Thin Films
Room 317 - Session TF1-MoA

Thin Films for Energy

Moderators: Prof. Dr. Adriana Creatore, Eindhoven University of Technology, **Prof. Mark Losego**, Georgia Institute of Technology

2:00pm **TF1-MoA-3 TFD Messier Mid-Career Award Lecture: Growth Mechanisms and Properties of Thin-Film Ceramics for Energy Applications***, Per Eklund,* Uppsala University, Sweden **INVITED**

This invited presentation for the AVS Thin Film Division's Russel F. Messier Mid-Career Award Lecture gives an overview of my research in the energy area and fundamental growth mechanisms. For thermoelectric devices, I present an overview of our work on multicomponent CrN-, ScN-, and $Ca_3Co_4O_9$-based thin films. The semiconducting early transition metal nitrides have emerged as an unexpected class of materials for thermoelectric energy harvesting. CrN exhibits n-type conduction with a high power-factor enabled by a high electron concentration thermally activated from N vacancies, and alloys can be made of rocksalt-$Cr_{1-x}Sc_xN$. Multicomponent alloying of ScN and CrN in alloys such as CrMoVWN or combinations thereof offer further possibilities for tailoring the thermoelectric properties and growth conditions. We have developed textured and nanoporous hase-pure $Ca_3Co_4O_9$ thin films. These can further be deposited on flexible mica substrates, enabling flexible inorganic thermoelectric thin films that withstand repeated bending, and as free-standing films.

For growth on mica, an outstanding question is the growth of stress-free epitaxial films by van der Waals epitaxy (vdWE). Unlike conventional epitaxy, vdWE allows stress-free growth of thick films with oriented crystals without dislocations even for large film-substrate lattice mismatches. However, vdWE of non-layered materials is often presumed or claimed on layered substrates such as mica without experimental evidence. We have shown that the growth of rocksalt ScN and NiO films on mica(001) occurs by conventional epitaxy, which should be the default assumption for non-layered materials unless vdWE isexplicitly proven. In contrast, for layered materials on mica, the situation is far more complex, and an atomistic understanding of film/substrate interface structure that explains and predicts vdWE has remained elusive. We have unveiled atomistic interface mechanisms for vdWE of MoO_3 and VO_2 on mica showing negligible strain buildup in continuous epilayers, confirming vdWE. Ab initio computations showing interface energy minima for these orientations correlate with high cross-interface proximity between Mo atoms in alpha-MoO3 and K in mica conducive for maximal vdW attraction. These insights on interface structure and energetics provide a framework for predicting vdWE for different film/substrate combinations and designing of stress-free and/or standalone epitaxial films of layered materials on layered substrates such as mica.

2:45pm **TF1-MoA-6 Enhancing Energy Storage Performance via Minimal Doping in $SrTiO_3$ Thin Films***, Saeed Almishal, Joseph Petruska, Jon-Paul Maria,* Penn State University

We investigate a controlled minimal doping strategy for enhancingenergy storage performance in Mn-substituted SrTiO3 thin films by introducing nanoscale polarization disorder through Ti/O defect dipoles.We develop robust X-ray fluorescence calibration methods, enabling reliable quantification of Mn concentrations down to ~0.25% in bulk ceramics. We subsequently grow thin films by pulsed laser deposition on Pt/sapphire substrates,monitoring crystalline qualitywithX-ray diffractionandsurface roughness using atomic force microscopy.We additionally utilizeX-ray photoelectron spectroscopyfor chemical analysis and scanning electron microscopy to measurefilm thickness.We systematically characterize our thin film capacitors with tungsten-top electrodes through polarization-electric field measurements, breakdown testing, and energy storage analysis as functions of dopant concentration, film thickness, and measurement frequency. We identify an optimal Mn concentration of 1.75% at 350 nm thickness, providing the best compromise between polarization, breakdown field, efficiency, and reproducibility, delivering room temperature recoverable energy density ~87 J/cm3 at remarkably high 86% efficiency, compared to pure SrTiO3 ~5 J/cm3 and ~ 30% respectively, when measured at 10KHz frequency. Overall, our results demonstrate that minimal chemical perturbations can produce substantial enhancements in energy storage behavior.

3:00pm **TF1-MoA-7 Interfacial Engineering of the HTL-Perovskite Interface in Perovskite Solar Cells Using Atomic Layer Deposition***, Alexandra Hurd, Md Aslam Uddin, Oluka Okia, Neil Dasgupta,* University of Michigan, Ann Arbor

Perovskite solar cells (PSCs) are the leading low-cost, easily manufacturable photovoltaic alternative to commercial silicon, with efficiencies rivaling that of silicon. However, the interface between the perovskite absorber and hole transport layer (HTL) remains a critical barrier for the long-term operational stability of p-i-n PSCs. Nickel oxide is a highly effective inorganic HTL due to its high hole mobility, wide bandgap, and intrinsic stability. However, the trivalent nickel states required for hole conductivity are thought to contribute to perovskite degradation at the NiO-perovskite interface via redox and acid-base reactions[1]. Some strategies have been implemented in the literature to passivate this interface, including self-assembled monolayers, other organic and inorganic interlayers, and doping of the NiO[2,3]. However, there are limited studies that employ chemical control of the HTL-perovskite interface via vacuum processing methods to improve interfacial stability.

This work explores atomic layer deposition as a method for precise tuning of the nickel oxide film and NiO-perovskite interface. By performing post-deposition anneals in different gaseous environments, we control surface oxidation states of NiO. We examine trends between HTL electrochemical properties and interfacial stability for NiO-only and NiO with an ultrathin inorganic buffer layer. Surface energy and chemistry of the films are characterized by water contact angle goniometry and XPS, respectively. We conduct heat and light stability tests of encapsulated HTL-perovskite junctions and characterize degradation using X-ray diffraction and photoluminescence spectroscopy. Interfacial toughness of the interface is also characterized with mechanical testing. By identifying trends in interfacial stability and toughness with various NiO surface properties, we inform interfacial engineering of the interface to improve operational stability of PSCs and take steps toward their commercialization.

[1]Boyd, C., et al., Joule, (2020), 4(8), 1759-1775

[2]Zhou W., Fang Y., et al., Solar Energy Materials and Solar Cells, (2026), 296, 114079

[3]Zhou P., et al., Solar RRL, (2019), 3, 1900164

3:15pm **TF1-MoA-8 Regulating early-stage chemistry enables certified open-circuit voltage of 847 mV in wide-bandgap kesterite Cu2ZnSnS4 thin-film solar cells***, Ao Wang, Kaiwen Sun, Xiaojing Hao, Martin Green,* University of New South Wales, Australia

On the path to carbon neutrality, increasing photovoltaic (PV) penetration requires continuous cost reduction and efficiency advancement. It drives the need for developing earth-abundant, stable, and low-cost wide-bandgap materials that are compatible with Si-based tandem cells. Wide-bandgap kesterite Cu_2ZnSnS_4 (CZTS) is widely regarded as a promising candidate, yet its certified efficiency remains capped below 11.5% with an open-circuit voltage (V_{OC}) under 750 mV. Although researchers have long identified reducing the V_{OC} deficit as critical, achieving substantial improvement in this emerging technology has proven challenging.

In this work, we overcome this long-standing bottleneck by simultaneously achieving a certified V_{OC} of 847 mV and a record efficiency of 12.4% (previous results summarized in Table 1). This work sets a new benchmark for wide-bandgap CZTS, delivering a certified V_{OC} near 850 mV, which is the first beyond 800 mV and nearly 100 mV higher than the prior record.

Table 1. Certified results of wide-bandgap Cu_2ZnSnS_4 solar cells

V_{OC} (mV)	Efficiency (%)	Bandgap (eV)	Reference
731	11.0	1.50	Nat Energy 3, 764–772 (2018)
748	11.4	1.53	Nat Energy 10, 255–265 (2025)
709	11.5 (active-area)	1.50	Nat Energy 10, 630–640 (2025)
847	12.4	1.57	This work

More importantly, we reveal why the widely adopted strategy of designing a Cu-poor/Zn-rich composition, though guided by numerous theoretical calculations, has failed to deliver substantial performance advancement. Despite the well-controlled initial global composition, the spatial local chemistry before crystallization is more critical and can deviate significantly. In practice, the strong reactivity of Cu with S during annealing often leads to a Cu-rich surface, making it difficult to preserve the designed composition.

Here, we employ a 'structured two-stage Cu' strategy that enriches Cu-S bonding at the film surface, thereby lowering the driving force for Cu out-diffusion. The stabilized environment simultaneously suppresses diffusion-induced secondary phases and segregation, bridging the gap between

global design and local chemistry to ensure the desired crystallization chemistry and pathway. Consequently, benign defects are promoted while detrimental species are suppressed, leading to a significant enhancement of the effective carrier lifetime.

Beyond CZTS or even Cu-based chalcogenides, this strategy is expected to apply broadly to multinary thin-film materials containing elements with contrasting chemical reactivities. Furthermore, the concept is not limited to vacuum deposition, but can also guide solution processing and other scalable fabrication methods.

3:30pm **TF1-MoA-9 Perovskite Photovoltaics on Flexible Foils: Reliability, Scaling, and Pathways to Market***, Vivek Babu,* Verde Technologies **INVITED**
Metal-halide perovskite photovoltaics have attracted strong interest because they combine high efficiency with the potential for lightweight, flexible, and low-cost manufacturing. These features create a unique value proposition for applications where conventional silicon photovoltaics are limited by weight, rigidity, or installation constraints. Examples include space power, high-altitude platforms, unmanned aerial vehicles, and building- or vehicle-integrated photovoltaics.

However, moving perovskite photovoltaics from promising laboratory devices to reliable products requires solving challenges beyond initial power conversion efficiency. Flexible thin-film foils introduce practical constraints related to substrate handling, film uniformity, mechanical robustness, encapsulation, interconnection, and long-term environmental stability. As device area increases from small cells to mini-modules and panels, local defects and non-uniformities can strongly affect yield, reproducibility, and reliability.

In this invited talk, I will discuss the opportunities and barriers for commercializing flexible perovskite solar modules on polymer and metal foils. The presentation will focus on the connection between application requirements, manufacturing choices, and reliability expectations. Particular attention will be given to the challenges of scaling laboratory processes to larger-area flexible formats, maintaining device performance across the full panel area, and developing test protocols that reflect real operating conditions such as thermal cycling, humidity, illumination, mechanical stress, and radiation exposure.

Finally, I will discuss possible pathways toward market adoption, including the role of pilot-line manufacturing, inline quality control, accelerated reliability testing, encapsulation strategies, and early application targets where lightweight and flexible solar modules can provide clear system-level value. The goal is to highlight what is needed for flexible perovskite photovoltaics to move from high-performance prototypes toward manufacturable and bankable energy products.

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