Renewable Energy and Energy Storage
Room Naupaka Salon 4 - Session RE2-MoM

Surfaces and Interfaces in Photovoltaics

Moderator: Elisa Miller, National Renewable Energy Laboratory

10:20am **RE2-MoM-8 Stabilizing Zinc Powder Anodes via Functional Mxene Towards Flexible Zinc-Ion Batteries***, **ZIXUAN YANG**,* Deakin University, Australia*; Z. Wang,* RMIT University, Australia*; J. Razal,* Deakin University, Australia

The global energy crisis demands the development of sustainable and efficient energy storage technologies. Zinc-ion batteries (ZIBs) have emerged as a promising alternative to traditional lithium-ion batteries due to their intrinsic safety, environmental benignity, and the abundance of zinc resources. Among the available anode materials, zinc powder offers distinct advantages over conventional zinc foil, such as enhanced flexibility and processability, which are critical for flexible energy storage devices. However, zinc powder anodes face significant challenges, including dendrite growth, corrosion, and limited cycling stability, which hinder their widespread application.To overcome these issues, we propose a strategy to functionalize zinc powder anodes with MXene, leveraging their high conductivity and ease of surface modification. This functionalization improves the electrochemical performance of zinc powder by facilitating efficient charge transfer, mitigating dendrite formation, and enhancing cycling stability. The MXene-functionalized zinc powder anodes demonstrate remarkable structural integrity and electrochemical efficiency over extended cycling, positioning them as a stable and reliable option for flexible ZIBs.By addressing the fundamental limitations of zinc powder anodes, this study provides a viable solution for next-generation flexible energy storage systems, contributing to the broader goal of resolving global energy challenges through the development of sustainable, high-performance battery technologies.

10:40am **RE2-MoM-9 Hard X-Ray Photoemission Spectroscopy Possibilities at Scienta Omicron***, **Tamara Sloboda**,* Scienta Omicron, Sweden*; P. Amann,* Scienta Omicron, Germany*; M. Lundwall, D. Allansson,* Scienta Omicron, Sweden*; X. Zhang, A. Yost,* Scienta Omicron

X-ray photoemission spectroscopy (XPS) is a powerful method in investigations of chemical nature of materials' surfaces. During the past decade, increased attention has been shown to hard X-rays in the photoelectron spectroscopy (HAXPES) field which opens a path towards increased information depth and allows probing high binding energy core levels. This promoted the investigation of buried interfaces occurring in, e.g., device electronics or the work with elevated pressure or solid-liquid interfaces is difficult as the energy of the created photoelectrons is not high enough and scattering inside the material bulk limit the detected signal intensity.

This talk will give an overview on the Scienta Omicron HAXPES Lab system. Having access to HAXPES and XPS X-ray sources enables measurements of different core levels of the same element, including deep core levels. After excitation, electrons with enough kinetic energy escape the material and reach the detector. With an XPS source, the kinetic energy of most elements is low, thus the obtained information is very surface sensitive. However, with high energy X-rays it is possible to be both surface and bulk sensitive, as electrons stemming from deep core levels will have lower kinetic energy and contain more surface sensitive information. Similarly, electrons stemming from shallow core levels will have higher kinetic energy and contain more bulk sensitive information. This is especially valuable when detecting artefacts formed by sample exposure to different environments (e.g. air, moisture, heat, cold etc.) or by preparation steps known to induce chemical changes on the surface (e.g. sputtering). Scienta Omicron's HAXPES Lab uses a monochromatic Ga Ka metal jet source with excitation energy of 9.25 keV, therefore enabling artefact-free investigations with superior information depth, which clearly extends beyond limits of conventional XPS surface analysis. This unlocks a comprehensive and effective characterization of materials. Combined with a hemispherical electron analyzer with a ±30 degree acceptance angle, investigation of buried interfaces, operando devices and real-world samples becomes easily achievable.

Over the years it has proven invaluable in research of semiconductor materials in thin film electronic devices including the operando characterization of bias induced changes in chemical composition of material interfaces. Other applications include polymer materials, metal surfaces and coatings, or even food processing and pharmaceutical industry. This presentation will give an overview of the HAXPES Lab system and common applications of HAXPES method.

11:00am **RE2-MoM-10 Low Dos Tails Dominate Band Alignments in State-of-the-Art Cd(Se,Te) Solar Cells***, **Craig Perkins**,* National Renewable Energy Laboratory

As the efficiency of single junction CdTe-based solar cells approaches the thermodynamic limit, further device improvements depend heavily on identifying the limiting aspects of cell architectures.Device modeling is the main tool for apportionment of efficiency losses and for guiding research into which aspects of cell designs need improvement.State-of-the-art device models though require numerous input parameters related to both bulk and interfacial properties, many of which are not known.Detailed characterization of an interface in any completed thin film solar cell presents a challenge but is particularly difficult in CdTe-based solar cells where the heterojunction is formed first, evolves during subsequent processing, and ultimately gets buried between mm-thick glass and microns of other materials.In this contribution, we show how an unusual sample preparation method coupled with electron spectroscopic methods was used to tease out details of the front interface of new record efficiency CdTe solar cells.A combination of X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS), low energy inverse photoemission spectroscopy (LEIPS), and Auger electron spectroscopy (AES) was used to probe the electronic and structural properties of the front oxide-Cd(Se,Te) interface in fully completed solar cells.Prior to our destructive analysis of the front interface, operating cells were fully characterized by transport measurements, which when modeled, allowed independent assessment of band positions measured by surface analytical techniques.Band alignments based mainly on X-ray excited valence band spectra do not agree with alignments estimated from device modeling, whereas measurements using UPS-derived band edges do agree.A major conclusion from this is that low density of states (DOS) tails can be missed by X-ray excited valence band measurements, even when XPS data are used in conjunction with theoretical total DOS.The low DOS tails detected directly by UPS are found to be present in several different materials and structures found in modern CdTe solar cell designs, including SnO_2, a material used widely in other solar cell designs as well as in gas sensors and other electronic devices.It is believed that the low DOS band edges critical to this work are present in many other electronic materials.For that reason, our work has important implications for the use of electron spectroscopy in understanding and improvement of a wide variety of semiconducting devices.

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