PCSI

Room Keahou I - Session PCSI-WeA2

Materials for Catalysis, Energy Storage, and Energy Harvesting

Moderator: Mitsuru Takenaka, The University of Tokyo, Japan

2:35pm **PCSI-WeA2-14 Scalable Si-Based Metal-Insulator-Semiconductor Photoanodes for Water Oxidation Fabricated Using Nanosphere Lithography and Thin Film Reaction***, Edward Yu,* ***Yunho Choi****, Shang-Hsuan Wu, Joseph Risberg, Suhun Kim,* University of Texas at Austin

Photoelectrochemical (PEC) water splitting is a promising approach for converting solar energy into storable hydrogen, offering a sustainable alternative to fossil-based hydrogen production. PEC cells rely on semiconductor materials to absorb sunlight and generate mobile charge carriers that drive the hydrogen and oxygen evolution reactions. Si-based photoelectrodes are especially attractive due to their optimal bandgap, high charge mobility, long diffusion lengths, and cost-effective, scalable manufacturing process. To improve the stability of Si-based PEC cells, metal-insulator-semiconductor (MIS) structures have emerged as a promising approach [1]. MIS photoanodes integrate ultrathin insulating layers that protect the Si surface while maintaining charge transfer efficiency. The thickness of the insulator is critical:ultrathin layers facilitate effective charge tunneling, whereas thicker layers enhance long-term stability in corrosive environments.

In our previous work, we demonstrated that localized conduction paths formed via an Al/SiO$_2$ thin-film reaction enable low-resistance charge extraction through thick insulating layers, while also providing excellent stability and scalability to full-wafer photoanodes [2]. However, the performance of such photoelectrodes can be limited by nonuniformity in thin-film reaction behavior. We have now demonstrated a method for creating more controllable and uniform localized conduction paths on the photoanode by employing nanosphere lithography (NSL), a low-cost and highly scalable patterning technique. NSL is used to create a patterned mask for Al deposition that enables the density and locations of Al/SiO$_2$ thin-film reactions and consequently metal catalysts to be precisely controlled, leading to improvements in both photocurrent density and onset voltage. Moreover, a technique we have recently developed for extremely rapid large-area nanosphere monolayer formation [3] makes this patterning approach easily scalable to fabrication of full-wafer photoanodes and therefore, highly promising for large-scale PEC applications.

2:40pm **PCSI-WeA2-15 Development of Bi$_2$Te$_3$-based Thermoelectric Thin Films Using Advanced Pulsed Laser Deposition System***,* ***Yakubu Sani Wudil,*** King Fahd University, Saudi Arabia

This study presents the pulsed laser deposition of n-type selenium (Se)-doped bismuth telluride (Bi$_2$Te$_{2.7}$Se$_{0.3}$) and n-type bismuth telluride (Bi$_2$Te$_3$) nanostructures at varying substrate temperatures. The effects of substrate temperature on the structural, morphological, and thermoelectric properties of these nanostructures were systematically explored. Density functional theory (DFT) simulations were conducted to examine the electronic structures, partial, and total densities of states of the unit cells of the compounds. Surface and structural characterization revealed highly crystalline nanostructures with pronounced grain boundaries. A comparative analysis underscores the impact of Se inclusion on the thermoelectric performance of the Bi$_2$Te$_3$ matrix. The study also highlights the substrate temperature-dependent variations in the thermoelectric figure of merit (ZT). Notably, the room temperature thermoelectric power factors (PF) of 2765 $\mu W/mK^2$ for pure Bi$_2$Te$_3$ and 3179 $\mu W/mK^2$ for Se-doped Bi$_2$Te$_3$ demonstrate their promise for cooling and power generation applications. The Se-doped Bi$_2$Te$_3$ exhibited a room temperature ZT value of 0.92, representing a 30% improvement over the pure phase. This enhancement is attributed to the reduction in thermal conductivity due to increased phonon scattering at the interfaces in the doped material.

2:50pm **PCSI-WeA2-17 Minimizing Ion/Electron Pathways Through Ultrathin Conformal Holey Graphene Encapsulation in Li- and Mn-Rich Layered Oxide Cathodes for High-Performance Lithium-Ion Batteries***,* ***Heejoon Ahn,*** 222 Wangsimni-ro, Seongdong-gu, Republic of Korea*; Sungwook Kim,* Hanyang University, Korea

Lithium-ion batteries (LIBs) are increasingly favored due to their attractive features. The design of the cathode in LIBs plays a critical role in determining cell capacity, operating voltage, and overall cost. Lithium- and manganese-rich (LMR) cathode materials stand out as promising candidates for the next generation of cathode materials due to their ability to operate at high voltages and provide capacity exceeding 250 mAh g^{-1}. However, despite these appealing characteristics, LMR faces challenges in commercialization due to factors such as poor rate capability and rapid capacity and voltage decay during cycling. These are closely associated with the fundamental structural issues arising from the two distinct phases of LMR materials, slow reaction kinetics and structural degradation occurring through side reactions between the electrode and electrolyte. In this study, we introduce a carbon encapsulation technique that integrates polyethylenimine (PEI) and holey graphene onto the LMR surface, aiming not only to augment electrical conductivity but also to facilitate ionic conductivity. Despite its low carbon content of 0.1 wt%, the suggested PEI/holey graphene-encapsulated LMR demonstrates enhanced cycle stability and rate performance for the LMR electrode. Moreover, the thin and uniform PEI/holey graphene encapsulation layer serves a dual purpose by easing the movement of Li^+/e^- on the LMR surface and providing a protective barrier against physical and chemical aggressions. Throughout cycling assessments, the PEI/holey graphene-encapsulated LMR mitigates the leaching of transition metals, mitigating microcrack formation and irreversible structural alterations compared to bare LMR. Consequently, the proposed PEI/holey graphene encapsulation emerges as an attractive technology for high-performance LIB design, concurrently elevating the cycle stability and rate performance of LMR electrodes.

2:55pm **PCSI-WeA2-18 Development of High-Performance Hydrogen Generation Catalyst Based on Fluorine-Doped Tin Oxide Aerogel***,* ***Hyung-Ho Park,*** Yonsei University, Korea

The electrochemical hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are efficient methods for generating clean, sustainable, and dense energy sources. Nørskov's theoretical study states that Pt is the most effective catalyst for HER due to its low Gibbs free energy (ΔG ~0) or moderate M-H bonding toward H* adsorption. Unfortunately, its scarcity and high cost limit its practical use. To overcome these drawbacks, high surface area carbon in the form of core-shell, wrapped, or dispersed structures has been used as a metal catalyst support, forming complexes with the metal and providing impressive resistance against corrosion.

In this presentation, an "aerogel" system is introduced to fabricate an ultra-low-density and highly porous metal support of SnO$_2$.[1] The aim is to meet the fundamental criteria for an ideal metal support structure, including resistance to corrosion, high conductivity, high porosity, large specific surface area, and strong metal-support interaction. SnO$_2$ aerogel was synthesized using a sol-gel method, leveraging the benefits of an aerogel system to impart three significant advantages to SnO$_2$: ultra-low density, which reduces the electrode's weight; a large surface area to achieve optimal metal catalyst dispersion; and high porosity, facilitating ion insertion and mass transfer. Additionally, anion doping of SnO$_2$ with fluorine at the atomic level during synthesis was conducted to improve conductivity. This doping resulted in an observable bandgap expansion, and the one-step synthesized F-doped SnO$_2$ (F-SnO$_2$) exhibited higher conductivity, significantly reducing the electrochemical charge transfer resistance compared to undoped SnO$_2$. Subsequently, a sputtering technique was used to deposit nanometer-scale Pt on the colloidal F-SnO$_2$ surface. The resulting hybrid structure (F-SnO$_2$@Pt) demonstrated enhanced HER activity and impressive catalytic stability even after prolonged oxidation activity.[2]

[1] V. G. Parale, T. Kim, H. Choi, V. D. Phadtare, R. P. Dhavale, K. Kanamori, H.-H. Park, Adv. Mater. **2307772** (2024).

[2] T. Kim, S. B. Roy, S. Moon, S. Yoo, H. Choi, V. G. Parale, Y. Kim, J. Lee, S. C. Jun, K. Kang, S. Chun, K. Kanamori, H.-H. Park, ACS Nano. **16**, 1625 (2022)

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