

## Undergraduate Poster Session

### Room Ballroom BC - Session UN-ThP

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### UN-ThP-1 Nitrogen Plasma Treated-Polylactic Acid: Examining pH Variations During Degradation, *Imaandeeep Bual, Morgan Hawker, California State University, Fresno*

Polylactic acid (PLA) is a promising biodegradable polymer that degrades at a faster rate than conventional fossil fuel polymers and can combat the growing issue of plastic pollution. Moreover, it is an excellent alternative to the growing issue of microplastics because it can be readily degraded through hydrolysis. Although PLA is biodegradable, it induces environmental change when degrading. Specifically, the degradation of PLA in soil via hydrolysis has been shown to lower the soil's pH, adversely affecting plant growth. Previous research demonstrates that certain plants containing nitrogen-processing bacteria use nitrogen moieties to raise the pH of soil. Furthermore, PLA has been shown to degrade at an accelerated rate in alkaline conditions. We hypothesize PLA degradation can be induced by introducing nitrogen functional groups on the surface via nitrogen plasma treatment (NPT), which can then act as Lewis bases upon degradation. The impact of NPT on PLA degradation has not been previously investigated at large.

This study examined the change in pH as NPT PLA degraded in room temperature DI (deionized) water. PLA films were fabricated and plasma treated in an inductively-coupled plasma reactor using nitrogen gas as the precursor. Plasma treatment parameters including 30 W, 328 mTorr, and two minutes of treatment time were selected based on previous literature and optimized to maximize nitrogen incorporation. NPT PLA films and untreated control films were then submerged in 10 mL of DI water at room temperature to initiate degradation. Changes in pH of NPT and control PLA films were compared after degradation. Previous results showed no significant difference in pH change associated with one week of degradation of PLA between control and NPT films, necessitating longer-term degradation studies of NPT PLA film degradation with a specialized pH probe. Collectively, NPT shows potential to alter the chemical degradation of PLA when compared to native PLA degradation.

### UN-ThP-2 Studying Dna Base Pairing by Examining Adenine and Thymine Through Electrospray-Ionization Mass Spectrometry, *Connor McIlvain, S. Alex Kandel, University of Notre Dame*

Examining molecular interactions in solution can give insight into intermolecular forces with applications to cluster formation and crystallization. Electrospray-ionization mass spectrometry (ESI-MS) allows for the study of non-covalent molecular clustering patterns as electrospray is a soft enough ionization technique to preserve molecular clustering. Cluster stability is expected to decrease with size; however, large, unusually stable clusters, called magic number clusters, occasionally occur and are disproportionately represented in the mass spectra. Adenine and thymine are Watson-Crick base pairs, so the interactions driving their assembly deserve further study. Alone, adenine displays expected exponential cluster decay with size, except in the case of adenine trimers, which are disproportionately disfavored. Adenine dimer and tetramer formation could be explained by both Watson-Crick and Hoogsteen binding. The expected exponential cluster decay is also observed for thymine, with the exception of the dimer, which is disproportionately represented. Together, adenine and thymine display the same clustering tendencies with the addition of adenine:thymine clusters. In this case, the exponential decay is disrupted by the formation of magic number clusters, the 3:1 adenine:thymine tetramer, and the 3:2 adenine:thymine pentamer. Trimers of all kinds were still underrepresented. This clustering behavior indicates a high level of noncovalent intermolecular interaction outside of traditional Watson-Crick base pairing. This system is further studied through the introduction of the nontraditional base pair 6-O-methylguanine (6-OMG) with thymine to better understand the forces around Watson-Crick base pairing and Hoogsteen binding. These solution clustering experiments have the potential to improve the current understanding of molecular self-assembly, even outside of traditional Watson-Crick base pairing, and could further be augmented by future scanning tunneling microscopy experiments.

### UN-ThP-3 Investigation of Spinel and Sapphire Plasma Etching for Development of Anti-Reflection Nanostructures, *Sean Campbell, Thomas Hutchens, Stephanie Alvarez, Jacob Hay, Tyler Benge, Ishwar Aggarwal, The University of North Carolina at Charlotte*

In the field of high-energy lasers, there is a need for optical windows that exhibit high transmittance in the visible to mid-wave-infrared wavelength range (MWIR). This can be done with the patterning of nanoscale anti-reflective (AR) structures onto spinel and sapphire substrates. AR structured surfaces (ARSS) have shown to exhibit higher laser damage thresholds compared to thin-film AR coatings. The substrates are etched with a reactive ion plasma etcher and subsequently characterized with the help of a Fourier Transform Infrared Spectrometer (FTIR). Different etch chemistry and their respective etch rates were investigated, as well as optical transmission performance of the materials at visible to MWIR wavelengths. Future work involves masking of the substrate via photoresist and fine-tuning the scalability of the masking and etching process to larger substrate form factors.

### UN-ThP-4 Suppressing the Hydrophobic Recovery of Polyurethane Treated with Ar/O<sub>2</sub> Plasma, *Deevyam Malik, Morgan Hawker, California State University, Fresno*

Polyurethane (PU) is well-suited for indwelling catheters due to its durability and flexibility. However, its inherent hydrophobicity promotes thrombosis and biofouling, leading to complications such as catheter-related bloodstream infections and venous occlusions. Plasma surface modification can improve PU's hydrophilicity by incorporating polar functional groups. PU, however, exhibits significant hydrophobic recovery within one day after treatment with air, N<sub>2</sub>, O<sub>2</sub>, and Ar plasma precursors, meaning the polymer reverts to its original hydrophobic state after treatment. Studies on polydimethylsiloxane demonstrate that while individual feedgases (Ar and O<sub>2</sub>) enhance hydrophilicity, their combination in an argon/oxygen (Ar/O<sub>2</sub>) plasma mixture more effectively reduces hydrophobic recovery. This effect has not, however, been examined for PU. Extending this approach to PU has the potential to slow down aging after plasma modification.

This study investigates the influence of varying Ar/O<sub>2</sub> plasma precursor concentration on PU's hydrophobic recovery, incorporating an optimized 7% Ar / 93% O<sub>2</sub> composition by pressure— previously shown to mitigate hydrophobic recovery on polydimethylsiloxane. PU samples were plasma-treated using a radio-frequency low-pressure reactor (25 W, 2 min, 300 mTorr), with systematically varied argon composition in the feedgas. Samples were aged for 12 days, with water contact angle (WCA) measurements taken at 1, 2, 3, and 4 hours post-treatment, followed by measurements at 1, 4, 7, and 12 days. Contact angle goniometry was used to assess wettability as a function of aging. Preliminary results indicate that 100% Ar plasma achieves the greatest hydrophilicity and the greatest reduction in hydrophobic recovery compared to other feedgas compositions, with water contact angles increasing from 39.24±0.74° to 55.24±0.97° over 12 days. By enhancing the longevity and effectiveness of plasma treatment, this work aims to improve the performance and efficacy of PU in antibacterial catheters.

### UN-ThP-5 Freshwater Biofouling Analysis of Nano-Textured and Anti-Reflection Coated Windows, *Stephanie Alvarez, Thomas Hutchens, Sean Campbell, Jacob Hay, Tyler Benge, Ishwar Aggarwal, University of North Carolina at Charlotte*

Most high performance optical components, like lenses and windows are designed for sterile, low-contaminate environments, however, optical systems used by the Navy often operate in harsh marine and sandy environments. Improving the lifespan of optical elements in these conditions is essential. Optical elements with anti-reflective (AR) coatings or structured surfaces, which feature nano-textured elements, are particularly vulnerable to degradation. This study aims to evaluate the impact of submerged environments on these components. Long term testing was conducted on five 1-inch-diameter fused silica windows with different surface treatments: a polished blank, a hydrophilic "web-like" AR, a hydrophobic "moth-eye" AR structured surface (ARSS), a commercially available ARSS and a thin-film AR coating. Samples produced in-lab are done through high-vacuum mask deposition and plasma etching to produce the AR structured surface desired. Prior to submersion, the contact angles and optical transmission spectra of each window was measured. The samples were placed in a flotation housing unit and submerged in a semi-controlled biological freshwater environment for 30 days. Once removed, the windows were analyzed for biofouling accumulation and changes to optical performance. This experiment aims to identify how surface coatings

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and nano-structures influence the biofouling resistance of optical elements, providing insights into improving optical components durability in challenging environments.

**UN-ThP-6 Sol-Gel Hyper-Hydrophilic Anti-Fog Coatings Study & Model Of Surface Condensation Vs. Current Anti-Fog Strategies To Maximize Time-To-Fog & Optical Properties On Medical Lenses, Nicole Herbots, Sio2 Innovates LLC / Inifinitum BioMed LLC / UV One Hygienics Inc. / Arizona State University Department of Physics; Arya Bhakta, SIO2 Innovates LLC / Case Western Reserve University; Shreyash Prakash, Sio2 Innovates LLC / Inifinitum BioMed LLC; Viraj Amin, Sio2 Innovates LLC / Inifinitum BioMed LLC / University of Missouri-Kansas City School of Medicine; Ashwin Suresh, Sio2 Innovates LLC / Inifinitum BioMed LLC / University of Arizona Department of Physiology; Srivatsan Swaminathan, Sio2 Innovates LLC / Inifinitum BioMed LLC / Arizona State University / Icahn School of Medicine at Mount Sinai; Visheshwar Swaminathan, Sio2 Innovates LLC / Inifinitum BioMed LLC / UV One Hygienics Inc.; Dora D. Suppes, Mark Russell-Hill, Inifinitum BioMed LLC / UV One Hygienics Inc.; Robert J. Culbertson, Arizona State University Department of Physics; Eric J. Culbertson, Providence Santa Rosa Memorial Hospital / SIO2 Innovates LLC**

Endoscope lenses easily fog within closed body cavities, disrupting the visual field during surgery within minutes. Lens opacification is due to water vapor condensation, which forces surgeons to remove the scopes, wipe their lenses, and reinsert them. Repeated scope wiping and reinsertion increases infection risks, length of surgery and OR use, and tissue scarring due to prolonged air exposure.

Current strategies to inhibit fogging, such as alcohol-based coatings and heating, introduce complications. For example, alcohol solutions evaporate quickly and irritate damaged tissue due to their acidity. Another strategy is to pre-heat endoscope lenses; this requires reheating due to the cooling of small diameter lenses (2- 12 mm) connected to 30-200 mm endoscopes. Textured lens surfaces rapidly wear and are very difficult to clean and sterilize.

This work has developed a phenomenological model for fogging on smooth surfaces: the SEE (or Surface Energy Engineering) model with direct surface energy measurements. SEE has guided development and testing of new *hyper-hydrophilic* sol-gel coatings, KnoxFog<sup>1</sup>, using two key properties to inhibit fogging. First, coating' surfaces are *super-hydrophilic*, meaning molecules condense in 2D sheets (Frank-Vander Merwe Growth Mode) instead of 3D droplets (Volmer-Weber Growth Mode). Second, nanopores in the Sol-Gel absorb water as the condensate thickens. This combination yields a lasting anti-fog coating, where water condenses for 2+ hours into a continuous, flat film, free of optical distortion and droplets, even when exposed to blood and tissue debris.

Using four pairs of endoscopes *in vitro*, at T= 38±2°C, the time-to-fog (TTF) of a pair of identical endoscopes whose lens is coated with KnoxFog is compared in a closed cavity *simultaneously* with a pair of bare lenses and two pairs using the current anti-fog strategies. TTFs of KnoxFog coatings exceed 131 min with a variation of < 1 %. TTFs of bare lenses average less than 8 ± 8 min. *In these same simultaneous conditions of water evaporation*, a variation of 100% can occur in surgery due to a lack of controlled surface conditions on bare lenses. KnoxFog™ improves TTF by 1625 ± 1% over bare lenses, reduces by two orders of magnitude the TTFs unpredictability of bare lenses, and improves over lens tip heating, whose TTF averaged less than 1 min *in the same conditions*, and on alcohol-based coatings, whose TTF averages 47.5 min with a variability of 56%.

*In vivo* animal studies show that KnoxFog performance significantly increases TTFs and optical clarity while reducing the need for frequent lens cleaning from blood and tissues.

<sup>1</sup> Trademark owned by SIO2 Innovates

**UN-ThP-7 Exploring the Optoelectronic Properties of VS<sub>2</sub> Grown Beyond Traditional CVD Methods, Amari Gayle, Kedar Johnson, Elycia Wright, M.K. Indika Senevirathna, Michael D. Williams, Clark Atlanta University**  
Vanadium disulfide (VS<sub>2</sub>), which belongs to the family of transition metal dichalcogenides (TMDs), has garnered significant interest from researchers due to its fascinating properties. These include metal-insulator transition behavior, room-temperature ferromagnetism, a unique layered structure, and metallic conductivity. Additionally, VS<sub>2</sub> can form highly crystalline materials. With advances in achieving a more precise structure of this semiconducting material, VS<sub>2</sub> nanomaterials have the potential to be the most efficient TMDs for various photonic and optoelectronic applications. Chemical vapor deposition (CVD) has proven to be a valuable technique for synthesizing 2D materials. Its straightforward approach, alignment with

industry standards, and capability to generate high-quality crystalline samples make it an excellent choice for both researchers and manufacturers. This study examines the optoelectronic properties of VS<sub>2</sub> grown on various substrates using the chemical vapor deposition (CVD) technique, going beyond traditional methods. It identifies optimal growth parameters, including growth temperature and carrier gas flow rate. The characterization tools utilized in this research include photoluminescence, Raman spectroscopy, and confocal laser optical microscopy. These tools are employed to analyze the surface morphology, structural quality, phonon modes, and bandgap of the samples.

**UN-ThP-8 An Investigation into the Optoelectronic Properties of Layered and Vertically Aligned MoS<sub>2</sub>-MoSe<sub>2</sub> Heterostructures on Different Substrates, Elycia Wright, Clark Atlanta University; Kedar Johnson, Clemson University; Amari Gayle, Robin Rouseau, M.K. Indika Senevirathna, Michael D. Williams, Clark Atlanta University**

Two-dimensional transition metal dichalcogenide (TMD) materials offer exciting opportunities for various applications, particularly due to their unique layer-sensitive band structures, valley-selective optical coupling, and remarkable catalytic activities. Their notably large exciton binding energies and strong nonlinear optical responses underscore their potential. Moreover, by strategically stacking different monolayer TMD materials, we can create heterostructures that allow tuning band gaps across visible to infrared spectrum. This approach enhances their optoelectronic properties and opens new avenues for advancements in fields such as optoelectronics and photonics.

This research investigates the optoelectronic properties of MoSe<sub>2</sub>-MoS<sub>2</sub> heterostructures grown on various substrates, including gallium nitride (GaN) and sapphire, using the chemical vapor deposition (CVD) technique. The study also examines how the choice of substrate affects the growth of layered versus vertically aligned heterostructures. We utilize CVD techniques because they have proven more effective for producing samples with extensive monolayer growth than the commonly used exfoliation method. By analyzing the differences in bandgap, the Raman and infrared (IR) vibrational modes, we aim to reveal the unique properties of these heterostructures.

**UN-ThP-9 Correlation Analysis of In Situ Atomic Layer Deposition Mass Spectrometry Data for Surface Reaction Analysis, Ayelen Mara, Eric Bisse, Parag Banerjee, University of Central Florida**

Atomic Layer Deposition (ALD) enables precise, conformal thin-film coatings on high-surface-area nanoparticle powders through sequential, self-limiting reactions. However, coating nanoparticle beds presents unique challenges, including precursor diffusion limitations, particle agglomeration, and extremely high surface areas (reaching ~10s of m<sup>2</sup>/g). These factors complicate the ALD process, making it essential to monitor reaction progress and identify saturation ("end-pointing") within the powder bed.

In this work, we employ quadrupole mass spectrometry (QMS) as an *in situ* diagnostic tool to study Al<sub>2</sub>O<sub>3</sub> ALD on ZnO nanoparticle powder beds. Using trimethylaluminum (TMA) and ozone (O<sub>3</sub>) as precursors at a deposition temperature of 120 °C, we track methane (CH<sub>4</sub>) evolution—a key reaction byproduct—to gain insights into surface reaction kinetics and saturation behavior. Furthermore, we develop multivariate analysis tools to interpret ALD reaction dynamics in powder bed reactors with the hope of enabling better process control and optimization.

**UN-ThP-10 Naturally Derived Polymers for Biomedical Applications: Stabilizing Hydrophilicity after Nitrogen-Plasma-Treatment, Mina Abdelmessih, Morgan Hawker, California State University, Fresno**

Poly(lactic acid) (PLA) and chitosan (CS) are popular biopolymers that display tremendous potential for scaffolding applications in the biomedical field. Both polymers are renewable: PLA is produced from renewable feedstock, while CS is obtained through the deacetylation of chitin. The use of these polymers in biomedical-related applications such as scaffolding is promising due to their non-toxicity *in vivo* and biodegradability. Additionally, they each contain distinct mechanical and degradation properties suitable for different applications. However, both polymers have a hydrophobic surface, which restricts their biomedical implementations where cell adhesion is critical (e.g., in applications related to tissue and bone engineering). There is some evidence that cell adhesion and growth are facilitated by hydrophilic surfaces. Radio-frequency nitrogen plasma treatment displays promise in increasing the polymers' hydrophilicity, but also displays potential aging instability with hydrophobic recovery. This poses a significant problem for applications of the treatment especially when

considering storage-induced aging. Approaches to prevent this phenomenon in PLA and CS are widely unexplored.

This work investigated the impact of various aging conditions (storage in vacuum, cold temperature, and air) on the surface hydrophilicity of PLA and CS after exposure to nitrogen plasma. Films were prepared as model substrates using the solvent-casting method, and treated in a RF plasma reactor under optimized parameters (power, pressure, and treatment time). After treatment, the films were aged in the different aging environments for two weeks. Throughout the aging period, multiple surface analyses were conducted on samples exposed to the various preservation environments, including untreated samples as controls. Surface wettability analysis utilizing water contact angle goniometry displayed that vacuum aged PLA films and cold temperature aged CS samples possess the least hydrophobic recovery in comparison to other aging conditions. Surface chemical composition of PLA and CS samples was examined using x-ray photoelectron spectroscopy. These treatment preservation methods to PLA and CS have potential to positively impact their future use in the biomedical field as scaffolds.

**UN-ThP-11 Identifying XPS and FTIR trends in Calcium Lanthanum Sulfides via Machine Learning.** Taylor Cook, Brian Butkus, Alexandros Kostogiannes, Andrew Howe, Eric Bissel, Andrew Cooper, Hayat Soufiani, Romain Gaume, Kathleen A. Richardson, Parag Banerjee, University of Central Florida

Calcium Lanthanum Sulfide (CLS) is being studied as a potentially strong material in the field of Long Wave Infrared (LWIR) optics. Derived from the  $\gamma$ -La<sub>2</sub>S<sub>3</sub> structure and doped with CaS, we can achieve a stable CLS structure<sup>1</sup>. However, via X-ray photoelectron spectroscopy, we can see substitutional oxygen impurities within the CLS structure.<sup>2</sup> Subjecting multiple iterations of CLS powders and ceramics to metrology testing – XPS, and FTIR for example – we can gather a database on the properties of the compound. This database consists of 60+ powders and ceramic CLS samples, each with different compositions aimed at optimizing fitting to an ideal composition that provides the highest optical transmission.

This study focuses on the correlation between points of this database, focusing on correlations made between XPS and transmission gathered via FTIR. Machine learning is a useful process in determining these correlations with such a large database, as the algorithm can be trained to search for specific connections and properties.<sup>3</sup> If successful, we hope to see a direct correlation between the transmission of the CLS and the substitutional oxygen content.

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**UN-ThP-12 Bacterial Infection Detection in Drops Flattened into Thin Films by Super-hydrophilic Collection Surfaces using Macroscopic DNA/RNA Epi-Fluorescence: A hand-held sensor for Bacterial Infection Diagnosis: BacteroBug™, Arya Arya Saravanan, SiO2 Innovates/Arizona State University, Life Sciences & BioChemistry; Sriram Rajesh, SiO2 Innovates LLC; Nila Kathiravan, SiO2 Innovates LLC/InnovaBug LLC; Sudharshini Ram, Nithish Prakash, SiO2 Innovates LLC/InnovaBug LLC/ViroBug LLC; Viraj Amin, SiO2 Innovates LLC/InnovaBug LLC/University of Missouri - Kansas City (School of Medicine); David Guo, SiO2 Innovates LLC/Innovabug LLC/Drexel University/University of Arizona School of Medicine; Eric J. Culbertson, SiO2 Innovates LLC/InnovaBug LLC/Microbe Lab-On-Chip LLC; Robert J. Culbertson, Arizona State University Department of Physics; Nicole Herbots, SiO2 Innovates LLC/InnovaBug LLC/Microbe Lab-On-Chip LLC/Arizona State University**

In 2025, the gold standard for bacterial infection diagnosis, developed in the 70s, is plate culturing. State-of-the art infection diagnostics use the universally accepted Colony Forming Units (CFUs) counting on cultured plates, which requires 10-30 mL of blood, urine, sputum, etc... and 2-3 days for results.

However, about 40% of all positive cultures are false positives due to contamination from skin pathogens and handling in blood, urine, sputum, etc... during collection or environmental contaminations.

Per the NIH, false positives are "independently associated with increased subsequent laboratory charges (+20%) and IV antibiotic charges (+39%)". The excess of diagnosed infections costs US hospitals about \$20+Billions/year in 2025. False positives lead to administration of antibiotics in healthy patients, leading to antibiotic resistance, and to more than 48,000 US deaths/ year.

New, reliable methods are needed for bacterial detection, loads, infection diagnosis.

The present research investigates whether Macroscopic DNA Epi-Fluorescence (MaDRE) can be used for bacterial detection, and whether macroscopic epi-fluorescence intensity scales quantitatively with bacterial load in small volume drops using fluorophores developed for fluorescence microscopy. To sort detected microbes by class, 3 fluorophore combinations are designed to detect DNA/RNA in live bacteria and protozoa, RNA in viruses, and fungi-specific proteins.

A quantitative study was thus conducted to establish whether a MaDRE-based device is viable in accuracy and reproducibility. An initial stock solution in Luria Broth is diluted logarithmically into 10 bacterial serial loads from 1.0 to 10<sup>-9</sup> for calibration. Next, MaDRE's sensitivity is tested on these 2 x ten bacterial loads, to establish whether 520 nm fluorescence intensity of safe green DNA fluorophores I<sub>g</sub> scales reproducibly with bacterial concentration. The two sequential experiments were conducted by applying four 0.1 mL identical drops from each of the 20 solutions on 2 hyper-hydrophilic prototype strips.

I<sub>g</sub> is normalized to the 497 nm excitation intensity, I<sub>b</sub>, before and after 0.1 mL dye drops are applied, as RG/B. The difference between post-dye R<sub>Raw</sub> and pre-dye R<sub>Bgd</sub> yields the net R<sub>Net</sub>

R<sub>Net</sub> averages of 8.5 ± 2.1 for 300k *E.Coli* CFU/mL, and 3.6 ± 0.34 for 100 k *E.Coli* CFU/mL. Thus, R<sub>Net</sub> decreases 250% with a decrease of one order of magnitude in bacterial load. Pre-dye R<sub>Bgd</sub> averages = 1.8 ± 0.25, thus lower by a factor 2 to 4 than post-dye R<sub>Net</sub>.

Hence, the normalized fluorescence ratio R<sub>G/B</sub> scales with bacterial concentration consistently using 0.15 mL drops, and a handheld, small volume device is presently prototyped, BacteroBug™.

**UN-ThP-13 Machine Learning for Designing 'Undesirable' Metal-Organic Frameworks, Satya Kokonda, Charter School of Wilmington**

Many crucial processes are too complex for computational modeling, requiring experimentation to identify promising materials. Here, a general methodology for application specific material design is presented, while photocatalysis is presented as a specific case-study. Metal-Organic Frameworks (MOFs) are a subset of highly promising porous nanomaterials, used in a variety of 'unmodellable' applications. Reinforcement learning generated 60,000 novel MOFs optimized for CO/H<sub>2</sub>O selectivity. A predictor funnel system was created, iteratively removing low-scoring MOFs to 10,986 potential candidates, improving computational efficiency by 276%. Graph neural networks predicted features for creating a fitness function incorporating stability, catalytic ability, material cost, sustainability, and adsorption while allowing the inclusion of application specific design criterion. This designed function provides a computational method to model photocatalytic performance- and filtered down to two promising

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MOFs which each pass a myriad of synthesis criteria, first a Cr-based MOF with photocatalyst score 230% higher than the control. Second, a Zn-based MOF outperforms the best control across all relevant metrics, demonstrating robustness against variable fitness functions. Furthermore, analysis revealed insightful design patterns, such as the significant influence of metal cluster N262 on catalytic performance, providing a method for future work to narrow the chemical space. By incorporating industrially applicable features such as cost or stability of the material, this work successfully designs industrially promising materials in otherwise unmodellable processes such as drug delivery, while paving a method for multi-objective optimization incorporating 260% more features than prior work.

**UN-ThP-14 Statistical Optimization of Polynomial Fits for Carbon Bonding Analysis in XPS**, *Garrett Lewis, Matthew Linford, Alvaro Lizarbe*, Brigham Young University; *David Aspnes*, North Carolina State University

X-ray photoelectron spectroscopy (XPS) is a valuable tool for surface-level chemical analysis, particularly effective in assessing carbon hybridization states through the D-parameter, which distinguishes  $sp^2$  and  $sp^3$  bonding. Because this analysis involves differentiation, proper signal smoothing is critical to minimize the effects of noise. In this work, we explore high-order polynomial fitting as a general approach to prepare carbon Auger data for D-parameter analysis. To enhance reproducibility and reduce subjectivity, we introduce an algorithmic method for identifying the most suitable polynomial orders for smoothing. This approach evaluates the underlying structure of the data to balance over- and underfitting without relying on visual judgment. The results demonstrate that using statistical tools to guide polynomial selection leads to more reliable analysis of carbon bonding in XPS data. While developed for carbon Auger analysis, this method can be extended to other contexts where spectral smoothing is required for derivative-based measurements.

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