Advances in Battery Engineering, Interface Design, and Characterization Mini-Symposium
Room 319 - Session BT2+AS+SS+TF-FrM

Materials and Devices for Energy and Sustainability

Moderators: Alexander Kozen, University of Vermont, **Chuan-Fu Lin**, Catholic University of America

10:30am **BT2+AS+SS+TF-FrM-10 Nanoscale Investigation of Thin Film CdSeTe/CdTe Solar Cells Using High Resolution Cathodoluminescence**, ***Michael Walls,*** Loughborough University, UK

Thin film cadmium telluride is the most successful second-generation photovoltaic technology with annual manufacturing capacity approaching 25GWp.The record conversion efficiency has been improved to 23.1% by using a transparent n-type buffer layer and by adding selenium to form a CdSeTe alloy at the front of the absorber to create a band gap gradient.Group V doping, usually with arsenic, has been used to increase carrier concentration in the CdSeTe absorber.

The success of the device fabrication is highly dependent on optimizing the crucial high temperature cadmium chloride activation process.This process transforms the performance of the device by dramatically recrystallizing its polycrystalline microstructure and improving its electrical properties.The effects of the treatment include; increased grain size, randomization of grain orientation, removal of defects such as stacking faults, chlorine passivation of grain boundaries and interfaces, diffusion of selenium, etc...As a result of the recent improvements in device composition and the effect of the chlorine activation process, the microstructure of CdSeTe/CdTe solar cells has become increasingly complex.

High resolution cathodoluminescence (CL) enables the observation of defects and their precise location.By combining CL with high resolution transmission electron microscopy (HRTEM) together with complementary techniques such as EDX and EBSD, we can correlate the defect emissions with microstructural disorder.Also, for the first time, it is now possible to map Urbach energy on the nanoscale. Using these techniques, we will show how selenium and chlorine passivate the grain boundaries and how arsenic doping affects grain recrystallisation.We will show the precise shape of the band gap gradient and how it fluctuates with the selenium concentration.We will also show how the introduction of selenium and arsenic into the absorber causes a high density of new defects to occur.

10:45am **BT2+AS+SS+TF-FrM-11 MOF-derived B-doped NiCo2O4 Nanosheets for Enhanced Water Splitting Reaction**, *Krishna Modi,* ***Anand Joshi,*** Parul University, India

The development of stable, earth-abundant, and effective electrocatalysts for sustainable hydrogen generation is crucial. Herein, the rational design of MOF-derived B-doped $NiCo_2O_4$ nanosheets is studied as a bifunctional electrocatalyst for alkaline water splitting. Initially, MOF-derived $NiCo_2O_4$ nanosheets were directly grown on the Ni foam using a simple hydrothermal technique. Boron impurities then were incorporated into the scaffold structure of $NiCo_2O_4$ nanosheets using a chemical reduction process. The morphology of the as-deposited nanostructure on Ni foam was studied using scanning electron microscopy. The SEM images confirm the vertically aligned nanosheet formation of MOF-derived B-doped $NiCo_2O_4$ on Ni foam. An electrochemical water splitting study reveals that the B-doped $NiCo_2O_4$ electrocatalyst shows enhanced cathodic hydrogen generation reaction and anodic oxygen evolution reaction properties compared to pristine $NiCo_2O_4$ catalysts. Introduction of a B atom effectively modulates the electronic structure of $NiCo_2O_4$, which enhances the intrinsic activity. Electrocatalysts display the low overpotential and excellent stability of 75 hours in an alkaline medium. This work provides the groundwork for a unique method of fabricating a strong self-supported and vertically stacked porous structure with plenty of active sites ideal for the inexpensive alkaline electrolyzer.

11:00am **BT2+AS+SS+TF-FrM-12 MLIPs-Accelerated Theoretical Investigation of Electrochemical Hydrogen Evolution on CoCrFeNi(111) High-Entropy Alloy Surface**, ***Ahmad Arshadi,*** *Ye Xu,* Louisiana State University

High-entropy alloys (HEAs) offer a vast compositional space for replacing precious metal electrocatalysts, but fundamental understanding of their surface reactivity continues to lag behind the pace at which these alloys are being tested. Equimolar CoCrFeNi evolves H_2 in acid within about 160 mV of Pt and outperforms each of its constituent metals, but the origin of that activity is not fully understood. We model and investigate the electrochemical hydrogen evolution reaction (HER) on the (111) facet of the HEA with large (6×6) unit cells. Machine-learning interatomic potentials (MLIPs) accelerate configurational sampling and transition state calculations, and the energetics are verified with density functional theory (DFT) calculations. Grand canonical Monte Carlo (GCMC) simulation of the surface configurations and a microkinetic model based on the Volmer–Tafel mechanism together allow us to simulate the polarization curves. A full monolayer of H occupying the threefold hollow sites persists throughout the HER regime and is kinetically inactive. HER instead requires protons being deposited on weakly binding secondary sites populated beyond one monolayer, and proceeds on a subset of those sites at ambient temperature. The simulated polarization curves successfully reproduce the small activity gap measured between CoCrFeNi and Pt.

11:15am **BT2+AS+SS+TF-FrM-13 Integrated Hardware for Gas Monitoring: A Multisensor Embedded System for Biogas Composition Analysis**, ***Allan Fonseca,*** *Marco Cavallari,* UNICAMP, Brazil

The growing demand for renewable energy has driven the development of more efficient systems for the energy recovery of organic waste, with biogas standing out as a promising alternative for both energy generation and greenhouse gas mitigation [1]. Brazil has an estimated technical potential of 84 billion Nm^3 of biogas per year [2], while Germany, the global leader, operates over 9,500 biogas plants [3]. However, commercial analyzers are generally imported and costly [4], limiting their adoption in small and medium-sized rural installations and community biodigesters.

This work presents an embedded hardware system for biogas composition analysis — whose main component, methane, has a calorific value of 35.8 MJ/m^3 [2] — featuring multisensor acquisition, digital processing, and wireless communication. An analog front-end conditions signals from electrochemical and semiconductor sensors for methane (up to 100% vol.), hydrogen (up to 1000 ppm), and oxygen (0–25% vol.), followed by 12-bit analog-to-digital conversion, processing on a low-power microcontroller with integrated Wi-Fi/Bluetooth, and local display on an OLED screen. The firmware applies digital filtering (moving average and Kalman filter) and calibration for offset, gain, and thermal drift compensation.

Experimental validation was performed in a lab-scale anaerobic digestion reactor (up to 0.3 bar, 55°C, 150 rpm) using standard gas cylinders to assess measurement error, sensitivity, stability, and repeatability. The prototype was built on a compact printed circuit board (52.75 × 45.5 mm) in partnership with M. Lima Engenharia, aiming at future commercial biogas field-monitoring solutions. Results indicate the technical feasibility of the proposed system as an affordable, modular national alternative to imported analyzers, contributing to the democratization of biogas quality monitoring in Brazil.

References

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[3] Fachagentur Nachwachsende Rohstoffe e.V., Biogas in Germany (2025).
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11:30am **BT2+AS+SS+TF-FrM-14 Vacuum Assisted Swirl Flow Separation and Flash Evaporation Apparatus Enabling Desalination Applications for High-Salinity Brines and Forever Chemicals**, ***Chinmay Chavan,*** Texas A&M University*; Ashok Thyagarajan,* Southwest Research Institute*; Vijay Dhir,* University of California at Los Angeles*; Debjyoti Banerjee,* Texas A&M University

Clean-room operations often require water remediation to reduce environmental footprint (e.g., separation of “forever chemicals” before discharging the waste water to local eco-systems). Conventional thermal desalination platforms typically use static flash evaporation and vapor separation processes in separate large chambers. Operators widely use static methods such as Multi-Stage Flash (MSF), Multi Effect Distillation (MED), and Reverse Osmosis (RO) for desalination. These methods create large footprints and drive up the production costs of purified water. The study aims to develop a novel desalination apparatus that uses flash evaporation and swirl flow separation in the same chamber (dynamically), resulting in smaller form factors and thus lower desalination costs of seawater, remediation of produced water, and hyper-saline sources. The aim of this experimental study is to leverage hot saline water from sources such as solar ponds as an input to develop a desalination platform. Tests for saline feed water with salinity levels varying from 2-20% salt by mass (20-200 g/kg) are compared in this study. Vacuum is maintained in the

downstream chambers to enable flash evaporation at lower temperatures. Downstream in the condenser, pure water with salinity as low as 0.001% salt by mass (e.g. potable water <0.05% salinity) is collected. This work was used to evaluate the efficacy of the design and the thermal-hydraulic performance of this desalination platform by determining the thermal efficiency, phase separation efficiency, and collection efficiency values for a set of specified experimental conditions. Several experiments were performed with feed-water ranging from 65-90ºC and flow-rates from 0.05-0.25 GPM to ensure repeatability of the experimental results. Performance analysis is carried by evaluating variation in thermal efficiency, collection efficiency, separation efficiency and water recovery with varying salinity conditions. The comparison between high and low salinity experiments highlights the insensitivity of the apparatus in handling variation in feed-water salinity concentrations. By testing this novel swirl flow apparatus, the aim of this study is to provide a better solution for commercial utilization to purify produced water and similar extremely high salinity brines.

11:45am **BT2+AS+SS+TF-FrM-15 Geothermal Silica-Based Superhydrophobic Glass Coatings for Water Collection in Solar Stills**, ***Floryan ROMAIN***, *Christelle YACOU, Joelle LEVALOIS-GUTZMACHER,* Université des Antilles, Guadeloupe

Freshwater availability is a growing concern in coastal and island regions, where seasonal shortages can affect water supply. [1]Passive solar stills offer a low-cost and low-energy approach to freshwater production, but their performance is limited by the condensation efficiency of the glass cover. Surface modification can promote dropwise condensation and facilitate water shedding[2], thereby improving water collection[3].

In this study, amorphous silica recovered from the Bouillante geothermal plant in Guadeloupe [4] was functionalized with octadecyltrichlorosilane (OTS), a non-fluorinated hydrophobic agent, and deposited on glass by dip-coating. Two geothermal silica nanoparticles, NPs-250 and NPs-20, were investigated and compared with commercial silica NPs-5 after OTS functionalization. The resulting surfaces showed similar superhydrophobic properties, with static water contact angles reaching values close to 162° (Fig. 1), demonstrating the potential of geothermal silica for the preparation of hydrophobic glass coatings.

The influence of the glass coating and of the solar still design on water collection was first evaluated using OTS-functionalized commercial silica (NPs-5@OTS). With the first-generation device, coating the glass cover increased the collection flux from 5.73 ± 1.16 to 14.4 ± 1.04 × 10^{-2} g cm^{-2} h^{-1}, corresponding to a 151% increase. With the redesigned second-generation device, the flux increased from 28.0 ± 1.6 to 46.56 ± 3.65 × 10^{-2} g cm^{-2} h^{-1}, corresponding to a 66% increase (Fig. 2). A water collection experiment performed with geothermal silica (NPs-20@OTS) in the second-generation device gave a collection flux of 44.27 ± 1.19 × 10^{-2} g cm^{-2} h^{-1}, comparable to that obtained with NPs-5@OTS under the same conditions, the difference between the two coatings falling within the standard deviation.

These results show that both surface modification and solar still design influence water collection. More importantly, the comparable performance obtained with geothermal and commercial silica highlights the potential of locally recovered geothermal silica as an alternative material for superhydrophobic glass coatings in passive solar water collection.

Acknowledgments: Territorial Collectivity of Martinique, Office de l'Eau Guadeloupe, GTSI, COVACHIM-M2E, the Bouillante Geothermal Station, and ETH Zurich (ScopeM).

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