. These innovations not only achieve exceptional electrical conductivity and corrosion resistance but also play a pivotal role in significantly reducing the CO2 footprint of critical components. Ultimately, this talk aims to contribute to the ongoing discourse in the energy sector, demonstrating how advanced materials and coatings can facilitate the widespread adoption of hydrogen as a clean energy carrier.

10:40am **TS1-1-MoM-3 Intermediate-Temperature Proton-Conducting Solid Oxide Fuel Cells and Electrolyzers for Clean Energy***, **Sheng-Wei Lee [swlee@ncu.edu.tw]**, Chung-Jen Tseng, Szu-Yuan Chen,* National Central University, Taiwan **INVITED**

The solid oxide cells (SOCs), which can operate in fuel cell or electrolyzer mode, is a promising technology to store electrical energy as chemical energy and to reconvert it into electricity upon demand. In recent years, extensive efforts have been devoted to developing proton-conducting SOCs (P-SOCs) that operate in the low-to-intermediate temperature range (400-800 ℃). Compared to the conventional oxygen ion-conducting SOCs (O-SOCs) that require high operating temperature (800- 1000 ℃), this scheme enables more reliable sealing, use of cheaper materials for interconnect, and a better control of electrode/electrolyte interactions, thus prolonging the operational lifetime of SOCs.

In this presentation, a variety of nanostructured electrode for P-SOCs is demonstrated via nano-engineering and have demonstrated their excellent cell performance. For example, we present a nanofiber-derived functional anode and cathode for proton-conducting SOFCs. The significantly lower polarization resistance elements indicate that the nano-fibrous electrode has superior catalytic activity for HOR and ORR. We also use PS nanospheres as pore former to fabricate an LSCF cathode with graded porosity, thus greatly improving the cell performance. In addition, we employ spin-coating technique and pulsed laser deposition (PLD) with doping strategy to fabricate thin-film electrolyte for P-SOCs. A bulk heterojunction GCCCO-BCZY layer with a domain width of ∼5 nm by PLD via spontaneous phase separation is demonstrated as an electrolyte/cathode interlayer, which effectively increases the interfacial area between the two distinct phases and facilitates proton transport across the interface. Finally, we also discuss the SOC performance when fed with a variety of fuels and in the electrolysis mode.

11:20am **TS1-1-MoM-5 Development of Anode Electrodes for Water Electrolysis by Electroplating***, Pei-Chi Lin, Chieh-Fu Huang, **Yong-Song Chen [imeysc@ccu.edu.tw]**,* National Chung Cheng University, Taiwan **INVITED**

Anion exchange membrane water electrolysis (AEMWE) has drawn much attention recently as a sustainable and cost-effective method for hydrogen production. Unlike proton exchange membrane water electrolysis, AEMWE employs non-precious metal as catalysts, which can significantly reduce material costs. However, it remains challenging to develop efficient and durable anode electrodes that can withstand alkaline environments while maintaining high performance in the oxygen evolution reaction (OER). In this study, stainless steel paper (SSP) is employed as the porous transport layer (PTL) of the anode in AEMWE. The effects of various surface modifications on SSP are investigated to assess their impact on electrochemical performance, including heat treatment, acid treatment, and electroplating.

Surface morphology, Brunauer–Emmett–Teller (BET) surface area, and current-voltage (I-V) characteristics are analyzed across treatments to evaluate their impact on catalytic activity. Results indicate that electroplating nickel (Ni) onto acid-treated SSP significantly enhances anode performance, achieving over a 10% increase in efficiency compared to untreated SSP. This enhancement is attributed to the increased specific surface area provided by acid treatment, combined with the catalytic benefits of Ni from electroplating. BET analysis supports that acid treatment creates a rough surface on the SSP fibers, thereby increasing active surface area. Additionally, I-V curves demonstrate that Ni-electroplated, acid-treated SSP exhibits lower overpotentials and higher current densities. This approach utilizes low-cost, commercially available stainless steel, supporting the potential for mass production and enhancing the economic feasibility of AEMWE in hydrogen production applications.

12:00pm **TS1-1-MoM-7 Development of Three-Dimensional Lithium Metal Composite Electrode with Lithiophilic ALD Coating***, Yu-Lun Cheng, **Chih-Liang Wang [wangcl@mx.nthu.edu.tw]**,* National Tsing Hua University, Taiwan

Lithium (Li) metal is widely regarded as an ideal anode material for lithium-ion batteries thanks to its high theoretical capacity (3860 mAh/g) and low electrochemical potential (-3.04 V vs. standard hydrogen electrode). However, practical use is limited by challenges such as lithium dendrite growth, volume expansion, and dead lithium, which degrade performance. This study addresses these issues by applying atomic layer deposition (ALD) of zinc oxide (ZnO) onto electrospun carbon nanofibers (CNFs) to create a high-performance, three-dimensional (3D) lithium metal composite anode. Polyacrylonitrile (PAN) was first electrospun to form the CNF framework. The lithiophilic properties of CNFs were systematically explored by adjusting the number of ALD ZnO cycles. The 3D lithium metal composite anodes were then produced by infusing molten lithium into the ZnO-coated CNFs. These composite electrodes showed excellent electrochemical performance, including low overpotential and extended cycle life in symmetric cell tests. In full-cell tests with $LiFePO_4$, the 3D Li composite anode delivered higher capacity than traditional Li metal foil. Overall, the combination of electrospinning and ALD techniques demonstrates substantial potential in creating 3D lithium metal composite electrodes, offering improved lithium diffusion, current distribution, battery stability, cycle life, and rate performance.

Topical Symposium on Sustainable Surface Engineering
Room Town & Country B - Session TS1-2-MoA

Coatings for Batteries and Hydrogen Applications II

Moderators: Chen-Hao Wang, National Taiwan University of Science and Technology, Taiwan , **Martin Welters**, KCS Europe GmbH, Germany, **Fan-Bean Wu**, National United University, Taiwan

1:40pm **TS1-2-MoA-1 The Effect of the Transition Metal Dopant on the Microstructure and Electrochemical Performance of Magnetron Sputtered Electrodes for Solid Oxide Fuel Cells Applications***, Justyna Kulczyk-Malecka [j.kulczyk-Malecka@mmu.ac.uk], Katharina Steier, David Shaw, Kleitos Panagi, Peter Kelly,* Manchester Metropolitan University, UK

The electrolytic energy conversion has become one of the main technologies considered to deliver actions on reducing CO_2 emissions in the energy, heavy-duty transportation and industrial processes sectors. The electrolytic cells (fuel cells and electrolysis cells) can be utilised in energy conversion, generation, and storage, which has been demonstrated at scale in many regions around the world already. Solid oxide cells are typically composed of porous ceramic matrix and Ni metal catalyst fuel electrodes, dense ceramic electrolytes, such as YSZ or GDC, and perovskite air electrodes. These cells operate at relatively high temperatures (typically 600-850°C) and, therefore do not require precious metal group catalysts to drive the reaction forward in both electrolysis (H_2 generation) and fuel cell (energy conversion) modes. Moreover, they are more versatile in terms of required fuel type allowing utilisation of hydrogen as well as alternative fuels, such as methanol, ammonia, or biogas.

In this work, thin (~3 µm) nanostructured cermet anodes consisting of YSZ-Ni and GDC-Ni were doped with transition metals to study their influence on coatings microstructure and electrochemical performance. The anodes were deposited onto commercial YSZ electrolyte support cells using oblique angle pulsed DC reactive magnetron sputtering. The coating microstructure was evaluated using FIB-SEM and TEM and focused on the triple-phase boundary evolution in relation to the amount of the added dopant (0-5 wt.%). The chemical composition of the coatings was assessed using EDX, XPS and XRD analysis. The polarization curves were obtained from SOFC single stack assemblies under hydrogen and air flows for anode and cathode, respectively, at operating temperatures of 850°C to evaluate the electrochemical performance of the deposited films.

2:00pm **TS1-2-MoA-2 Investigation of $Ba_{0.5}Ce_{0.3}Zr_{0.18}Y_{0.01}Yb_{0.01}O_{3-\delta}$ /$Y_{0.2}Ce_{0.8}O_{2-\delta}$ Composite Coatings for the Electrolyte of Solid Oxide Fuel Cell***, Yen-Yu Chen [yychen@mail.npust.edu.tw], Ke-Hsing Wang,* National Pingtung University of Science and Technology, Taiwan

Solid oxide fuel cells (SOFCs) are one of the potential power generation devices for the sources of renewable energy. In this study, the composite coatings consisted of $BaCe_{0.7}Zr_{0.12}Y_{0.1}Yb_{0.1}O_{3-\delta}$ (BCZYYb) and $Y_{0.2}Ce_{0.8}O_{2-\delta}$ (YDC) were developed by a colloidal coating process as the electrolyte for SOFC. Both of the powders of BCZYYb and YDC were synthesized by the solid-state reaction methods. The well dispersed suspensions after refined by the planetary ball method were spin coated on the porous NiO/$BaZr_{0.85}Y_{0.15}O_{3-\delta}$ (BZY) substrates, which were prepared by a die pressing method after pre-sintering at 1200^{o}C for 1 h. Several properties were analyzed including microstructures, crystallographic phases, and electrical performance. The BCZYYb/YDC composite coatings still showed duel-phases including perovskite-type BCZYYb and fluorite-type YDC after sintered at 1550oC for 24 h, The coating layer shows high density after sintered. And the thickness of the coating layers are around several µm. The composites show ionic conductive behaviors from the temperature between $500\sim800^{o}$C. The details will be reported in the presentation.

2:20pm **TS1-2-MoA-3 Unveiling the ORR Mechanism on Co Single-Atom Catalysts Using Operando Raman Spectroscopy with Catalyst-Coated Membrane (CCM) Methodology***, Sun-Tang Chang [suntang925@gmail.com], Yi-Qing Chu, Zih-Jhong Huang, Chen-Hao Wang,* National Taiwan University of Science and Technology, Taiwan

In this study, operando Raman spectroscopy was employed to investigate the mechanism of the oxygen reduction reaction (ORR) on a cobalt single-atom catalyst (Co-SAC). The Co-SAC was synthesized and utilized as a cathode catalyst for an alkaline anion exchange membrane fuel cell (AAEMFC). The results demonstrate excellent ORR activity, with an electron transfer number of 3.96 and J_{iming} is 5.5 $mAcm^{-2}$. X-ray absorption spectroscopy (XAS) revealed that the Co-SAC features a Co-N5 coordination structure, with cobalt in the +3 oxidation state. Furthermore, wavelet transform (WT) analysis confirmed the presence of isolated cobalt single atoms.

To minimize interference from the electrolyte during Raman laser measurements, the catalyst-coated membrane (CCM) method was adopted. This approach effectively prevents direct interaction between the laser and the electrolyte while ensuring efficient OH^- group transfer to the catalyst. Additionally, in the operando setup, electrochemical impedance spectroscopy (EIS) was integrated with Raman spectroscopy. This combination enabled a detailed observation of the ORR mechanism and the evolution of surface phenomena under different applied biases.

This study represents a significant breakthrough in unveiling the ORR mechanism, particularly for Co-based single-atom catalysts.

2:40pm **TS1-2-MoA-4 Study on Mo_xN Thin Films Deposited by HiPIMS and RF Sputtering with Heteroatom Doping for Hydrogen Evolution Reaction Catalysts***, Hung-I Wu [a8794191@gmail.com],* National Yunlin University of Science and Technology, Taiwan*; Ying-Hsiang Lin,* National United University, Taiwan*; Shih-Hung Lin,* National Yunlin University of Science and Technology, Taiwan*; Fan-Bean Wu, Chi-Yueh Chang,* National United University, Taiwan*; Thi Xuyen Nguyen, Chia-Ying Su, Ruei-Chi Lin, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan*; Wan-Yu Wu,* National United University, Taiwan

In recent years, materials such as transition metal oxides and nitrides have been popular in catalyst research. Compared to scarce noble metals, molybdenum-based materials not only have more abundant resources but also exhibit excellent activity[1], making them highly suitable to replace the costly noble metal catalysts (Ru, Ir, RuO_2, IrO_2). Molybdenum nitride (MoN) possesses outstanding corrosion resistance and electronic conductivity[2], allowing it to perform the hydrogen evolution reaction (HER) in acidic media. If different elements like Ti, Co, Ni, and V are doped into Mo_xN as a substrate, a synergistic effect is expected to further enhance HER performance. Additionally, when attaching catalysts to electrodes, one must consider the uniformity of surface coverage and adhesion on electrodes of various shapes. As is well known, sputtering offers advantages such as uniform coating, easy control of film thickness, and excellent adhesion. Therefore, using this method to prepare catalyst thin films on electrodes is the optimal choice.

In this study, we employed RF sputtering and High Power Impulse Magnetron Sputtering (HiPIMS) techniques to deposit Mo_xN thin films for comparison. Initially, we deposited Mo_xN thin films using HiPIMS and found in preliminary results that the HiPIMS-deposited Mo_xN thin films exhibited an overpotential of 415 mV at η=10 during hydrogen evolution reaction (HER) tests in 0.5M H_2SO_4. Energy-dispersive X-ray spectroscopy (EDS) analysis revealed that the Mo and N contents in the Mo_xN thin films were 60 at.% and 40 at.%, respectively. Grazing-incidence X-ray diffraction (GIXRD) results indicated that the thin films have a face-centered cubic (FCC) structure similar to Mo_3N_2. Building on these Mo_xN results, we will further explore the impact of varying the N/Mo ratio on HER performance. Additionally, we plan to attempt doping other elements into Mo_xN to observe the changes induced by doping.

3:00pm **TS1-2-MoA-5 Ternary FeCoNi / Graphene Composites as Electrocatalysts for Highly Efficient Hydrogen Evolution Reaction***, Yu Tsung Lin [asd881228@gmail.com], Jow Lay Huang, Sheng Chang Wang, Yu Min Shen,* National Cheng Kung University (NCKU), Taiwan

As a consequence of the depletion of fossil fuels, the escalating energy crisis has driven researchers to explore innovative energy. To address this problem, exploring hydrogen energy generation via water splitting emerges as a promising solution. This process involves the hydrogen evolution reaction (HER), a multi-electron transfer process necessitating catalysts to facilitate efficient rates. Despite noble metals have conventionally served this purpose due to their favorable Gibbs free energy, their prohibitive costs pose challenges for widespread adoption and commercialization. In response, our investigation focuses on HER within alkaline electrolytes, aiming to engineer alternative electrocatalysts that are both cost-effective and efficient.

Transition metals from the first row are active centers for the HER due to their 3d orbital, exhibiting excellent activity. Among them, nickel (Ni) and cobalt (Co) shows the most promising potential because the hydrogen adsorption energy of them approaches that of Pt. Furthermore, recent studies have indicated that the incorporation of third transition metals, such as iron (Fe), can further enhance the HER activity. This is attributed to the synergistic effect among the three metals. Additionally, it can be observed that a large number of studies use two-dimensional carbon materials as supports. Graphene, a highly conductive 2D material, serves as an excellent supporting matrix due to its high surface area, facilitating efficient electron transfer during HER. Consequently, we synthezised ternary FeCoNi-LDH/graphene composite by hydrothermal method and measured the HER performance in 1.0 M KOH electrolyte.We used X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and transmission electron microscope (TEM) to determine the crystal structure and morphology of the composite. The results demostrate that we successfully synthesized FeCoNi-LDH/graphene. In addition, Linear Sweep Voltammetry (LSV) were employed to confirm the HER performance. The overpotential and Tafel slope is -386.6 mV and 85.8 mV/dec, respectfully.

3:20pm **TS1-2-MoA-6 Ti-Cr-N Nanopyramid/Nitrogen-Doped Carbon Quantum Dot/Stainless Steel Mesh as a Flexible Supercapacitor Electrode***, **Rajesh Kumar [rgangwar1997@gmail.com]**, Bhanu Ranjan, Krishan Kumar, Satyam Shankhdhar, Davinder Kaur,* Indian Institute of Technology Roorkee, India

Nitrogen-doped carbon quantum dots (N-CQDs) incorporated into highly conductivetransition metal nitride offer enhanced electrochemical performance, delivering high energy density and outstanding electrochemical stability. The present study reports a high-performance supercapacitor electrode consisting of electrophoretic anchoredzero-dimensional N-CQDs with reactively co-sputtered titanium chromium nitride nanopyramids (Ti-Cr-N) thin film on flexible stainless-steel mesh (SSM) substrates. The nanopyramids of N-CQDs/Ti-Cr-N offer remarkable electrochemical performance through Li^+ storage, ascribed to the abundant electroactive sites and enhanced synergism between the high specific surface area of N-CQDs and higher conductivity of Ti-Cr-N.Subsequently, the N-CQDs/Ti-Cr-N/SSM electrode in 1M Li_2SO_4 aqueous electrolyte exhibits an excellent gravimetric capacitance of 393.8 $F.g^{-1}$ at a specific current density of 0.32 $A.g^{-1}$. Further, the N-CQDs/Ti-Cr-N/SSM heterostructure outperforms other multi-cationic-based supercapacitors with a maximum energy density of 41.41 $Wh.kg^{-1}$ and a superior power density of 7.0 $kW.kg^{-1}$. Impressive electrochemical stability of ~88.6% is retained by the heterostructure even after 5000 continuous charge-discharge cycles. Insights into charge-storage mechanisms highlight the dominance of surface-limited capacitive and pseudocapacitive kinetics, with fewer contributions from diffusion-controlled faradaic processes. Furthermore, an exemplary mechanical stability of ~99.98% over 1200 bending cycles demonstrates the N-CQDs/Ti-Cr-N/SSM heterojunction's excellent resilient structural strength, validating the present electrode potential for high-performance flexible supercapacitor application.

4:00pm **TS1-2-MoA-8 Effects of Nb Content on the Water Splitting Performance of FeNiMoWNb$_x$ High Entropy Coating Grown by Magnetron Sputtering***, **Naveen Karuppusamy [naveen10111@gmail.com]**,* Ming Chi University of Technology, Taiwan*; Bih-Show Lou,* Chang Gung University, Taoyuan City, Taiwan*; Jyh-Wei Lee,* Ming Chi University of Technology, Taiwan

Hydrogen fuel is an alternative green energy to neutralize the carbon emission and to fulfill the global energy demand. Electrochemical water splitting is a technique to produce hydrogen comprising of both oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), where OER is a bottleneck reaction in water splitting for efficient performance. Thus, it is necessary to prepare a suitable catalyst with an excellent water splitting performance. Though RuO_2 is a benchmark catalyst for OER performance, scarcity and cost of resources are limited to the use of RuO_2 in water splitting performance. Transition-metal based electrocatalyst already garners attention due to its excellent redox properties, earth abundant and cost-effective, which makes it suitable for alternative catalyst.

In this study, FeNiMoWNbx high entropy alloy (HEA) coatings with different Nb contents were fabricated on carbon cloth (CC) at high inclined angle using magnetron sputtering technique. The composition of Nb is altered with changing the RF power from 0 to 100 W. Chemical composition of FeNiMoWNbx was analyzed by the field emission electron probe microanalyzer (FE-EPMA). Phase analysis and crystallinity of FeNiMoWNbx were analyzed with glancing angle X-ray diffractometer (GA-XRD). Surface roughness and cross-section morphologies of FeNiMoWNbx films were examined using atomic force microscope (AFM) and field emission scanning electrochemical microscopy (FE-SEM). The OER performance of FeNiMoWNbx films was investigated with the polarization curve obtained in 1 M KOH and 1 M KOH + 3.5 wt.% NaCl aqueous solution. FeNiMoWNbx thin films exhibited a superior OER performance with low overpotential in 1 M KOH and 1 M KOH + 3.5 wt.% NaCl solution. The effects of Nb concentration in FeNiMoWNbx film and the sputtering inclined angle on the kinetics of OER performance was discussed. This works provides the strategy for the fabrication of cost effective FeNiMoWNbx HEA thin film catalyst for efficient water splitting performance.

4:20pm **TS1-2-MoA-9 Pseudocapacitive Storage in Molybdenum Oxynitride Nanostructures Reactively Sputtered on Stainless-Steel Mesh Towards an All-Solid-State Flexible Supercapacitor***, **Bhanu Ranjan [branjan@ph.iitr.ac.in]**, Davinder Kaur,* Indian Institute of Technology Roorkee, India

Exploiting pseudocapacitance in rationally engineered nanomaterials offers greater energy storage capacities at faster rates. The present research reports a high-performance Molybdenum Oxynitride (MoON) nanostructured material deposited directly over stainless-steel mesh (SSM) via reactive magnetron sputtering technique for flexible symmetric supercapacitor (FSSC) application. The MoON/SSM flexible electrode manifests remarkable Na^+-ion pseudocapacitive kinetics, delivering exceptional ~881.83 $F.g^{-1}$ capacitance, thanks to the synergistically coupled interfaces and junctions between nanostructures of Mo_2N, MoO_2, and MoO_3 co-existing phases, resulting in enhanced specific surface area, increased electroactive sites, improved ionic and electronic conductivity. Employing 3D Bode plots, b-value, and Dunn's analysis, a comprehensive insight into the charge-storage mechanism has been presented, revealing the superiority of surface-controlled capacitive and pseudocapacitive kinetics. Utilizing PVA-Na_2SO_4 gel electrolyte, the assembled all-solid-state FSSC (MoON/SSM||MoON/SSM) exhibits impressive cell capacitance of 30.7 $mF.cm^{-2}$ (438.59 $F.g^{-1}$) at 0.125 $mA.cm^{-2}$. Moreover, the FSSC device outputs superior energy density of 4.26 $\mu Wh.cm^{-2}$ (60.92 $Wh.kg^{-1}$) and high power density of 2.5 $mW.cm^{-2}$ (35.71 $kW.kg^{-1}$). The device manifests remarkable flexibility and excellent electrochemical cyclability of ~91.94% over 10,000 continuous charge-discharge cycles. These intriguing pseudocapacitive performances combined with lightweight, cost-effective, industry-feasible, and environmentally sustainable attributes make the present MoON-based FSSC a potential candidate for energy-storage applications in flexible electronics.

References:

1. Bhanu Ranjan and Davinder Kaur, Small, 20 (20), 2307723 (2024). https://doi.org/10.1002/smll.202307723

2. Bhanu Ranjan and Davinder Kaur, ACS Applied Materials & Interfaces, 16 (12), 14890-14901 (2024). https://doi.org/10.1021/acsami.4c00067
3. Bhanu Ranjan and Davinder Kaur, ACS Applied Energy Materials, 7 (10), 4513-4527(2024). https://doi.org/10.1021/acsaem.4c00563
4. Bhanu Ranjan and Davinder Kaur, Journal of Energy Storage, 71, 108122. (2023). https://doi.org/10.1016/j.est.2023.108122
5. Bhanu Ranjan, Gagan Kumar Sharma, and Davinder Kaur, Applied Surface Science, 588, 152925 (2022). https://doi.org/10.1016/j.apsusc.2022.152925
6. Bhanu Ranjan, Gagan Kumar Sharma, and Davinder Kaur, Applied Physics Letters, 118 (22), 223902 (2021). https://doi.org/10.1063/5.0048272

7. Bhanu Ranjan, Gagan Kumar Sharma, Gaurav Malik, Ashwani Kumar, and Davinder Kaur, Nanotechnology, 32 (45), 455402 (2021). https://doi.org/10.1088/1361-6528/ac1bdf

4:40pm **TS1-2-MoA-10 Applicability of MoS$_2$-Asic Heterostructure for Durable Supercapacitance and NO$_2$ Gas Sensing in Harsh Environment***, **Habeebur Rahman [h_rahman@ph.iitr.ac.in]**,* Indian Institute of Technology Roorkee (IIT Roorkee), India*; Gagan Kumar Sharma,* Indian Institute of Technology Roorkee, India*; Preetam Singh,* CSIR-National Physical Laboratory Delhi, India*; Davinder Kaur,* Indian Institute of Technology Roorkee, India

In the present work, the heterostructure of molybdenum disulfide (MoS_2)with amorphous silicon carbide (aSiC) on stainless steel (SS) and Si substrates was fabricated using a DC magnetron sputtering system. This unique heterostructure was examined for energy storage and NO_2 gas sensing applications suitable for harsh environmental conditions. The 2D MoS_2 nanostructured with dissolution resistive aSiC supercapacitor electrode delivers 1.5-fold enhancement in the gravimetric capacitance, a voltage window enlargement from 0.8V to 1.8 V, and an excellent stability of more than 4,000 charge-discharge cycles. Further, the high concentration

NO_2 gas sensing performance of the MoS_2-aSiC on Si substrate revealed the stable and recoverable response at high operating temperatures. Therefore, loading aSiC with 2D MoS_2 enables durable electrode material for energy storage and NO_2 gas sensing applications in adverse conditions. The as-fabricated heterostructure was systematically studied by various material and electrochemical characterizations.

5:00pm **TS1-2-MoA-11 One Step Fabrication of Highly Ordered Binder Free Vanadium Oxide Thin Film Cathode for Next Generation Micro Batteries***, **Ananya Bansal [ananya_b@ic.iitr.ac.in]**,* Indian Institute of technology Roorkee, India*; Ramesh Chandra,* Indian Institute of Technology Roorkee, India

The increasing demand for microelectronics has significantly driven the advancement of thin film energy storage devices, specifically batteries. Till now, a range of materials have been investigated for lithium-ion batteries, with vanadium oxide emerging as a promising material. Vanadium oxides are known for multiple oxidation-reduction states during electrochemical reaction, hence, can promote multiple diffusion of Lithium ions resulting in high energy and power density. In this work, binder-free Vanadium oxide (V_2O_5) has been synthesized by reactive DC magnetron sputtering on aluminium foil substrate. Vanadium target (99.99% pure) is bombarded with high-energy Ar^+ ions which dislodge atoms from the vanadium surface. These ejected atoms then react with oxygen ions to form highly pure V_2O_5 and deposit onto a substrate, forming a thin film. The deposited layers were analyzed for their structural and surface morphology using XRD and SEM techniques. Highly ordered brick like nanostructures were observed during SEM analysis. X-ray photoelectron spectroscopy measurements were carried out to understand the chemical bonding of the cathode. The surface of vanadium oxide obtained from this binder-free approach helps us to create a high-quality cathode-electrolyte interface with high wettability (33.3^o). Cyclic voltammetry (CV), galvanostatic charge-discharge (GCD) cycling, and electrochemical impedance measurements were used to investigate the capacity and cycling stability of the V_2O_5 cathode in 1 M lithium hexa-flouro-phosphate. As a result, it can be interpreted that this binder-free technology can be used to fabricate efficient lithium free cathode for new generation thin film batteries.

5:20pm **TS1-2-MoA-12 Research Coating Conductive Material on SiO_x@rGO Composite Materials as Anode Material in Lithium-Ion Batteries***, **Yi-Ling Chen [n56124155@gs.ncku.edu.tw]**,* National Cheng Kung University (NCKU), Taiwan

With the advancement of technology, lithium-ion batteries have emerged as a future energy storage technology with the gradual development of electric vehicles. Silicon-based materials, due to their high theoretical capacity, energy density (~4200mAh/g), and natural abundance, are considered as candidates for negative electrode materials in lithium-ion batteries.

In this study, our research team successfully prepared reduced graphene oxide (rGO) using the Hummer method and incorporated commercial SiO_x micron-sized powder to synthesize SiO_x@rGO composite material as an anode for lithium-ion batteries. The initial charge capacity was measured at 1487 mAh/g, with a discharge capacity of 1060 mAh/g, yielding an initial coulombic efficiency of 71%. After 40 cycles, the capacity retention remained at 91%. However, there are currently no theoretical studies addressing the lithiation process and lithium ion insertion/extraction mechanisms in SiOx materials.

Therefore, in our study, we not only explore the use of SiO_x@rGO composite material as an anode to improve the theoretical capacity and energy density of lithium-ion batteries but also aim to enhance the electrical conductivity and electrochemical performance of the battery. Conductive materials such as copper, gold, and platinum will be deposited on the prepared SiO_x@rGO anode material. These conductive coatings will provide additional electrons, creating a driving force for lithium ion diffusion into the anode material during discharge to achieve charge conservation. This process is expected to enhance the capacity and cycling stability of lithium-ion batteries. We will characterize the materials using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), and transmission electron microscopy (TEM). Furthermore, charge-discharge and cycling performance tests will be conducted on the lithium-ion batteries to investigate the effect of the conductive materials on their performance. Cyclic voltammetry will be employed to observe the electrochemical reactions during charge and discharge cycles.

This study conducts a theoretical analysis of SiO_x@rGO composite material as an anode for lithium-ion batteries by coating it with conductive materials, aiming to provide valuable reference data for both commercial and academic purposes.

Topical Symposium on Sustainable Surface Engineering
Room Town & Country C - Session TS3-TuA

Circular Strategies for Surface Engineering

Moderators: Marcus Hans, RWTH Aachen University, Germany, **Nina Schalk**, Montanuniversität Leoben, Austria

2:00pm **TS3-TuA-2 Scalable Solar-Thermal Synthesis of High-Yield Flake Graphite and Hydrogen**, ***Timothy S. Fisher [tsfisher@ucla.edu]***, University of California Los Angeles, USA **INVITED**

Current industrial processes for power, fuel, and commodity production are responsible for massive, ongoing CO_2 emissions that adversely affect the stability of Earth's climate with potentially disastrous consequences. Increased use of hydrogen as a fuel and chemical building block promises to reduce CO_2 emissions in critical sectors, but contemporary hydrogen production technologies also involve high greenhouse gas emissions. This talk considers a process in which concentrated radiation from a simulated solar source converts methane and similar hydrocarbons to high-value synthetic flake graphite and hydrogen gas. Methane flows within a photo-thermal reactor through the pores of a thin substrate irradiated by several thousand suns at the focal peak. The methane decomposes primarily into hydrogen while depositing highly graphitic carbon that grows conformally over ligaments in the porous substrate. The direct heating of the porous substrate serves to capture the solid carbon into a readily captured and useful form while maintaining active deposition site density with persistent self-catalytic activity. The talk will cover topics including solar irradiation profile modeling and measurements, chemical kinetics, gas-phase diagnostics, material characterization, product yields, and solar-to-chemical efficiency.

2:40pm **TS3-TuA-4 Developing Next Generation Sustainable Flexible Food Packaging Materials**, ***Peter Kelly [peter.kelly@mmu.ac.uk]***, Manchester Metropolitan University, UK; *Carolin Struller,* Bobst Manchester Ltd, UK; *Glen West,* Manchester Metropolitan University, UK; *Nick Copeland,* Bobst Manchester Ltd, UK; *Gwyneth Spence,* Manchester Metropolitan University, UK

Flexible food packaging materials are complex surface engineered products that must meet demanding quality criteria yet be produced at very high volume and low cost. Until recently, typical flexible packaging material might consist of an inner heat sealable polyethylene (PE) film, then combinations of adhesives to hold the laminated structure together, inks for printing product details, a topcoat, a barrier layer and finally an outer polymer film, such as polyethylene terephthalate (PET). The barrier layer provides extended shelf life to the food product by preventing moisture and oxygen ingress, which spoils the product over time. Barrier layers can be organic layers (e.g. polyvinylidene chloride (PVdC)) deposited by wet chemical techniques, aluminium foil layers or as in the case here, either aluminium or aluminium oxide ('AlOx') coatings deposited by thermal evaporation techniques. These coatings are deposited at very high rates (line speeds are up to 1000m/min) and over very large areas (up to 4.85m wide x 100km long rolls) in roll-to-roll vacuum systems. Average barrier layer thicknesses are 40-50nm for Al films and 8-15nm for AlOx layers.

As a consequence of the mixed materials used in conventional flexible packaging, most products cannot be recycled and go to landfill or are incinerated. The increasing demand for sustainable packaging products has led Bobst and other companies in the packaging value chain (ranging from raw material producers and convertors to brand owners and retailers) to develop new products that meet the criteria of 'recyclable, reusable or compostable'.

This paper describes progress towards mono-material polyolefin-based solutions for fully recyclable polymeric packaging and paper-based products, which are suitable to be processed in the existing paper recycling stream. In both cases, the Bobst oneBARRIER PrimeCycle PE product and the FibreCycle paper-based product provide high barrier performance and meet international recyclable standards. In addition to the development of these products, extensive life cycle analyses (LCAs) have been undertaken on each stage of the manufacturing process to allow accurate and comparable assessments to be made of the environmental impact and sustainability of the product.

3:00pm **TS3-TuA-5 PFAS Free Anti-Stick Coatings for Superior Electrosurgical Performance**, ***Noora Manninen [noora.manninen@oerlikon.com]***, Oerlikon Surface Solutions, Liechtenstein; *Sanna Tervakangas,* Oerlikon Surface Solutions, Finland; *Klaus Boebel,* Oerlikon Surface Solutions, Liechtenstein

Per- and polyfluoroalkyl substances (PFAS) are a large class of thousands of synthetic chemicals currently used in a wide variety of products (e.g. food packaging, cookware, textiles, medical devices, semiconductor components, batteries, among many others). PFAS contain carbon-fluorine bonds, which are one of the strongest chemical bonds in organic chemistry, meaning they are very attractive in different consumer products as they can resist to degradation. Nevertheless, the degradation resistance also persists once they are disposed. Currently PFAS are increasingly detected as environmental pollutants and some are linked to negative effects on human health, which has led to the current restriction proposal by European Chemical Agency (ECHA).

The restriction on use of PFAS will require the development of new solutions, which must fulfill health and environmental requirements. Medical devices are one of the main fields of use of PFAS, where PTFE based coatings are widely used, among many applications as anti-stick coatings in electrosurgical devices. In the current work existing coating solutions already in use for medical market and approved by regulatory authorities (e.g. FDA) have been tested (e.g. TiN, CrN, DLC, Parylene C) and compared to new coating solutions under research and development. The main goal is to obtain coatings with good anti-stick performance, which ideally can be re-used as multiple use devices, opposed to concept of single-use devices, which are discarded after each surgery generating large amount of waste. In order to fulfill the requirements for multiple use devices the coatings must stand multiple cleaning and sterilization cycles meaning they must have good corrosion properties as well as good abrasion resistance.

In the present study the coatings are characterized regarding their surface energy given that this surface property is connected with anti-sticking properties, and also functional tests are performed in a test set-up consisting of an electrosurgical unit (ESU) where coatings anti-stick performance is tested against pork liver. Additionally, the corrosion and abrasion resistance of the coatings are evaluated under autoclave and alkaline cleaning conditions and under abrasive cleaning test condition in order to resemble the lifecycle of multiple-use electrosurgical devices.

4:00pm **TS3-TuA-8 Design of Defect Structure in an Epitaxial VN Bilayer Film by Tailoring Nitrogen Concentration and Interfacial Strain**, ***Marcus Hans [hans@mch.rwth-aachen.de]***, *Damian Holzapfel,* RWTH Aachen University, Germany; *Zhuo Chen,* Erich Schmid Institute of Materials Science, Austria; *Soheil Karimi Aghda, Michal Fečik,* RWTH Aachen University, Germany; *Daniel Primetzhofer,* Uppsala University, Sweden; *Zaoli Zhang,* Erich Schmid Institute of Materials Science, Austria; *Jochen Schneider,* RWTH Aachen University, Germany

A $V_{0.48}N_{0.52}/V_{0.54}N_{0.46}(001)$ bilayer has been grown epitaxially on MgO(001) by reactive high power pulsed magnetron sputtering at a temperature of 400 °C in an industrial-scale deposition system. Based on ion beam analysis, atom probe tomography, X-ray diffraction, high-resolution transmission electron microscopy data as well as *ab initio* calculations, it is demonstrated that the defect structure is affected by the nitrogen concentration and interfacial strain. Strain at the $MgO/V_{0.48}N_{0.52}$ interface is caused by a lattice parameter mismatch of ~2.3% as predicted by density functional theory. The experimentally determined lattice parameter difference is only ~1.3%, hence, the interfacial strain is partially relaxed by formation of misfit dislocations. Consequently, the dislocation density in $V_{0.48}N_{0.52}$ is reduced from ~0.20 nm^{-2} to ~0.10 nm^{-2} within a distance of ~10 nm from the $MgO/V_{0.48}N_{0.52}$ interface. The dislocation density is reduced to ~0.04 nm^{-2} at the $V_{0.48}N_{0.52}/V_{0.54}N_{0.46}$ interface and < 0.01 nm^{-2} in the $V_{0.54}N_{0.46}$ layer within a distance of ~35 nm from the interface due to strain relaxation. Based on the here presented findings, it is evident that control of the nitrogen concentration and interfacial strain allows for the design of layered architectures with a variation in dislocation density by two orders of magnitude.

4:20pm **TS3-TuA-9 Low Friction Sputtering Coatings, a Sustainable Option to Reduce Energy Consumption and Harmful Lubricant Usage**, ***Albano Cavaleiro [albano.cavaleiro@dem.uc.pt]***, University of Coimbra, Portugal **INVITED**

From the more than 500 EJ of the World energy consumption, 20% regards losses due to friction in mechanical contacts[1]. The obvious solution to decrease friction, the use of liquid lubricants, rises increasing concerns to the environment due to their harmful impact. Therefore, alternatives that can either provide a decrease of the friction in solid contacts or a reduction/removal of the usage of liquid lubrication, will have a significant and positive impact in both saving of energy and protection of the environment.

Low friction coatings were intensively developed in last decades as solutions for applications where liquid lubrication is restricted (space, food industry, vacuum,...) as well as a tool for removing either the usage of liquid lubrication or the extremely harmful additives of lubricant oils. As friction is a surface phenomenon, the main advantage of low friction coatings is that they can be applied over the currently used materials for mechanical applications without significant changes of the components and devices.

In this talk several examples related with the development and application of sputtering coatings in mechanical applications (moulding, cutting, forming,...) with main objectives of decreasing friction and reducing the harmful impact of oil lubricants, will be presented. The sliding mechanisms, in particular the understanding of tribolayers formation, will be addressed and connected to different concepts which were in the basis of the coatings development.

[1] K. Holmberg, A. Erdemir, Influence of tribology on global energy consumption, costs and emissions, Friction 5 (2017) 263–284

Topical Symposium on Sustainable Surface Engineering
Room Palm 5-6 - Session TS2-WeA

(Photo)electrocatalysis and Solar/Thermal Conversion

Moderators: Atasi Dan, National Institute of Standards and Technology (NIST), USA, **Arnaud Le Febvrier**, Uppsala University, Sweden, **Carlos Tavares**, University of Minho, Portugal

2:00pm **TS2-WeA-1 Flexible Thermoelectrics: Transforming Wearables, Space Exploration, and IoT***, André Pereira [ampereira@fc.up.pt],* University of Porto, Portugal **INVITED**

Flexible thermoelectric (TE) materials are at the forefront of advancing wearable electronics, space exploration, and the Internet of Things (IoT), offering a sustainable and efficient means of converting thermal gradients into electrical energy. Recent research has explored innovative designs and materials to overcome challenges in flexibility, efficiency, and scalability. A pivotal development is the radial flexible thermoelectric device powered by high-power laser beams, showcasing photo-thermoelectric conversion for wireless energy transfer. This approach provides a transformative solution for applications in space exploration, particularly for powering CubeSats and remote sensing systems.

Advances in hybrid thermoelectric materials have also driven significant progress. Nanostructured Bi_2Te_3 composites, integrated with polymer matrices like PVA, have demonstrated enhanced thermoelectric performance and printability. Devices fabricated with these materials achieve excellent mechanical flexibility and are well-suited for low-power wearable devices and printed electronics. The optimization of hybrid materials and ink formulations has enabled the realization of scalable, printable thermoelectric generators (TEGs) with customizable geometries.

Furthermore, the development of functional thermoelectric inks has opened avenues for high-throughput manufacturing of flexible µ-TEGs. These devices exhibit improved thermoelectric properties, mechanical stability, and adaptability to various substrates, ensuring seamless integration into IoT sensor networks and wearable platforms. The interplay of material innovations, device architecture, and advanced manufacturing techniques underscores the potential of flexible thermoelectrics in addressing global energy challenges while enabling novel functionalities in emerging technologies.

This work highlights the role of multidisciplinary approaches in transforming the capabilities of thermoelectric devices, paving the way for their adoption in dynamic environments and applications demanding autonomy and efficiency.

Acknowledge:

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References:

M. Almeida “Touch Empowerment: Sistema termoelétrico e-Tattoo autossustentável para mapeamento de temperatura” (2024) – Advanced Science

Printed Flexible µ-Thermoelectric Device Based on Hybrid Bi2Te3/PVA Composites

AL Pires,et al. ACS applied materials & interfaces 11 (9), 8969-8981

A Photo-Thermoelectric Twist to Wireless Energy Transfer: Radial Flexible Thermoelectric Device Powered by a High-Power Laser Beam

2:40pm **TS2-WeA-3 Alloy/Phosphate Heterostructure as High-Performance Hydrogen Evolution Reaction Electrocatalyst***, **Yung Hsun Yen [N56124210@gs.ncku.edu.tw]**,* National Cheng Kung University (NCKU), Taiwan*; Thi Xuyen Nguyen,* National Cheng Kung University (NCKU), Taiwan*; Jyh Ming Ting,* National Cheng Kung University (NCKU), Taiwan

With the rising demand for sustainable energy, the development of efficient electrocatalysts for the hydrogen evolution reaction (HER) has become increasingly important. Also, achieving cost-effective water electrolysis in industrial scale is crucial for large-scale green hydrogen production. In this study, we have investigated metal alloy/phosphate heterostructure HER electrocatalysts. Alloy is first synthesized using a two-step hydrothermal process, followed by thermal annealing. Phosphate is then electro-deposited on the surface of as-prepared alloy. The obtained catalyst demonstrates excellent catalytic activity toward HER with a low overpotential of 28.4 mV at 10 mA cm^{-2} and small Tafel slope of 42.1 mV dec^{-1}. Under a high current density of 500 mA cm^{-2}, the catalyst requires an only ultra-low overpotential of 186.3 mV.Stability tests using AEMWE having the heterostructure OER electrocatalyst are performed under 1 M KOH electrolyte and 1 M KOH + 0.3 M NaCl electrolytes.After 1000-h of test at 500 mA cm^{-2}, negligible voltage drops are demonstrated under both electrolyte conditions. The excellent HER performance and cost-effective of the synthesized catalyst is highly desirable for real water splitting for sustainable hydrogen production.

3:00pm **TS2-WeA-4 Ni-Co Based Catalysts for the Upcycling of Polyethylene Terephthalate***, **Ruei Chi Lin [a0979116476@gmail.com]**,* National Cheng Kung University (NCKU), Taiwan*; Thi Xuyen Nguyen,* National Cheng Kung University (NCKU), Taiwan*; Jyh Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Plastic waste management represents a critical environmental issue. Electrochemical upcycling of polyethylene terephthalate PET waste into high-value chemicals has received great attention recently. However, the development of highly active and selective catalysts remains challenging. In this study, we have developed a noble metal-free Ni–Co based electrocatalyst, synthesized via a hydrothermal method, for ethylene glycol oxidation reaction (EGOR). The EG is derived from PET. With its high surface area and tunable electronic structure, the obtained catalyst exhibits an excellent potentials of 1.25 V and 1.31 V at current densities of 10 mA cm$^{−2}$ and 100 mA cm$^{−2}$, respectively. PET is effectively transformed into potassium terephthalate with excellent Faradaic efficiency and selectivity under high current density.Meanwhile, zero-gap membrane electrode assembly closed-loop flow reactor has been used to achieve outstanding stability of PET upcycling in PET hydrolysis at 100 mA cm^{-2}. This work highlights the excellent potential for electro-reforming PET plastic waste into valuable chemicals with simultaneous reduced-cost hydrogen production.

3:20pm **TS2-WeA-5 Single Atom Ag Bonding between PF3T nanocluster and TiO_2 leads the Ultra-stable Visible-Light-Driven Photocatalytic H_2 Production***, **Tsan-Yao Chen [chencaeser@gmail.com]**, Fan-Gang Tseng,* National Tsing Hua University, Taiwan*; Jyh-Pin Chou,* National Taiwan University, Taiwan

Atomic Ag cluster bonding is utilized to enhance the interface between PF3T nanoclusters and TiO2 nanoparticles. At an optimized Ag loading of 0.5 wt% (Ag/TiO2), the Ag atoms are uniformly dispersed on the TiO2 surface, generating a high density of intermediate states within the bandgap. This forms an efficient electron channel between the terthiophene groups of PF3T and TiO2 in the hybrid composite (denoted as T@Ag05-P). The enhanced interface broadens the photon absorption bandwidth and facilitates core-hole splitting by enabling photon-excited electrons (from excitons in PF3T) to inject into the conduction band (CB) of TiO2. These features enable a remarkable H2 production efficiency of 16,580 µmol h$^{−1}$ g$^{−1}$ and exceptional photocatalytic stability, with no degradation observed under visible light exposure for 96 hours. Compared to the hybrid material without Ag bonding (TiO2@PF3T), the H2 production yield and stability improve by 4.1-fold and 18.2-fold, respectively, representing the best performance among similar materials with comparable component combinations and interfacial reinforcement strategies. This innovative bonding approach opens new opportunities for advancing photocatalytic hydrogen production technologies.

3:40pm **TS2-WeA-6 Transition Metal-Based Electrocatalysts for Sustainable Oxygen Reactions in Green Energy Applications***, **Emma Björk [emma.bjork@liu.se]**,* Linköping University, IFM, Sweden **INVITED**

Water splitting and recombination are pivotal processes in the transition toward green, renewable, and fossil-free energy production. These reactions are limited by the kinetics of the oxygen reactions—the Oxygen Evolution Reaction (OER) and the Oxygen Reduction Reaction (ORR)—which creates a significant demand for efficient electrocatalysts. Efforts are focused on developing abundant, cost-effective alternatives to the noble metal catalysts currently in use. In this presentation, the possibility to use transition metal oxides, e.g. Co, Ni, and Mn oxides, as oxygen catalysts will be discussed.

The first part will cover multicomponent films, e.g. CoCrFeNi and MnCrFeNi, as catalytically active, corrosion-resistant coatings. The films were synthesized via magnetron sputtering and subsequently subjected to electrochemical activation through anodization, enhancing their catalytic activity towards both ORR and OER. Anodization also altered the ORR mechanism in CoCrFeNi and MnCrFeNi films, shifting it from a (2+1) electron pathway in as-deposited films to either a 4- or 2-electron pathway in anodized films. These changes are attributed to modifications in active sites and film structure. Substituting Co with Mn slightly improved OER performance but did not affect the ORR activity significantly.

The films also demonstrated excellent corrosion resistance in alkaline and neutral chloride environments, attributed to the formation of a protective oxide layer. The corrosion performance was influenced by film composition and structure, particularly grain size. For example, lattice distortion in CoCrFeNi enhanced resistance in NaCl, while smaller grain sizes improved the corrosion resistance in KOH.

The second part of the talk focuses on increasing catalytic activity of transition metal oxides by introducing nanoporosity to enhance the number of active sites. Nanoporous materials, which often have specific surface areas exceeding 100 m^2/g, were synthesized via hydrothermal treatment methods to create nanoporous MOx (M = Cr, Fe, Co, Ni, Ce) and $NiCo_2O_4$ oxygen electrocatalysts. Optimizing pore size in nanoporous NiO revealed a critical balance between the number of active sites and the diffusion of reactants and products. NiO with a pore size of 3.3 nm achieved the lowest overpotential (335 mV at 10 mA/cm^2), outperforming a commercial Ir/C catalyst under similar conditions.

The different ORR pathways on the various catalysts enable product selectivity, and we have designed electrochemical cells for an oxygen pump, hydroxyl radical generation, and H2O2 production using nanoporous transition metal oxides, air, water, and KOH.

4:20pm **TS2-WeA-8 Bi-Based Photocatalysts Obtained by Reactive Sputtering for the CO_2 Photoreduction – from Thin Films and Composites to Nanoparticles***, **Angélique Bousquet [angelique.bousquet@uca.fr]**, Sara Ibrahim, Jean-Michel Andanson, Pierre Bonnet,* Institut de Chimie de Clermont-Ferrand, France*; Mireille Richard-Plouet,* Institut des Matériaux, France*; Maryline Le Granvalet,* Institut des Matériaux de Nantes, France*; Sébastien Roth, Audrey Bonduelle,* Institut Français du Pétrole, Energies Nouvelles, France

To reduce the CO_2 emission into atmosphere is a major issue to mitigate the current climate change. Moreover, be able to photo-convert CO_2 into more valuable species and form clean solar fuels and molecules would be a step forward to the industry decarbonation. Among the photocatalysts investigated to photoreduce CO_2, Bi-based materials have demonstrated their interest to selectively form CO, a molecular building block which can further be used to obtain methanol, acetic acid, aldehyde and even fuels...

In this study, we investigated the deposition of Bismuth oxyfluoride thin films by reactive radiofrequency magnetron sputtering of a pure Bi target in $Ar/O_2/CF_4$ atmosphere. We demonstrated, that it is possible to obtain coatings of various crystallized compounds ($Bi_7O_5F_{11}$, $BiO_{0.5}F_2$, BiF_3...) depending on the injected flow rates of O_2 and CF_4 reactive gases. More interesting, is the possibility to form composites of these compounds with a controlled content of metallic Bismuth nanodomains by reducing the reactive gas flow rates. Hence, we obtained in one step heterojonctions that presents enhanced photocatalytic activities thanks to potential plasmonic effect. The composition, structure and morphology of these coatings were studied by XRD, Raman spectroscopy, XPS, TEM and SEM. Their optical properties, especially their band gap, were determined from UV-visible spectroscopy and ellipsometry. Experiments of photodegration of pollutants into water shows that an optimum of metallic content has to be found to enhance the photocatalytic properties of the Bi-based materials[1]. The CO_2 photoconversion measurements, perfomed at IFPEN, on these materials demonstrate a photon conversion efficiency close to the one of TiO_2 P25 from Degussa, but with a high selectivity to form CO (= 90% and 10% of H_2).

To go further, we now working on nanostructuration of these materials in order to increase the contact surface with CO_2 gas using an original method: the reactive sputtering onto liquid. If this technique was already investigated to form dispersion of metallic nanoparticles into liquid, we suceeded for the first time to use it in reactive mode to obtain dispersion of sperical, well-crystallized oxyfluoride nanoparticles with a mean size ranging from 6 to 8 nm and presenting a photocatalytic response[2]. These particules may be dispersed on porous support paving the way of high surface specific aera system for CO_2 photoreduction.

[1] S. Ibrahim, et al., 2023, hal-04037069v1.

[2] S. Ibrahim, et al., Nanoscale, 15, 2023, 5499 - 5509

4:40pm **TS2-WeA-9 Effect of Crystallographic Texture on Dealloying Kinetics and Nanoporous Gold Thin Film Composition***, Ezgi Hatipoğlu,* Max-Planck Institut für Nachhaltige Materialien, Germany*; Ayman A. El-Zoka,* Imperial College London, UK*; Jochen Schneider,* Materials Chemistry, RWTH Aachen, Germany*; Baptiste Gault, **Aparna Saksena [a.saksena@mpie.de]**,* Max-Planck Institut für Nachhaltige Materialien, Germany

With rising concerns regarding climate change, the demand for cleaner and sustainable fuels is increasing. Hydrogen is the most popular candidate for clean energy for a carbon-neutral economy. Hydrogen production via water splitting reaction is a promising route where catalysts play a vital role in improving the energy conversion efficiency of the reaction. Nanoporous metals offer an important platform for tailoring composition and surface-to-volume ratio, both aspects critical for applications in catalysis. Here, AgAu films were deposited at 400°C either (111)-textured or untextured. Upon chemical dealloying to form the nanoporous structure, atom probe tomography reveals that the textured film retains a higher Ag concentration within the nanoligaments, whereas the untextured film already exhibits coarsening , indicating a faster reaction kinetics, and a lower Ag content. Our study highlights the potential of microstructure engineering in tailoring the properties of nanoporous metals for possible future catalytic and electrochemical applications.

Topical Symposium on Sustainable Surface Engineering Room Golden State Ballroom - Session TS1-ThP

Coatings for Batteries and Hydrogen Applications Poster Session

TS1-ThP-1 Room Temperature DC Sputtered V_2O_5-Based Flexible Robust and Transparent Electrode Over Polymeric PVA Substrate for Green Supercapacitor Applications*, Habeebur Rahman [h_rahman@ph.iitr.ac.in]*, *Davinder Kaur,* Indian Institute of Technology Roorkee, India

This work presents a flexible, robust, and transparent electrode for green supercapacitor device. For biodegradability, a polymeric polyvinyl alcohol (PVA) substrate was utilized for the supercapacitor electrode development. To ensure a robust electrical connection, partially embedded copper contact was made during the substrate development. The vanadium pentoxide active layer was sputter coated at room temperature for the supercapacitor transparent electrode formation. In particular, the active element was fabricated in two different layers possessing an interface in between that assisted in the current collection. The sputtered components were systematically studied using various materials characterization tools. The two similar electrodes were then assembled with an aqueous Na_2SO_4 electrolyte-soaked glassy fiber separator to form the supercapacitor device. The two electrode mode electrochemical measurements demonstrated a wide 1.3 V voltage window with a remarkable 178.7 F/g specific capacitance at 10 mV/s scan rate. It delivered 9.6 kW/kg power density at 3.5 Wh/kg energy density. It retains the 82 %, and 67.3 % capacitance after 10,000, and 18,000 charging-discharging cycles respectively. Further, the device exhibited negligible performance loss upon bending, twisting, and stretching and showed excellent stability with device-to-device variation. In addition, the biodegradability of the electrode was tested in water and moist soil, which illustrated quick degradation. The transparency of the electrode was determined by UV Vis spectroscopy that demonstrated 70 % transmittance in the visible region. Therefore, the biodegradable PVA substrate, environment-friendly Na^+ ion charge storage, and non-toxic V_2O_5 active layer combined together to procure a green energy storage device. The excellent mechanical flexibility of the device and the transparent nature of the electrode make it suitable for modern-day advanced energy storage technology.

TS1-ThP-2 Y-doped $Li_7La_3Zr_2O_{12}$(Y-LLZO) Based all Solid-State Lithium Ion Battery Prepared by Colloidal Coating Processes*, Yen-Yu Chen [yychen@mail.npust.edu.tw]*, *Guang-Yi Yao,* National Pingtung University of Science and Technology, Taiwan

All solid-state lithium ion batteries (ASSLIBs) were widely investigated due to safety issue and higher electrical performance. In this study, Y-doped $Li_7La_3Zr_2O_{12}$ (Y-LLZO)-based solid electrolyte coatings on the $LiCoO_2$ (LCO)-based cathode substrate with C/Si anode printed on the coatings were prepared. The Y-LLZO powders were synthesized by a solid-state reaction method. Several properties were analyzed including microstructures by scanning electron microscopy (SEM) and transmission electron microscopy, crystal phases by the X-ray diffraction (XRD) method, electrical performance by electrochemical impedance spectroscopy (EIS) and battery testing system. The Y-LLZO coatings after sintered at 1100°C for 12 h show highly dense configuration on the LCO-based cathode substrate. The thicknesses of the coating layers are around several to ten more micrometers. Only a few of pores can be found in the coating layers. The crystal phases after sintering were including the major LLZO garnet and a rare of $La_2Zr_2O_7$ phases. The interface between Y-LLZO and LCO grains shows slightly inter-diffusion behavior. The electrical conductivity of Y-LLZO is around 10^{-4}~10^{-5} $S{\cdot}cm^{-1}$. The more details will be reported in the presentation.

TS1-ThP-3 MXene Based Thin Film Nonstructural Composite for Oxygen Evolution Electrocatalysis*, Md Zaved Hossain Khan [zaved.khan@just.edu.bd]*, *Romzan Ali,* Jashore University, Independent Road, Jashore, Bangladesh

There is a continuous high demand for an effective electrocatalytic-oxygen evolution reaction (OER) to mitigate energy crises by offering renewable energy sources. Metal oxide and metal carbide are well regarded electrocatalysts for water splitting; however, they produce sluggish reaction kinetics and further require higher energy to launch OER reaction. The transitional metal carbide MXene coupled with earth abundant metal oxide show good catalytic performance overcoming potential barrier by enhancing reaction kinetics. Therefore, MXene ($Ti_3C_2T_x$) coupled earth-abundant metal oxide nanocomposite ($Zn_{0.92}Cu_{0.04}Ni_{0.02}O_2$) based electrocatalyst for OER is presented in this work for the first time. $Ti_3C_2T_x$ enhances electroconductivity, offers large surface area, increases the number of active sides of the electrocatalyst and enhances the electrocatalytic performances. A simple hydrothermal method was used for the fabrication of the electrocatalyst $Zn_{0.92}Cu_{0.04}Ni_{0.02}O_2$@MXene. The proposed electrocatalyst exhibits an extremely low overpotential of 169.5 mV at $10mAcm^{-2}$ and long-term stability (higher than 10 hours) in an acidic condition in 1M H_2SO_4 solution. This work demonstrates a facile and an effective strategy to boost up the electrocatalytic performance of OER in an acidic medium aiming for the design of efficient and cost effective electrocatalyst.

TS1-ThP-4 Pseudocapacitive Kinetics in Synergistically Coupled MoS_2-Mo_2N Nanowires with Enhanced Interfaces towards All-Solid-State Flexible Supercapacitors*, Bhanu Ranjan [branjan@ph.iitr.ac.in]*, *Davinder Kaur,* Indian Institute of Technology Roorkee, India

Pseudocapacitive kinetics in rationally engineered nanostructures can deliver higher energy and power densities simultaneously. The present report reveals a high-performance all-solid-state Flexible symmetric supercapacitor (FSSC) based on MoS_2-Mo_2N nanowires deposited directly on stainless-steel mesh (MoS_2-Mo_2N/SSM) employing Direct current (DC) Reactive Magnetron Co-sputtering technology. The abundance of synergistically coupled interfaces and junctions between MoS_2 nanosheets and Mo_2N nanostructures across the nanocompositeresults in greater porosity, increased ionic conductivity, and superior electrical conductivity. Consequently, the FSSC device utilizing Polyvinyl alcohol-sodium sulfate (PVA-Na_2SO_4) hydrogel electrolyte renders an outstanding cell capacitance of 252.09 $F.g^{-1}$ (44.12 $mF.cm^{-2}$) at 0.25 $mA.cm^{-2}$ and high rate performance within a wide 1.3 V window. Dunn'sand *b*-value analysis reveals significant energy storage by surface-controlled capacitive and pseudocapacitive mechanisms. Remarkably, the symmetric device boosts tremendous energy density ~10.36 $\mu Wh.cm^{-2}$(59.17 $Wh.kg^{-1}$), superb power density ~6.5 $mW.cm^{-2}$ (37.14 $kW.kg^{-1}$), ultrastable long cyclability (~93.7% after 10,000 Galvanostatic charge-discharge (GCD) cycles) and impressive mechanical flexibility at 60°, 90°, and 120° bending angles.

References:

1. Bhanu Ranjan and Davinder Kaur, Small, 20 (20), 2307723 (2024). https://doi.org/10.1002/smll.202307723
2. Bhanu Ranjan and Davinder Kaur, ACS Applied Materials & Interfaces, 16 (12), 14890-14901 (2024). https://doi.org/10.1021/acsami.4c00067
3. Bhanu Ranjan and Davinder Kaur, ACS Applied Energy Materials, 7 (10), 4513-4527 (2024).https://doi.org/10.1021/acsaem.4c00563
4. Bhanu Ranjan and Davinder Kaur, Journal of Energy Storage, 71, 108122. (2023). https://doi.org/10.1016/j.est.2023.108122
5. Bhanu Ranjan, Gagan Kumar Sharma, and Davinder Kaur, Applied Surface Science, 588, 152925 (2022). https://doi.org/10.1016/j.apsusc.2022.152925
6. Bhanu Ranjan, Gagan Kumar Sharma, and Davinder Kaur, Applied Physics Letters, 118 (22), 223902 (2021).https://doi.org/10.1063/5.0048272
7. Bhanu Ranjan, Gagan Kumar Sharma, Gaurav Malik, Ashwani Kumar, and Davinder Kaur, Nanotechnology, 32 (45), 455402 (2021). https://doi.org/10.1088/1361-6528/ac1bdf

TS1-ThP-5 PVD-Coated Interconnects for Solid Oxide Electrolysers*, Giuseppe Sanzone [giuseppe.sanzone@teercoatings.co.uk]*, Teer Coatings Ltd, UK*; Kun Zhang,* University of Birmingham, UK*; Susan Field, Hailin Sun,* Teer Coatings Ltd, UK*; Jangwoo Seo, Hyo Ki Hwang, In-sung Lee,* E&KOA Co., Republic of Korea*; Parnia Navabpour,* Teer Coatings Ltd, UK

Achieving net-zero emissions by 2050 continues to be a significant challenge for the global energy sector. Hydrogen, and specifically green hydrogen can play a key role in decarbonisation, as it has the potential to be used as fuel for power and transportation. Green hydrogen can be produced in several ways using renewable energy sources like solar, wind or nuclear, through high- and low-temperature electrolysis, various thermochemical and photochemical processes. Water electrolysis is the most effective technique which is capturing the market's attention.

Amongst the electrolyser technologies, solid oxide electrolysers (SOE) are the most energy efficient. However, there are challenges related to their performance, lifetime, durability and cost, along with the scale-up from kW to MW level. The interconnect plays an important role as a current collector and a physical barrier that separates the electrodes between cells. It has to meet technical requirements such as matching thermal expansion coefficient to other (ceramic) layers, high thermal and electrical conductivities, formation of a dense low-resistive oxide layer in redox atmospheres, and high thermomechanical strength at elevated temperatures (600 to 900 °C). The metallic interconnects employed in the SOC stack operated usually suffer high temperature corrosion and Cr-evaporation in the steam-rich environment at high temperature, leading to material failure of interconnects and degradation electrolysis stack. There is a need to control the chromium (VI) diffusion from the metallic interconnects and its poisoning of the air electrode to achieve increased electrolyser durability and performance.

This work presents conducting, protective spinel oxide coatings deposited by PVD method in order to reduce chromium evaporation from the interconnects. These coatings benefit from a dense structure as well as scalability, allowing high performance and making them suitable for commercialisation. The effect of coating thickness and composition on high temperature stability and chromium evaporation rate from ferritic stainless steel has been investigated.

TS1-ThP-6 Porous $BiVO_4$ Thin Films Deposited by Radiofrequency Co-Sputtering as Photoanode for H_2 Production by Water Splitting, *Mathias Goutte,* ***Angélique Bousquet [angelique.bousquet@uca.fr]****, Eric Tomasella,* Institut de Chimie de Clermont-Ferrand, France*; Guillaume Monier,* Institut Pascal, France*; Thierry Sauvage,* CEMHTI, France

H_2 is consider as a potential new fuel which will participate to decarbonate the mobility sector. Unfortunately, this molecule is nowadays mainly formed from fossil gases, and so, does not meet criteria for the sustainable development. Efforts are then engaged to developp new clean H_2 synthesis technologies such as water photo(-electro)lysis. However, this latter method still suffers from low global efficiency because of limited properties of photoanode. Thanks to its band gap in the visible range (near 2.4 eV) and its low valence band, Bismuth vanadate $BiVO_4$ is one of the most promising candidate for this application.

In this paper, we studied the deposition of $BiVO_4$ thin films by radiofrequency magnetron co-sputtering of Bi and V targets into Ar/O_2 atmospheres. By tailoring the target powers, we were able to deposite coatings with various V/Bi ratios (determined by Rutherford Backscattering Spectroscopy). Since these as-deposited films are amorphous, thermal post-treatments were used to crystallize them. Interestingly, this treatment leads also to the developpement of porosity into the films thickness (observed by SEM), which will be beneficial to increase contact surface aera with water. After 2 hours at 450°C in air, XRD analysis shows that $BiVO_4$ in monoclinic phase is mainly formed. This phase could be associated to Bismuth or Vanadium oxides ones for non-stoechiometric films. The XPS also confirms these heterojunctions formation following the shift of binding energy positions. Analysis by ellipsometry and UV-visible spectroscopy shows, that the films exhibit direct band gaps between 2.4 and 2.6 eV, while flat band voltages from -0.05 to -0.13 V (vs RHE) are deduced from the Mott-Schottky technique. Hence, diagram with band positions can be drawn for each thin films, indicating that their valance band positions are convenient for O_2 production. Stoechimetric film, that exhibits the lower valence band, also presents the higher photo-current density of 0.05 mA/cm^2 at 1.3 V vs RHE and this current density remains high under irradiation for more than one hour, while significant drop of 75% has usually been reported for electrodes made from powder.

To go further, Bismuth metallic nanoparticles were added on the top surface of $BiVO_4$ thin film by sputtering the Bismuth target in pure Argon during very short times. The presence of metallic nanoparticles, thanks to heterojunction and plasmonic effect, highly enhances the measured photocurrent, keeping a good stability in time.

TS1-ThP-7 HiPIMS Deposition of Ti_xN Coatings for Oxygen Evolution Reaction Catalysts*, **Yi-Cho Tsai [ljesskoghjk@gmail.com]**,* National United University, Taiwan*; Ying-Hsiang Lin,* National United University, Taiwan*; Siang-Yun Li, Thi Xuyen Nguyen, Chia Ying Su, Ruei Chi Lin, Jyh-Ming Ting,* National Cheng Kung University, Taiwan*; Wan-Yu Wu,* National United University, Taiwan

Electrochemical reactions, particularly hydrogen and oxygen evolution reactions (HER/OER), are crucial for advancing clean energy technologies. However, current OER catalysts primarily rely on noble metals like Ir and Ru, which are expensive and less durable. Transition metal nitrides (e.g., Ti, Fe, Co, Ni) have gained attention due to their high conductivity and cost-efficiency. TiN, specifically, shows metal-like conductivity (3.34×10^{-7} Ω·cm), strong resistance to acids/alkalis, oxidation, and chemical inertness, making it ideal for OER.In this study, High Power Impulse Magnetron Sputtering (HiPIMS) was used to deposit TixN films on Ni foam, chosen for its high porosity (98%) and conductivity, to enhance the active surface area. HiPIMS, with its high plasma density and strong film adhesion, is superior to traditional DC sputtering, particularly for complex substrate structures. The TixN film with 63.1 at.% Ti content showed an overpotential of 377 mV at 50 mA/cm^2 (η10), a Tafel slope of 121.4 mV/dec, and a charge transfer resistance (Rct) of 3.05 Ω, outperforming commercial RuO_2 (421 mV). Further optimization of the Ti/N ratio revealed that a film with 52.6 at.% Ti and 47.4 at.% N had the best performance, achieving an overpotential of 333 mV, a Tafel slope of 97.8 mV/dec, and Rct of 1.95 Ω. This demonstrates that a near 1:1 stoichiometric ratio in TiN significantly enhances conductivity and electron transfer, thus improving OER efficiency.Preliminary analyses using EDX, XPS, XRD, TEM, and SEM suggest that adjusting the Ti/N ratio may impact the catalytic activity of the films. Based on the current test results, the optimized TixN films show promising potential in 1 M KOH electrolyte, indicating their prospective application as cost-effective and durable OER catalysts.

TS1-ThP-8 Enzyme-Catalyzed Thin-Film Coatings for Bipolar Plates*, **Chiara Nenninger [c.nenninger@biotec.rwth-aachen.de]**, Marisa Sárria Pereira de Passos,* Institute of Biotechnology, RWTH Aachen University, Aachen, Germany*; Philipp Niemietz,* Manufacturing Technology Institute (MTI), RWTH Aachen University, Aachen, Germany*; Thomas Bergs,* Manufacturing Technology Institute (MTI), RWTH Aachen University, Aachen, Germany; Frauenhofer Institute for Production Technology (IPT), Aachen, Germany*; Ulrich Schwaneberg,* Institute of Biotechnology, RWTH Aachen University, Aachen, Germany; DWI-Leibniz Institute for Interactive Materials e.V., Aachen, Germany

Thin-film coatings are applied to almost all material surfaces to enhance their physical and chemical properties, as corrosion resistance and conductivity. Protection of metal materials used in batteries and bipolar plates from highly corrosive environments using functional coatings can extend their lifetime and improve performance. Despite advances in coating technologies, challenges remain in achieving uniform surface functionalization, broad material compatibility, control over film thickness, scalability and sustainability.

Within this work, a biological method for the surface-confined polymerization of thin-film coatings using immobilized enzymes was developed. A fusion protein consisting of an enzyme, a linker and an adhesion-promoting peptide (AP) [1] was immobilized via dip- or spray-coating from an aqueous solution at room temperature and atmospheric pressure. The enzyme catalyzes the polymerization reaction, that “automatically” stops at approximately 30 nm. The self-termination of the polymerization reaction occurs when the immobilized enzyme becomes encapsulated by the coating, thereby controlling the film thickness.

The scalability of this method was demonstrated by coating a stainless-steel plate measuring 30 × 100 × 0.02 cm. The performance of the bio-based coatings was assessed on different metal alloys used in bipolar plates for hydrogen fuel cells through an alternating corrosion test, including climate storage and salt spray test, an acid resistance test, a pencil hardness test and a pull-off adhesion test. The coatings exhibited sheet resistance values within the range of 109 – 8250 $k\Omega\ sq^{-1}$.

This work presents a novel enzymatic coating approach for materials used in bipolar plates and battery applications that need protection from highly corrosive environments. The coating method is resource- and energy-efficient due to the use of enzymes as catalysts in aqueous environment, at room temperature and atmospheric pressure. The method has the potential to be transferred to other materials and coatings by engineering or exchanging the AP, the enzyme, or by selecting alternative monomers.

Reference

[1] M. Mao, L. Ahrens, J. Luka, F. Contreras, T. Kurkina, M. Bienstein, M. Sárria Pereira De Passos, G. Schirinzi, D. Mehn, A. Valsesia, C. Desmet, M.-A.S. Beltrán, D. Gilliland, U. Schwaneberg, Material-specific binding peptides empower sustainable innovations in plant health, biocatalysis, medicine and microplastic quantification, Chem. Soc. Rev. (2024) 10.1039.D2CS00991A. https://doi.org/10.1039/D2CS00991A.

TS1-ThP-9 Sustainable Lithium-Ion Batteries: Constructing Biochar-Based Conductive Networks for LMFP Cathodes*, **I-Hung Hsu [hsusonic900322@gapp.nthu.edu.tw]**, Che-Ya Wu,* National Tsing Hua University, Taiwan*; Wen-Lin Wang,* Agri-Industrial Systems Technology Division, ITRI Central Region Campus, Taiwan*; Tzu-Ying Lin,* National Tsing Hua University, Taiwan

Recently, lithium-ion batteries (LIBs) have played a crucial role in sustainable energy storage and electric mobility. Lithium transition-metal phosphate materials ($LiMPO_4$, M = Fe, Mn, Co, Ni) are considered promising cathode candidates due to excellent cycle stability. Among cathode materials, lithium manganese phosphate ($LiMnPO_4$, LMP) exhibits higher operating voltage and energy density compared to commercial $LiFePO_4$. Nevertheless, $LiMnPO_4$ suffers from severe Jahn-Teller distortion, limiting Li-ion transport and causing Mn dissolution-induced electrolyte degradation. To modify the properties of the material, $LiMn_xFe_{1-x}PO_4$ (LMFP) has been developed to release the effect of Jahn-Teller distortion and Mn dissolution. Yet, its intrinsic properties of low electronic conductivity remain a challenge.

In this study, a novel biochar-based carbon coating strategy for LMFP cathodes is proposed, utilizing bamboo biochar and sucrose via a one-step solid-state synthesis. The microporous biochar layer provides a higher surface area to reduce the lithium-ion transport pathway.Biochar-sucrose-derived hard carbon conductive network observed via High-Resolution Transmission Electron Microscope (HR-TEM) morphology enhances the electronic conductivity and lithium-ion transportation. After modification of the combing biochar and LMFP, electric conductivity increased 20 times compared to the sample using only sucrose as the carbon coating precursor. Electrochemical analysis reveals that the biochar-coated LMFP cathode exhibits 25% higher initial capacity (130 mAh/g at 0.1C) compared to the pristine sample and approximately 100% capacity retention after 1000 cycles at 1C cycle test. Furthermore, the biochar coating effectively captures and retains dissolved transition metal ions, preventing electrolyte degradation and improving long-term cycling stability.

Compared to conventional fossil fuel-derived carbon additives such as carbon black and artificial graphite, biochar reduces greenhouse gas emissions by around 50% and decreases the reliance on fossil fuel-derived products. Biochar materials offer an eco-friendly alternative conductive material for next-generation LIBs. These findings demonstrate the potential of biomass-derived carbon coatings in enhancing both electrochemical performance and sustainability in lithium-ion battery technology.

keywords： Lithium-ion Battery, LMFP, Hard Carbon, Surface Modification, Biowaste-Derived Carbon.

TS1-ThP-10 Enhancing Performance of Solid-State Lithium-Ion Batteries with Glass Fiber-Reinforced Polymer Electrolyte*, **Fu-Wei Chang [vivian.henryscoffee@gmail.com]**, Tzu-Ying Lin,* National Tsing Hua University, Taiwan

Lithium metal batteries (LMBs) are regarded as promising next-generation energy storage devices due to their high theoretical capacity and power denstiy. However, lithium dendrite growth during cycling causes serious safety concerns. To address this, solid polymer electrolytes (SPEs) provide a safer alternative, with polyethylene oxide (PEO)-based SPEs receiving considerable attention. Nevertheless, their low ionic conductivity and crystallization at room temperature limit their performance, thereby hindering their practical application. In this study, a fiber network-reinforced composite polymer electrolyte (CPE) is developed by embedding PEO/LLZTO electrolytes onto a glass fiber cloth (GFC) membrane. FTIR spectroscopy, shown in Figure 1, indicates that the dissociation ratio of lithium salt increases after the combination of composite polymer electrolyte and glass fiber cloth. Lithium ions transport by coordinating with oxygen atoms in PEO and GFC. The integration of PEO electrolyte and GFC membrane introduces additional ion diffusion pathways, thus facilitating lithium transport ability. Li stripping/plating tests, as shown in Figure 2, were conducted at a current density of 0.05 mA cm^{-2} and 50°C. The voltage hysteresis of PEO-LiTFSI increased sharply after 100 hours. On the other hand, the CPEs with GFC maintained stable overpotential for over 300 hours. The scheme of the lithium mechanism is showed in Figure 3. These results indicate that original PEO-LiTFSI electrolytes suffer from uneven Li deposition, leading to dead Li formation and dendrite growth. In contrast, the PEO-LiTFSI-LLZTO@GFC electrolyte promoted uniform Li deposition, effectively suppressing dendrite formation. This research provides an effective way to fabricate CPEs with superior performance. It is convinced that the combination of polymer electrolyte, ceramic electrolyte, and glass fiber as the framework offers a new design for high-performance SPEs.

TS1-ThP-11 MoS_2 Coating Facilitating Delayed Activation and Fast Charge-Discharge Properties in Highly-Doped n-type SiNW Anodes for Lithium-Ion Batteries*, **Li An Kuo [m414002@gmail.com]**, Ta Jen Yen,* Department of Materials Science and Engineering, National Tsing Hua University, Taiwan

Silicon (Si) is considered a promising anode material for lithium-ion batteries due to its exceptionally high theoretical capacity (~3579 mAh/g), which is nearly ten times that of conventional graphite anodes. However, its practical application is hindered by significant volume expansion (~300%) during lithiation, leading to severe mechanical stress, particle pulverization, and unstable solid electrolyte interphase (SEI) formation, which result in rapid capacity fading and poor cycling stability. To address these challenges, protective coatings can be applied to enhance structural stability, mitigate side reactions, and improve charge transport, ultimately enabling more durable and high-performance Si-based anodes. In our study, we applied a dual modification to the silicon anode:

1. Introducing highly-doped n-type silicon nanowires (0.001-0.005 ohm·cm) by metal assisted chemical etching, as shown in Fig. 1. Heavy doping enhances electrical conductivity, reducing charge transfer resistance and enabling faster lithium-ion diffusion. The nanowire structure provides better mechanical flexibility, accommodating volume expansion more effectively and reducing particle pulverization.
2. Applying MoS_2 (Molybdenum Disulfide) coating by hydrothermal process, as shown in Fig. 1. We found that the application enhances the performance of lithium-ion batteries, particularly exhibiting two key characteristics.

1. Delayed Activation: The results of long-term galvanostatic charge/discharge (GCD) cyclic measurements in Fig. 3. show that the conversion reaction of MoS_2 proceeds gradually until approximately the 200th cycle. Subsequently, at around the 800th cycle, the alloying process of Si nanowires becomes the dominant factor influencing the electrochemical performance, leading to a continued increase in capacity. We speculate that is the result from a unique property of the MoS_2@SiNW heterostructure as shown in Fig. 4. We will use Raman measurements and X-ray absorption spectroscopy to explain these phenomena and compare them with the MoS_2@p-type SiNW anode.
2. Fast Charging/Discharging: MoS_2 has excellent electronic and ionic transport properties, which enhance the conductivity of SiNWs, reduce interfacial resistance, and enable rapid lithium-ion diffusion within the electrode. During the initial charge/discharge cycles, the MoS_2 coating acts as a protective layer, reducing direct contact between the electrolyte and SiNWs, which helps stabilize the formation of the solid electrolyte interphase (SEI) layer.
3. This design enhances the rate capability of lithium-ion batteries while extending electrode lifespan and reducing initial irreversible capacity loss.

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(Photo)electrocatalysis and Solar/Thermal Conversion Poster Session

TS2-ThP-2 Synthesis and Photocatalytic Efficiency of Bismuth-Copper Selenide Chitosan Microspheres for Micropollutant Degradation under Solar Radiation*, **Sayed Suliman Shah [ss.shah@unistra.fr]**,* The Molecular Innovation and Applications Laboratory (LIMA), University of Strasbourg, France

Among the top trending environmental concerns, water pollution has got a serious attention these days. Technological advancement in industrial sectors for manufacture of diverse products particularly micropollutants is the principle reason by discharging the wastewater of unit operations. In this context various percussive strategies have been followed among which photocatalysis is considered cheap, ideal and eco-friendly in nature . In this work, an effort has been made to have synthesize an effective catalyst bismuth-copper selenide chitosan microspheres via solvothermal process in order to degrade micropollutants in wastewater under solar radiations. The synthesized catalyst nano composite was fabricated withpolyaniline (PANI) being conductive in nature for better photocatalytic efficiency and characterized with FTIR, SEM, EDX and XRD. The photocatalytic nature of the catalyst was examined by varying different variables namely pollutant concentration, catalyst dose, pH, degradation time and batches.

TS2-ThP-3 Dual-Metal Doped Perovskite Oxides: High-Performance Fenton-Like Catalysts for Antibiotic Degradation*, **Thi Xuyen Nguyen [nguyenxuyen1511@gmail.com]**, Yong Yu, Chia-Ying Su, Jyh-Ming Ting,* National Cheng Kung University (NCKU), Taiwan

Water pollution from organic wastewater has become a significant global concern. The Fenton-like process is an effective and practical method for reducing organic pollutants. In this study, we synthesized a dual-metal of Cu and Mn co-doped in $LaFeO_3$ perovskite oxide using a simple co-precipitation method. The obtained $La(FeCuMn)O_3$ achieves a remarkable 90.3% removal rate of high-concentration tetracycline (40 ppm) within 30 min without requiring additional light irradiation. This performance is six times higher than that of pristine $LaFeO_3$ and surpasses that of single-metal-doped samples ($LaFeCuO_3$ and $LaFeMnO_3$). We found that the oxygen vacancies induced by doping can enhance the pollutant adsorption, while Cu^+ facilitates the regeneration of Fe^{2+} and Mn promotes charge redistribution. The synergistic effects of dual-metal co-doping substantially enhance Fenton activity.

TS2-ThP-4 3D Atmospheric Plasma Beam TiO_2 Lamination of Porous Structures for Manufacturing Electro-Photocatalytic Reactors*, **Yuri Glukhoy [glukhoy1@aol.com]**,* Nanocoating Plasma Systems Inc, USA*; Michael Ryaboy,* nanocoating plasma systems inc, USA

Nanocoating Plasma Systems has developed electro-photocatalytic (EPCO) reactor with matrix's honeycomb structure made from welded together quartz capillaries with ID 0.5 mm and 7 mm long/ Due to such a design component like electric field applied to the matrix can increase the area of disinfection. When exposed to moisture (water vapor) and light, TiO2 undergoes excitation that produces electron-hole pairs, which in turn react with water molecules to form $OH^{\cdot}$ and other reactive species, this reaction is further enhanced by the electric field which not only accelerates the production of hydroxyls but also drives their propagation into the surrounding space. This phenomenon called chain reaction is the process, where the ejected from the matrix and energized by a high voltage hydroxyl radicals collide with water molecules in the room to produce secondary hydroxyl radicals. It is essential for extending the disinfecting effects over larger areas and reducing pathogen concentrations rapidly. NPS have used the focused the RF plasma beam carrying the TiO2 nanoparticles is commonly employed to provide the 2D nanocoating for different application. However, transition to the TiO2 lamination of the 3D object like the matrix with the capillaries' holes with a high aspect ratio is complicated by the negative charge passivating the entrance of these holes and rejecting the beam. ionize gases and control plasma behavior at atmospheric pressure. This phenomenon called Debye Plasma Law makes impossible lamination of the matrix. To breach this law NPS has applied the auxiliary RF discharge at the exit of the capillary holes. It generates the hollow discharge inside the hole neutralizing the parasitic charge at the entrance. Therefore, the plasma beam is able to penetrate into the interior of the holes, where the TiO2 coating is deposited on the inner walls. This technique not only overcomes the challenges of applying uniform coatings to complex geometries (such as the small and intricate capillary structures) but also, taking in account the electrical component, ensures enhancing chain reaction to enlarge the disinfection area. Involving the RF plasma beam helps to solve another problem like a low photo-catalytic activity of the commercial TiO2 nanoparticles with a bandgap about 3.2 eV limited just by UV that includes just 4% of solar spectrum. Therefore, besides generation the fine plasma beam, the nitrogen plasma discharge provides the N-doping of the TiO2 nanoparticle generates the fine plasma beam particles reducing the bandgap up to 2.75 eV for absorption of all spectrum of visible spectrum.

TS2-ThP-5 Novel Self-Assembled Materials for Indoor Perovskite Solar Cells*, **Chieh-Cheng Lu [M12188029@mail2.mcut.edu.tw]**, Chih-Ping Chen, Yan-Ru Lin, Zhong-En Shi,* Ming Chi University of Technology, Taiwan, Republic of China

Perovskite Solar Cells (PSCs) have emerged as a research hotspot for next-generation solar technology due to their high efficiency and low-cost fabrication. This study employs hydrophobic hole transport materials as interfacial layers in p-i-n type perovskite solar cells. Among the four materials investigated, the first two (HYT-H and CIM-H) are molecular materials based on a carbazole (Carbazole) core, while the latter two (HYT oCl and CIM-oCl) are derivatives of the former materials with additional chloro-functional groups. Notably, CIM-oCl exhibits excellent crystallinity, reduced non-radiative recombination, and longer carrier lifetimes. Under AM1.5G conditions, the p-i-n type perovskite solar cell with a NiO_X / CIM oCl bilayer hole transport layer achieved an optimal efficiency of 19.19%. Among the materials, those with added chlorine (Cl) elements showed the most significant improvement in V_{OC}. Under a 3000K LED light source (1000 lux), CIM-oCl demonstrated the best efficiency performance at 37.37%.

TS2-ThP-6 Perovskite Solar Cell with Potassium Chloride Treated SnO2 Electron Transport Layer for Increased Efficiency*, **Akhil Prio Chakma [akhilprio.chakma@udc.edu]**, Biplav Dahal, Tewelde Semere, Hongmei Dang,* University of The District of Columbia, USA

Perovskite solar cells (PSCs) have emerged as a promising candidate for next-generation photovoltaicsdue to their low fabrication cost and high-power conversion efficiency (PCE). However, recombination losses and charge transport issues at the interface between SnO_2 electron transport layer (ETL) and perovskite absorber are hindering the performance improvement. The SnO_2 surface often has oxygen vacancies and other defects that act as trap sites for electrons. These defects can lead to charge recombination, reducing the efficiency of charge extraction. This study demonstrates that potassium chloride (KCl) surface treatment of SnO_2 helps passivate these surface defects. Potassium ions (K^+) can fill oxygen vacancies, reducing trap density, mitigating recombination losses, and decreasing hysteresis in the current-voltage (I-V) characteristics. Characterization using scanning electron microscopy (SEM), atomic force microscopy (AFM), kelvin probe force microscopy (KPFM) confirmed better surface morphology and larger grain sizes onKCl treated SnO_2 and the corresponding perovskite layer. X-ray diffraction (XRD) analysis further revealed enhanced crystallinity, which is evident by intense diffraction peaks and reduced full-width half maximum (FWHM) compared to control samples. Photovoltaic performance measurements demonstrated improvements in device performance after KCl treatment. The best performing KCl based PSCs showed a PCE of 21%, fill factor of 77%,open-circuit voltage (V_{OC}) of 1.08V, and short-circuit current density (J_{SC}) of 25 mA/cm^2. The KCl based PSCs demonstrated that average efficiency is about 25% higher than control samples. These results highlight the effectiveness of KCl surface treatment in enhancing charge extraction, enhancing crystalline, reducing recombination losses, and improving overall device performance, making it a promising strategy for advancing high-efficiency PSCs.

Keywords: Perovskite Solar Cells, Electron Transport Layer, Efficiency, Atomic Force Microscopy, Kelvin Probe Force Microscopy, Scanning Electron Microscopy, Forward Width at Half Maximum.

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