Applied Surface Science
Room Ballroom A - Session AS-ThP
Applied Surface Science Poster Session

AS-ThP-1 Scratching at the Surface of Leadership, ***Brian Strohmeier,*** Surface Science Solutions, LLC

In today's dynamic research and business environment, strong technical skills are essential, but insufficient, for sustained career growth. Many exceptional scientists find themselves promoted to first-level management roles because of their outstanding scientific achievements, usually without having any formal training in leading people. Although they are well-prepared in technical and scientific areas, the toughest challenges for new managers usually involve delicate interpersonal skills, such as active listening, conflict resolution, empathy, and emotional intelligence, rather than science itself. Such topics are rarely encountered in graduate-level education and almost never in undergraduate curricula. To thrive amid constant change, managers and technical leaders need to hone and adapt their leadership styles to optimize resource management for each situation, focusing on prioritizing, empowering, and motivating their teams. This poster presentation will highlight effective modern leadership skills and strategies that can enhance your personal long-term growth and boost your career success.

AS-ThP-3 Sample Preparation Checklists and Instrument Parameter Tables: Newly Published Aids to Reliable and Reproducible Surface Analysis Data, Paper Reviewing, and Information Reporting, ***Don Baer,*** Pacific Northwest National Laboratory*; Linda Dake,* retired

Several examinations of surface analysis information reported in the literature indicate a significant degree of flawed data analysis and a high degree of inadequate reporting regarding sample handling, instrument operation and analysis details. This poster provides information about two newly published “tools” intended to help address three issues:

1. Researchers and others with surface analysis needs, but unfamiliar with the sample handling requirements often present “damaged” samples for analysis.
2. Information about how a sample has been handled before and in preparation for surface analysis is often not provided, and may not be recorded, limiting the ability of others, looking at a data report or in a publication, to assess the reliability of the analyses.
3. Many publications do not contain either adequate sample or instrument information to assess the data quality or to verify adequacy for use in databases or AI input

To assist those unfamiliar with collecting and preparing samples for surface analysis and to assist surface analysts in collecting data that should be recorded, two checklists based on new ISO standards have been published in the open literature. The first checklist is designed to guide a sample owner in selecting, handling and transporting a sample to a surface analyst. The second checklist is intended to assist a surface analyst in obtaining and reporting information regarding sample treatment, processing and mounting for surface analysis. These are based on ISO standards 20579 part 1: Documenting and reporting the handling of specimens prior to analysis and ISO 20579 part 2, Documenting and Reporting the Preparation and Mounting of Specimens for Analysis. In addition to the reporting requirements, which include information about the sample history and analysis objectives, there are normative annexes that provide information about sources of sample contamination, ways to minimize contamination and expected or generally required components of sample handling to extract useful surface information.

A new series of papers in Surface Science Spectra is being published to help analysts and authors report the relevant instrument information and provide readers with the information needed to assess the meaning and quality of XPS data. Included in these papers are instrument parameter tables which provide both the “fixed” instrument parameters and those that are operator selected and need to be called out in reports and journal articles.

The poster will show the checklists and examples from published parameter tables.

AS-ThP-4 Atmosphere-Controlled Surface Engineering of $CuRh_2O_4$ Nanofibers For Alkaline Water Oxidation, ***Namhee Kim,*** *Hyeon Gyeong Jeon, Myung Hwa Kim,* Ewha Womans University, Republic of Korea*; Dasol Jin,* Jeonbuk National University, Republic of Korea

Controlling the surface chemical states of metal oxide electrocatalysts is critical for optimizing catalytic performance, yet Cu-based oxides pose a particular challenge since Cu readily shifts its oxidation state depending on the synthesis atmosphere. In this work, Cu-Rh bimetallic oxide nanofibers were prepared by electrospinning followed by post-annealing under controlled O_2/He flow, where the O_2 concentration was systematically varied to examine its effect on surface composition and phase evolution. AR-XPS analysis revealed that insufficient oxidation leaves Cu and Rh incompletely oxidized, while excess oxygen promotes unwanted secondary phase formation. Only at the optimized O_2 concentration were Cu^{2+} and Rh^{3+} simultaneously stabilized on the surface, and single-phase $CuRh_2O_4$ formation was verified by XRD and Raman spectroscopy. The phase-pure sample demonstrated superior oxygen evolution reaction (OER) activity in 1 M NaOH, outperforming commercial Ir/C, along with stable performance over extended operation. These results highlight that annealing atmosphere engineering is a straightforward yet powerful route to controlling surface chemical states and achieving phase-pure Cu-based spinel oxide electrocatalysts. This work was supported by the National Research Foundation of Korea funded by the Ministry of Science and ICT and the Ministry of Education. (NRF-RS-2018-NR031064 and RS-2025-16063688).

AS-ThP-5 Surface Chemical Characteristics of Electrospun Multicomponent Rutile Oxide Nanofibers for pH-Universal Oxygen Evolution Reactions, ***HyeonGyeong Jeon,*** *Namhee Kim, Youngmi Lee, Myung Hwa Kim,* Ewha Womans University, Republic of Korea

Lattice-entropy modulation in multicomponent oxide systems has attracted increasing interest as a strategy for tuning surface chemical environments and interfacial electrocatalytic properties. In this study, rutile-type $(RuIrCrMnSn)O_2$ nanofibers were fabricated via electrospinning followed by thermal treatment. Electron microscopy and elemental mapping analyses confirmed the formation of continuous fibrous structures with relatively uniform distributions of Ru, Ir, Cr, Mn, and Sn species throughout the oxide framework. X-ray diffraction, SAED, and Raman analyses supported the formation of rutile-related multicomponent oxide structures with broadened structural features associated with multication incorporation. X-ray photoelectron spectroscopy revealed mixed oxidation states and defect-related oxygen species on the oxide surface, indicating chemically diverse surface environments within the multicomponent oxide structure. Among the prepared samples, the $(RuIrCrMnSn)O_2$ nanofibers calcined at 400 °C exhibited overpotentials of 199.7, 244.4, and 330.1 mV at 10 mA cm^{-2} under acidic, alkaline, and neutral electrolytes, respectively. The optimized sample also maintained stable operation for up to 35 h in acidic electrolyte. These results suggest that multicomponent rutile oxide nanofibers can provide chemically diverse electrocatalytic interfaces for pH-universal oxygen evolution reactions. This work was supported by the National Research Foundation of Korea funded by the Ministry of Science and ICT and the Ministry of Education. (NRF- RS-2025-16063688).

AS-ThP-6 Industrial Problem Solving with Low-Cost ToF-SIMS, *Nick Long, Torsten Henkel,* SAI, UK*;* ***Aidan Harrison***, *Silverio Iacono,* SAI Americas

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is often perceived as a complex high-end research tool requiring extreme mass resolution and accuracy. However, lower cost ToF-SIMS systems with restricted mass resolution operating at high vacuum levels for increased sample throughput remain exceptionally powerful for troubleshooting the processing of materials in industrial environments. These instruments can provide actionable data for resolving production bottlenecks, including (but not limited to) those arising in the following application areas.

Resolving Adhesion Failures

Adhesion problems in industrial processes often stem from monolayer-level surface modifications that are invisible to bulk analysis techniques. Low-cost ToF-SIMS excels here by identifying functional group distributions at the interface. For instance, the technique can detect sub monolayer presence of mold release agents (such as silicones or stearates) which can negatively impact adhesion performance. Additionally, a detailed inspection of the mass spectra from such surface contaminants can distinguish any subtle molecular differences between them in order to identify likely sources.

Detecting and Identifying Industrial Cleaning Residues

In a production electronics environment, contamination issues which can affect the performance of assembled parts often involve residues left by cleaning processes. These residues will have distinct signatures or fragmentation patterns that can be measured by ToF-SIMS even without high-resolution mass separation, helping to trace the source of the issue back to a specific stage in the manufacturing line such as a contaminated wash bath.

Detecting and Identifying Corrosion under Painted Metal Surfaces

Filiform corrosion is an atmospheric corrosion affecting organic coated metals by producing “threadlike” residues beneath the coating. Scanning Kelvin Probes can detect problems beneath the coatings physically by measuring work functions but for absolute chemical identification of the surface corrosion products a Low-Cost ToF-SIMS can provide the necessary answers.

Optimizing LDPE Roll Packaging Efficiency

The efficiency of Low-Density Polyethylene (LDPE) roll packaging often depends on the controlled migration of additives, specifically slip agents such as erucamide. These additives must bloom to the surface in precise concentrations to reduce friction during high-speed packaging processes. Restricted mass resolution ToF-SIMS is highly effective at monitoring the surface coverage of these slip agents, helping to resolve any blocking issues in the packaging process.

AS-ThP-7 Analysis of Interfaces by Soft and Hard X-ray Photoemission, ***Jia Lu***, *Jennifer Mann, Sarah Zaccarine, Norb Biderman, Cesar Saucedo, Kateryna Artyushkova,* Physical Electronics USA

Recent developments of lab-based hard X-ray photoelectron spectrometers (HAXPES) have created new, accessible opportunities for routine analysis of technologically significant devices. A micro-focused, monochromatic Cr Kα X-ray source not only provides three times greater analysis depth in comparison to the traditional Al Kα X-ray source, but it also provides high sensitivity for small area analysis. Using a combination of soft and hard X-rays allows for the analysis of materials non-destructively for their in-depth compositional heterogeneities. For film thicknesses that require ion beam sputtering to reach buried interfaces and layers, Cr sources allow one to probe below the depth of ion beam damage.

This poster will showcase how combining soft and hard x-ray photoemission within a single laboratory instrument offers a robust, non-destructive solution for chemical state analysis across the surface to bulk depth range. By using the micro-focused, monochromatic Cr X-ray source with increased analysis depth, accurate bonding chemistry and stoichiometry ratio of Ti/Al flakes (less than 100µm in diameter) can be probed below the surface organic contaminations with high sensitivity. In combination with soft X-rays, hard X-rays provide improved insight of how the NiPt nanowire surface was affected by annealing and surface treatments. Using a combination of XPS and HAXPES, high accuracy was obtained for calculating the thin film layer thickness of carbon/HfO_2/SiO_2/Si substrate using *Strata*PHI. For depth profile analysis of tin oxide, Cr X-ray source shows lower degree of tin reduction in comparison to Al X-ray source, showcasing its capability to probe below the depth of ion beam damage.

AS-ThP-8 Ion Scattering Spectroscopy to Identify and Quantify Selective Internal and External Decorations of Pt Nanoparticles on Porous Carbon Supports, ***Alessio Cosenza***, *Ich Tran, Plamen Atanassov,* University of California Irvine

Determining whether metal nanoparticles are located on the external surface or within the internal pore network of porous supports remains a key challenge in applied surface analysis, catalyst design, and host–guest nanomaterials. This distinction is especially important for porous carbon-supported Pt catalysts, where nanoparticle locality affects accessibility, utilization, and stability. However, common characterization methods provide incomplete information. TEM and dark-field imaging give projected contrast through the specimen thickness, making internal and external nanoparticles difficult to distinguish. Secondary-electron imaging is more surface-sensitive, but remains qualitative and can be ambiguous for nanoparticles beneath nanometer-scale carbon shells. XPS provides surface and chemical sensitivity, but Pt beneath thin carbon shells can still contribute to the Pt 4f signal because of the finite information depth.

Here, we investigate ion scattering spectroscopy (ISS) as a direct surface-sensitive approach to distinguish externally exposed Pt nanoparticles from Pt shielded inside mesoporous carbon black supports. Pt nanoparticles with similar size distributions were synthesized either within the carbon shell/pore network or on the external carbon surface. Carbon supports with different shell thicknesses and graphitic structures were used to evaluate how nanoparticle confinement affects the ISS and XPS response.

For each matched internal/external Pt pair, the external-Pt catalyst was used as a local reference corresponding to fully externally accessible Pt. The Pt ISS signal of the internal-Pt catalyst was normalized by total Pt loading and compared with the corresponding external reference. This provides a semi-quantitative estimate of the fraction of Pt accessible to the outermost surface. The complementary XPS response was used to evaluate how much of the internal Pt population remains detectable through the carbon shell, providing an apparent Pt 4f visibility factor rather than a direct measure of external exposure.

The results show that ISS can resolve large differences in external Pt accessibility between nominally similar Pt/C catalysts and estimate the fraction of nanoparticles shielded within the pore/shell structure. In contrast, XPS and electron microscopy provide valuable complementary information but cannot alone quantify nanoparticle locality in these non-ideal porous systems. This work establishes ISS as a practical surface-analysis tool for evaluating nanoparticle placement in porous catalyst supports and suggests broader application to host–guest, core–shell, encapsulated catalyst, and carbon peapod-type nanostructures.

AS-ThP-9 Probing Energy Level Alignments in NFA Organic Solar Cells: Combined UPS and LEIPS Study on Blend Films, ***Yongsup Park***, *Seunggu Lee,* Kyung Hee University, Republic of Korea

Energy level alignment (ELA) in non-fullerene acceptor (NFA) organic photovoltaic (OPV) cells is crucial, as the offsets between HOMO and LUMO levels at the bulk heterojunction (BHJ) interface determine charge separation efficiency and significantly affect the open-circuit voltage (Voc). Traditionally, ELA has been measured using a combination of cyclic voltammetry (CV) and optical absorption (OA), despite their limited accuracy. More precise measurements can be obtained through UV photoemission spectroscopy (UPS) and low-energy inverse photoemission spectroscopy (LEIPS). However, most studies have focused on neat films, while ELA can differ significantly in blend films. In this study, we used UPS and LEIPS to measure the HOMO and LUMO levels for both neat and blend films of the donor-acceptor pairs (PM6:Y6 and PM6:L8-BO). The results reveal significantly different ELA in blend films compared to neat films, particularly when using conventional vacuum level alignment was applied to the neat films. These differences are discussed in the context of Voc estimation and the impact of the HOMO offset (ΔE_HOMO) on charge separation efficiency.

AS-ThP-10 Tuning Topography and Morphology of Mg2-MOF-74 Metal-Organic-Framework to Study Optimization of Carbon Capture Capabilities, ***Corbyn Stosich***, *Sean Lubner,* Boston University

In order to combat the climate crisis and keep global warming under the 1.5℃ threshold for human safety, it is imperative that our net carbon emissions reach not only zero, but be negative by 2050 [1], [2]. To accomplish negative emissions, carbon capture via direct air capture (DAC) and point capture are necessary and on the scale of gigatons per year [3]. This process is energetically exhaustive due to the thermal energy required to regenerate carbon capture materials, and these energy demands cannot be met by global energy production [2], [3].

Metal organic frameworks (MOFs) are a highly tunable class of materials that have demonstrated exciting abilities in adsorption of CO_2 for point capture and primarily DAC purposes. These materials have particularly high CO_2 capacity with incredibly fast kinetics. The tunable nanostructure inherent to MOFs allows for many ways to minimize the energy requirement of material regeneration.

In this work, we tweak synthesis environments of otherwise identical MOF materials (Mg_2-MOF-74) to study the resulting topography and morphology. This process is accomplished through heterogeneous crystallization on different substrates with varying temperature and polarity environments. We then characterize the resulting crystals by running BET, SEM, and NMR to identify both surface and chemical variances. We aim to isolate variables such as crystal length and orientation, porosity, pore percent, and surface area. These factors influence the MOF’s ability to capture CO_2 as capacity, kinetics, and selectivity are affected and measured by TGA and our house dynamic gas sorption system. By tuning the nanostructure of these materials, we aim to optimize these variables to alleviate the energy burden of sorbent regeneration.

References:

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AS-ThP-11 XPS Analysis of Plasma Exposed TiB2 and ZrB2 Substrates, ***Harry Meyer***, *Lauren Nuckols, Chad Parrish,* Oak Ridge National Laboratory

Deuterium and hydrogen plasma exposures were performed on ultra-high temperature ceramics TiB2 and ZrB2 using the PISCES-RF linear plasma device as early screening tests for first wall, plasma facing material applications. These ion plasma exposures were performed using 40 eV ion energies at 240, 525, and 800 ◦C sample temperatures and 90 eV ion energies at 240 ◦C sample temperatures to analyze TiB2 and ZrB2 sputtering and surface morphology evolution behavior. Post-plasma exposure chemistry characterization of the near surface (< 50 nm) region using x-ray photoelectron spectroscopy (XPS) shows transition metal enrichment, indicating boron preferential erosion, and resulting in reduced total sputtering yields compared to predicted assuming stoichiometric sputtering. Transition metal to boron fractions vary with plasma exposure temperature under the 40 eV ion energy exposure at different temperatures; metal enrichment is maximized at 800 ◦C and then minimized at 525 ◦C. Sputtering yield measurements of the 40 eV ion energy plasma exposed samples show that the samples with greater metal surface enrichment have lower sputtering yields, likely due to the rougher surfaces of the more metal-enriched samples leading to higher instances of prompt redeposition processes. XPS data was acquired on the as-exposed TiB2 and ZrB2 samples. Depth profiles were then done to track the amounts of T (or Zr) and B as a function of Ar-ion sputter depth. Data was finally acquired on the well sputtered sample surfaces. This abstract has been authored by UT-Battelle, LLC under Contract No. DE-AC05-00OR22725 with the U.S. Department of Energy.

AS-ThP-12 Thin-Film Characterization Using the Surface Analysis Toolbox: From Data to Answers, ***Jonathan Counsell***, Kratos Analytical Limited, UK

Thin films play a critical role in semiconductor devices and coatings due to their unique physical and chemical properties. Accurate characterization of these films is essential for understanding their behaviour and optimizing their performance. The surface analysis toolbox, including techniques such XPS, HAXPES and both destructive and non-destructive methods.

In this study, we utilize the surface analysis toolbox to characterize metal oxide and nitride thin films focusing on the interfacial regions where different materials meet. We employ XPS to determine the chemical states of elements in the thin films, particularly focusing on interfacial oxidation states. HAXPES is used to complement XPS by providing information on the elemental composition and depth profiling of the thin films.

By integrating these surface analysis tools, we capture detailed information about the chemical interactions and electronic configurations at the interfaces. Our work aims to bridge the gap between raw data and meaningful interpretations, providing a comprehensive understanding of the thin-film characteristics. Through optimized sample preparation and advanced data analysis techniques, we offer insights into the fundamental properties of thin films, enabling the development of more reliable and efficient semiconductor technologies.

AS-ThP-13 Cryo-XPS of nanoparticles. Vitrification... where speed is everything!, ***Chris Moffitt***, Kratos Analytical Inc.*; Liam Soomary,* kratos Analytical Inc, UK

Vitrification, a rapid cooling process that prevents ice formation, is crucial for preserving the structural integrity of nanoparticles during cryogenic applications. In this study, we employ Cryo-XPS (X-ray Photoelectron Spectroscopy) to investigate the surface chemistry and phase transformations of various nanoparticle types during the vitrification process. Our findings highlight the importance of ultrafast cooling rates in maintaining the desired physical and chemical properties of these materials. We discuss the challenges associated with achieving uniform vitrification across different nanoparticle sizes and compositions and propose strategies to optimize and improve experimental workflows during the vitrification process for enhanced material stability and performance. These insights are particularly relevant for applications in nanotechnology, biomedicine, and advanced materials science.

AS-ThP-14 Surface and Bulk Characterization of Organic Macrocyclic Coordination Compounds Using XPS and UPS Techniques, ***David Surman***, Kratos Analytical Inc.

Organic semiconductors have gained attention due to their potential for flexible, lightweight, and low-cost electronic applications. These materials enable charge transport via delocalized electronic states, a characteristic of their pi-conjugated molecular structures. Their utility includes various organic electronic devices, such as Organic Thin-Film Transistors (OTFTs) and Organic Photovoltaics (OPVs). The selection and performance of these materials depend on properties such as charge carrier mobility, energy level alignment, and stability. Here we utilize a combination of experimental methods - XPS and XPS imaging, to probe the surface and bulk properties of both blanket and printed organic semiconductor structures. We will discuss the relevance of scattered electron backgrounds and background subtraction for analytical clues. Also, we will explore the effects of deposition processes and the evolution of electrical properties as a function of depth using Argon cluster etching ultra thin layers. UPS is also used in with profiling to give not just an elemental distribution but also the electronic properties of these molecules as a function of depth, determining the work function of these materials, a critical parameter in optimizing charge injection and transport. A methodological approach to surface characterization will also be discussed, providing insights into the interfacial properties that govern device performance.

AS-ThP-15 Automatically Determining the Cutoff of the Transfer Function in Reciprocal Space for the Fourier Denoising of X-ray Photoelectron Spectroscopy Data, ***Tyler B. Andersen***, *Maxsym Gerashchenko, David E. Aspnes, Matthew R. Linford,* Brigham Young University

The Fourier denoising of X–ray photoelectron spectroscopy (XPS) data is valuable when optimal (low noise) XPS data cannot be collected. It should also prove to be important when preparing XPS data for analysis by artificial intelligence (AI). Because of its sigmoidal shape in reciprocal space, its adjustable position, and the shape of its Fourier transform in real space, the Gauss-Hermite transfer function is an excellent transfer function for denoising data. However, the position of this transfer function on a set of Fourier coefficients is determined manually by the user. In this work, we describe two algorithms for automating this positioning. It is believed that these algorithms will also work for other transfer functions, e.g, the brick wall filter function. In addition, these approaches should apply well to data from other techniques, for example, spectroscopic ellipsometry, low-energy electron scattering, and x-ray diffraction, among others.

AS-ThP-17 Heterointerface-Induced Charge Transfer Kinetics in Sputtered $Mote_2$-Mos_2 Nanocomposite for High-Performance Ambient No_2 Detection, *Sonika Kodan,* ***Ramesh Chandra***, Indian Institute of Technology Roorkee, India

The present research reports a nanostructured $MoTe_2$-MoS_2 n-n heterojunction-based gas sensor developed on a silicon (Si) substrate, demonstrating room-temperature (RT, 30 °C) nitrogen dioxide (NO_2) sensing. A controlled and one-step magnetron co-sputtering approach is utilized to deposit $MoTe_2$-MoS_2 nanocomposite thin film on a Si substrate, producing a uniform, dense, and porous nanoscale morphology. Herein, surface analysis and structural characterization of the $MoTe_2$-MoS_2/Si sensor reveal a rough, and defect-rich morphology with abundant exposed edge sites, which significantly enhances the availability of active adsorption sites for effective gas sensing. The developed $MoTe_2$-MoS_2/Si heterostructured sensor delivers an exceptional sensor response of 74.4% with an ultrafast response/recovery time of 7.5/2 s towards 25 ppm NO_2 at RT. Additionally, the present sensor showcases highly reproducible and consistent behavior over a wide range of NO_2 concentrations (1-60 ppm), along with remarkable selectivity against common potential interfering gases (H_2S, NH_3, CO, H_2) and a low detection limit of 700 ppb. This study provides critical insights into NO_2 sensing induced by heterointerface band modulation and defect-assisted adsorption at the sensor's surface, thereby providing a strong foundation for a reliable platform for high-performance NO_2 gas sensors based on the MoTe2-MoS2 heterostructure.

AS-ThP-18 ASSD Student Award Finalist Poster: Sen-Banerjee (SB) Number as a Unified Scaling Parameter for Deviant Density Enhancement in Nanofluids, ***Anusree Sen***, *Debjyoti Banerjee,* Texas A&M University

Nanofluids are attractive for modulating heat transfer (thermal management), energy storage (e.g., battery), transport, and radiation-shielding applications because adding nanoparticles can anomalously change the effective properties of a base fluid (neat solvent). In practice, measured property changes (e.g., density) do not match the classical two-

phase mixture model predictions. This mismatch is usually tied to interfacial effects near the particle surface that standard models do not include.

In this study, we evaluate the Sen-Banerjee number (S_B) as a practical scaling parameter for interpreting and predicting these anomalous density deviations. The analysis leverages a three-phase model of a nanofluid: the nanoparticle, the surrounding bulk liquid, and a compressed interfacial liquid layer formed at the solid-liquid boundary (this is also termed as the "*nano-Fin effect*" or "*nFE*"). We tested the framework across three representative nanofluid families, molten-salt nanofluids, poly-alpha-olefin nanofluids, and casein oleo-nanofluids, while varying nanoparticle shape, nanoparticle mass fraction, and interfacial-layer thickness.

A clear pattern emerges when surplus density is plotted against the Sen-Banerjee number (S_B). Interestingly, results from different systems and particle geometries collapse toward a common trend. At low S_B, density enhancement is stronger and highly sensitive to small changes in concentration. At higher S_B, the response gradually approaches classical mixture-rule behavior (two-phase mixture rule). Among the systems studied, casein oleo-nanofluids show the strongest deviations, consistent with their density contrast between phases. Overall, SB offers a physically meaningful and scalable way to compare nanofluids and guide formulation choices for targeted applications.

KEYWORDS: Sen-Banerjee number; nanofluids; deviant density; interfacial compressed layer; nano-Fin effect; thermophysical properties; scaling analysis; density enhancement, anomalous property, nFE.

AS-ThP-20 A Priori designed NiAg Single-Atom Alloys for Selective Epoxidation Reactions, ***E. Charles H. Sykes***, Tufts University

Ethylene oxide, produced through the partial oxidation of ethylene, is one of the highest-volume chemicals manufactured globally—and also one of the most carbon-intensive. While silver (Ag) catalysts can achieve high selectivity (~90%) for ethylene oxide, this requires a combination of promoters such as chlorine (Cl), which increases selectivity by 25%, cesium (Cs), and rhenium (Re). The reaction must also be run at low conversions (<15%) to prevent complete combustion of ethylene to CO_2. In this work, we present a theory-guided investigation showing that the incorporation of small amounts of nickel (Ni) into Ag(111) surfaces lowers the activation barrier for O_2 dissociation and facilitates the spillover of atomic oxygen onto the Ag surface. Temperature-programmed desorption (TPD) experiments confirm the facile dissociation, spillover, and desorption of O_2 on NiAg(111). Remarkably, and in contrast to previous studies, Ni enables the formation of atomic oxygen on Ag(111) under near-ultra-high vacuum conditions without the need for oxygen atomizers or reactive species like NO_2 or O_3. Ambient pressure X-ray photoelectron spectroscopy (AP-XPS) further reveals that Ni not only promotes O_2 activation and spillover but also stabilizes nucleophilic oxygen species, which are typically associated with total combustion pathways. Guided by these findings, we synthesized and tested supported catalysts, demonstrating that NiAg single-atom alloy nanoparticles improve both conversion and ethylene oxide selectivity by 25%—achieved without the use of Cl, the ubiquitous industrial promoter.

Reference

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