Undergraduate Poster Session
Room Central Hall - Session UN-ThP

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UN-ThP-1 Using Fourier Smoothing to Calculate D-Parameter for Carbonaceous Samples*, **Kristopher Wright**, M. Linford,* Brigham Young University

Carbon samples reveal much about their properties through surface analysis. X-ray photoelectron spectroscopy (XPS) has proven itself a reliable approach to analyzing surfaces of all material, including carbon samples. We can use the carbon Auger peak as an important tool for characterizing the ratio of sp2 to sp3 hybridization of carbon samples. This is accomplished through determining the D-parameter, which is related to the energy difference between the first derivative minima & maxima, and which is directly proportional to the sp2:sp3 ratio of the sample. The D-parameter has many important uses, such as determining graphite versus diamond composition in a material. In the past, the characteristically noisy auger peak has made the D-parameter difficult to determine. In this poster, will be looking at various carbon samples ranging from sp3 carbon (such as diamond), polymers, and sp2 carbon samples (like HOPG) using a new approach to determining the derivative of the Auger peak via a Gauss-Hermite Filter. The Gauss-Hermite Filter convolves the data with a transfer function by utilizing Fourier analysis to break down XPS data into its components, then multiplying these by the reciprocal of the transfer function. The result is a minimalization of high frequency noise while preserving the lower frequency components that are characteristic of the signal.

UN-ThP-2 Calcium Lanthanum Sulfide - An Investigation Via X-Ray Photoelectron Spectroscopy*, B. Butkus, **Taylor Cook**, A. Kostogiannes, A. Cooper, A. Howe, R. Gaume, K. Richardson, P. Banerjee,* University of Central Florida

Calcium lanthanum sulfides (CLS) are crucial in applications requiring high optical transmissivity in the long-wave IR regime. These ternary sulfides, forming solid solutions of CaS and La_2S_3 in a cubic Th_3P_4 phase, exhibit varying cationic vacancies depending on the Ca:La ratio to maintain stoichiometric balance and charge neutrality.

Using X-ray photoelectron spectroscopy (XPS), we analyzed the chemical and bonding states of hot pressed CLS ceramics. Our findings confirm the stoichiometry aligns with the expected Ca:La ~ 10:90 composition, revealing an intrinsic ≥10 at% oxygen impurity even under inert conditions. This suggests oxygen substitution for sulfur, particularly bonding with La, which may influence the material's optical properties as experimentally seen in the lower IR transmission of CLS and development of absorption bands in the long-wave IR regime. The interpretation and conclusions are made from data of over 30 CLS samples with varying compositions. A multivariate analysis of the composition also support the hypothesis that oxygen substitutes for sulfur in the CLS lattice.

This study highlights the persistent challenge of oxygen incorporation in CLS and suggests potential processing modifications to enhance material purity and performance.

UN-ThP-3 Avoiding Common Errors in X-ray Photoelectron Spectroscopy Data Collection and Analysis*, **Braxton Kulbacki**, J. Pinder,* Brigham Young University*; G. Major,* Texas Instruments*; M. Linford,* Brigham Young University

X-ray photoelectron spectroscopy (XPS) is the most popular surface characterization technique because of its ability to determine the composition and chemical state of the first 5-10 nm of various materials. Although widely used, correct collection procedure, technique and reporting are not widely understood. Experts in other scientific fields use XPS, but are often not experts in XPS as well, so technical errors such as incorrect data interpretation and presentation, incorrect reporting of instrumental parameters, unjustified conclusions and unjustified peak fittings are common. Publications with these errors have made experimental reproduction difficult and have caused a reproducibility crisis. The following presentation is intended to bring awareness to common errors observed. Some common examples include: data collection, peak fitting errors, background errors, data presentation errors and data reporting errors.

UN-ThP-4 Deposition of Cobalt-Doped Zinc Oxide Nanocrystals via Successive Ionic Layer Adsorption and Reaction*, **Luis Tomar**, K. Ye, S. Xie,* University of Central Florida*; M. Chang, J. Baillie,* University of Washington*; T. Currie, F. Liu, T. Jurca,* University of Central Florida*; D. Gamelin,* University of Washington*; P. Banerjee,* University of Central Florida

Transition metal doped semiconductors are highly desired due to new functionalities enabled by the dopants. For example, Co-doped ZnO has been shown to be a magnetic quantum dot [1]. These materials are typically synthesized in the form of nanoparticles [1], and the ability to synthesize these materials as high-quality thin film is desirable for their applications in optics and electronics. Successive ionic layer adsorption and reaction (SILAR) provides a simple approach to create transition metal doped semiconductors, while providing control over the film thickness and dopant concentration. SILAR works via a series of liquid-phase ionic reactions that are self-limiting, similar to atomic layer deposition [2].

This work aims to synthesize Co-doped ZnO films using a SILAR process. The approach involves adapting the mechanism of solution-based nanoparticle process into a SILAR process. While the solution process involves the rigorous mixing of the precursors to precipitate Co-ZnO nanoparticles, the SILAR process discretizes the use of these compounds into separate dip-coating steps. Thus, by simply controlling the solution concentration and number of cycles, films of various thickness are formed. The films are evaluated using ultraviolet-visible spectroscopy (UV-Vis), scanning electron microscopy, energy dispersive x-ray spectroscopy, and x-ray photoelectron spectroscopy to confirm the successful doping of the isovalent Co^{2+} in the ZnO lattice.

References:

[1] D. A. Schwartz, N. S. Norberg, Q. P. Nguyen, J. M. Parker, and D. R. Gamelin, “Magnetic Quantum Dots: Synthesis, Spectroscopy, and Magnetism of Co2+- and Ni2+-Doped ZnO Nanocrystals,” *Journal of the American Chemical Society*, vol. 125, no. 43, pp. 13205–13218, Oct. 2003, doi: https://doi.org/10.1021/ja036811v.

[2] Samantha Prabath Ratnayake, J. Ren, E. Colusso, M. Guglielmi, A. Martucci, and Enrico Della Gaspera, “SILAR Deposition of Metal Oxide Nanostructured Films,” *Small*, vol. 17, no. 49, Jul. 2021, doi: https://doi.org/10.1002/smll.202101666.

UN-ThP-5 Assessing and Recommending Standards to Improve Reproducibility in Thin Film Analysis; a Multi-Faceted Approach*, **Jacob Crossman**, M. Linford, J. Pinder,* Brigham Young University

Reproducibility is a key component of the scientific method requiring data collection to be repeatable by oneself and/or others. Also known as replication, reproducibility (or rather, a lack thereof) has established itself as a growing crisis in the scientific community—many studies are being published without providing sufficient information for an outside source to replicate and corroborate findings, thereby reducing confidence in those studies. The variety of scientific fields requiring vacuum technology, including thin film research, are not immune to the reproducibility crisis. Because thin film sciences are crucial to advancements in solar array, computer microchip, and LED technologies, it stands to reason that the scientific community should expect a high degree of transparency and reproducibility from this research. Techniques such as thin film synthesis using ALD or CVD and analysis via methods such as XPS, LEIS, or SE, must be reproducible both internally and externally. This means a researcher should be able to internally reproduce a material or measurement multiple times consistently. Additionally, should that researcher choose to publish his or her findings, he or she should provide sufficient information for an external researcher to reproduce those findings consistently and accurately. This system of reproducibility helps ensure the integrity of research. In this presentation, we pose recommendations and reminders to make sure reproducibility remains central to the research process. To ensure internal reproducibility, we recommend a thorough recording of procedures and tests for consistency. Creatively deploying physical and procedural measures, such as fitment jigs and SOPs are paramount to ensuring internal reproducibility. Externally, we suggest clarity in instrument parameter reporting (such as the tables found in certain SSS articles) and clear, complete supporting information. Any paper published should contain all the information necessary for someone else to perform the same experiment. With recommendations such as these in mind, researchers will continue to prioritize reproducibility and increase the transparency of their research to combat the replication crisis.

UN-ThP-6 Enhancing the Selectivity of Acetaldehyde Formation Using a Copper-based Model Catalyst*, **Joseph Loiselet**, A. Baber,* James Madison University

Acetaldehyde is a common intermediate in many industrial chemical syntheses. Current methods of acetaldehyde formation are inefficient and wasteful, leading to low product yields and unwanted by-products. In order to improve acetaldehyde yield and minimize other products, the dry dehydrogenation and dehydration of ethanol was observed using temperature programmed desorption (TPD). These reactions occurred on flat, roughened, and oxidized Cu(111) surfaces under ultrahigh vacuum (UHV) conditions. The reaction of ethanol over each surface was studied, and the oxidized Cu(111) most readily formed acetaldehyde and hydrogen at 350 K. A second reaction pathway formed ethylene and water at 350 K. The selectivity for acetaldehyde production was maintained over 80% throughout consecutive TPDs, yet the yield decreased continuously as the surface became less oxidized. Future experiments will study the reactivity of a partially oxidized Cu(111) sample using UHV-TPD.

UN-ThP-7 Optimizing XPS Analysis with Maximum Entropy for Determination of the D Parameter*, **Garrett Lewis**,* Brigham Young University

In spectroscopy, the aim is to gather insights through the examination of spectra that are ideally clear of distortions and free from noise. The Maximum Entropy filter is another technique to de-noise XPS that works by preserving both high and low-order coefficients. It achieves this by utilizing the trends established by the low-order Fourier coefficients and projecting them into the white noise region (high-order coefficients). X-Ray Photoelectron Spectroscopy (XPS) is a surface analytical technique used to survey the top 5-10 nm of a sample. In sample analysis, XPS unveils the carbon Auger peak, a product of secondary electron emission upon ejection of a core-level electron from a carbon atom, subsequently filled by an electron from a higher energy level. The carbon Auger peak is pivotal in assessing the D-parameter, a ratio between sp^2 and sp^3 hybridization in carbonaceous materials such as diamond and highly oriented pyrolytic graphite (HOPG). By utilizing the maximum entropy filter, we can demonstrate its effectiveness in enhancing data quality through smoothing, thereby aiding in the determination of the D-parameter via the carbon Auger peak. This improved understanding of material characteristics enhances their potential applications.

UN-ThP-8 Copper by X-Ray Photoelectron Spectroscopy (XPS) at Pass Energies from 10 – 200 eV*, **Annika Dean**, S. Jafari, M. Linford,* Brigham Young University

X-ray photoelectron spectroscopy (XPS) is an important analytical technique that provides chemical information about surfaces. XPS analyses of metallic copper were performed at different pass energies, ranging from 10 to 200 eV. The pass energy determines the kinetic energy at which the emitted photoelectrons pass through an analyzer and enter the detector. The pass energy determines the energy resolution of the experiment. While survey scans are generally taken at high pass energies, narrow scans are taken at lower pass energies to achieve a higher resolution. Higher resolution can aid in distinguishing between peaks that are close together, such as spin-orbit split peaks, or for identifying fine features in spectra. As expected, lower pass energies result in better resolution but lead to increased noise in spectra. Selecting an appropriate pass energy therefore includes considerations for both the spectral resolution and the desired signal-to-noise ratio.

UN-ThP-9 Structure of Benzyl Isothiocyanate Self-Assembled Monolayers on Au(111)/Mica Surfaces*, **Darya Moiny**, L. Tackett, L. Penland, D. Ovchinnikov, R. Farber,* University of Kansas

Benzyl isothiocyanate (BITC) is an aromatic thiolate of biological importance and is utilized in biofunctionalization, such as the bio fabrication of nanoparticles encapsulated with BITC as a method of drug delivery. Notably, the coexistence of both the stabilizing pi-pi interactions and destabilizing electron withdrawing cyanide group can influence the packing structure and formation of the SAM of BITC. While BITC can be used to modify Au surfaces for biological applications, there is little known about the molecular packing structure of BITC self-assembled monolayers (SAM) on Au surfaces.

In this work, tapping mode atomic force microscopy (AFM) was used to investigate the relationship between solution concentration and incubation time on the molecular structure of BITC SAMs. After initial characterization of Phasis epitaxial gold, Au(111)/Mica, to determine the structural properties of the Au surface, Au(111) was incubated in a 2 mM ethanolic solution for 24 hours. AFM revealed minimal structural evolution to the Au surface, suggesting that a BITC monolayer did not form. The sample was then placed back into solution for another 41 hours, bringing the total incubation time to 65 hours. Following the prolonged incubation in BITC, a linear pattern was seen across the surface, suggesting the formation of a BITC SAM. To understand the relationship between concentration and BITC SAM formation, the solution concentration was increased by a magnitude of 10. Similar to the 2 mM preparation, there was no noticeable structural evolution following a 24-hour incubation. Incubating the Au substrate for 65 hours in the 20 mM solution did, however, result in the characteristic linear pattern seen for the 0.2 mM sample preparation.After establishing that an incubation of 65 hours was needed to form a uniform BITC SAM, the solution concentration was increased to 0.2 M. Following a 65-hour incubation, a new ring-like pattern was seen across the surface suggesting the formation of a new structure at higher BITC concentrations. Ongoing work is focused on using ultra-sharp AFM tips to investigate SAMs formed following a 65-hour incubation in a 20 mM BITC solution to resolve the exact molecular structure of the BITC SAM. In addition to continued AFM imaging,Future work will focus on imaging the BITC SAMs using ultra-high vacuum scanning tunneling microscopy (UHV-STM) and scanning tunneling spectroscopy (STS) to further investigate the structural and electronic properties of the surface of the SAM at the atomic scale.

UN-ThP-10 Computationally Enhanced Experimental Investigation of Reactivity of Isomeric Butanol on TiO_2/Au(111)*, **Haley Frankovich**, E. Euler, L. Garber, A. Galgano, K. Letchworth-Weaver, A. Baber,* James Madison University

Biofuels can be used to reduce global dependence on fossil fuels while contributing to a carbon-neutral cycle. Biobutanol has low volatility and multiple transportation options which make it an attractive alternative fuel. Understanding the fundamental thermal catalysis processes of butanol over heterogeneous model catalysts can aid in the design of more efficient catalysts. To better understand the processes in play, temperature-programmed desorption (TPD), atomic force microscopy (AFM), density functional theory (DFT), and high-performance computing are used to investigate its reaction. This study aimed to examine the reactivity of different isomers of butanol, namely 1-butanol, 2-butanol, and isobutanol, when exposed to a TiO2/Au(111) surface. TPD was used to detect products, with 1-butanol showing little reactivity and elimination products, 2-butanol showing oxidation and elimination, and isobutanol yielding all products. The selectivity of the reaction was not altered during successive desorption experiments, indicating that the model catalyst was stable without reoxidation between experiments. AFM highlighted the morphology of the surface and shows the Au(111) crystal has ~0.13ML and 0.27ML of TiO2 with predominantly 1D wire like nanoparticles. Higher coverages of TiO2 result in more particles distributed across the surface indicating that the reactivity was influenced by butanol proximity to TiO2 nanoparticles rather than differences in size or shape. DFT calculations to investigate energetic trends and provide an atomic-scale understanding of the structure of butanol adsorbed on the surface are ongoing.

UN-ThP-11 Pulsed Laser Deposition of Ruthenium Oxide Thin Films for Electrocatalytic Splitting of Water for Oxygen and Hydrogen Evolution Reactions*, **Anansi Coleman**, D. Kumar,* North Carolina A&T State University

Wisdom Akande, Anansi Coleman, Ikenna Chris-Okoro, Sheilah Cherono, Mengxin Liu, and Dhananjay Kumar

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This presentation reports the synthesis, structural characterization and evaluation of electrocatalytic properties of crystalline ruthenium oxide(RuO2) thin films. The films were grown using Pulsed Laser Deposition technique on a variety of single-crystal substrates, sapphire(Al2O3) and titanium dioxide(TiO2) while varying oxygen pressures from 5mTorr to 50mTorr, and substrate temperatures from 400°C to 700°C. The films were structurally characterized using x-ray diffraction, x-ray photon spectroscopy and scanning electron microscopy. Cyclic-voltammetry and Linear-sweep-voltammetry were also measured and used to evaluate the electrochemical properties during OER, with the aim of providing insights into role crystal structure and surface orientation on the electrochemical properties of the films.

UN-ThP-12 Direct Printing of Oxide Nanoparticles Via Vapor Phase Microreactor Assisted Nanomaterial Deposition (V-MAND) and Its Application*, **Isaac Camp**, V. V. Doddapaneni, M. Dodge, S. Pasebani, C. Chang,* Oregon State University

Nanomaterial printing is gaining attention from the many properties nanomaterials are excellent for, such as catalysts, light absorbers/reflectors, and mechanical property modifiers compared to their bulk counter parts. Many traditional methods, such as inkjet printing and aerosol jet printing techniques, are being used to deposit and fabricate functional materials and devices. However, they require solvent dispersion of nanoparticles which can lead to carbon impurities and structural imperfections. Moreover, nanoparticle dispersion inks tend to have limited shelf-life, further limiting their applications. To address these challenges, different solventless and dry printing methods have been developed. Within this work, we developed a vapor phase microreactor assisted nanomaterial deposition (V-MAND) printing technology. This technology uses solventless or solid precursors and generates nanoparticles on-demand, transporting them to the desired surfaces from the print head. Furthermore, this V-MAND printer can be integrated into 3D printers to produce functional composites materials, such as high temperature alloys for aerospace and nuclear applications, and UV-resistant materials for food packaging applications.

UN-ThP-13 Optimizing Plasma Conditions for the Modification of Silk Fibroin Using Small and Large Molecule Precursors*, **Bethany Yashkus**, M. Corbett, J. Blechle,* Wilkes University

Silk materials show promise for use in biomedical applications because of their desirable mechanical properties, versatility, and accessibility. Their overall utility is limited, however, as the biological lifetime of silk materials remains uncontrolled. Plasma-enhanced chemical vapor deposition (PECVD) has previously been employed to modify silk films by altering the wettability of the surface. Significant work has been completed to explore the impact of gas composition and plasma conditions on the surface of these modified materials. Critically, the mechanism by which these modifications occur is an ongoing question due to a lack of gas-phase analyses. Here, optical emission spectroscopy (OES) is used to monitor the plasma during silk modification, with the hope of elucidating key reactive species.

Utilizing previously established conditions (Hawker, 2023) of acrylic acid and pentane precursors at 75 mTorr and 65 W revealed no observable spectral differences upon addition of silk films, providing little mechanistic insight. As such, this work will explore an expanded experimental parameter space, including pressure, power and time constraints, to probe for gas-phase reactive hydrocarbon species. Diagnostic calculations, such as relative densities and internal temperatures, will also be employed to further characterize the system. Additionally, small molecule precursor gases (namely N_2 and O_2) will be employed for direct comparison and ease of spectral analysis. Compiling diagnostic data across this expanded parameter space provides an opportunity for unparalleled insight into the mechanisms of silk fibroin surface modification.

UN-ThP-14 Epitaxial Lift-Off of Barium Hexaferrite Membranes*, **Clara Jackson Jackson**,* Clark Atlanta University*; E. Li, A. Park, D. Schlom,* Cornell University

Freestanding barium hexaferrite ($BaFe_{12}O_{19}$ or BaM) membranes are valuable for various technological applications, and their fabrication via Molecular-Beam Epitaxy (MBE) involves overcoming significant challenges, particularly in the epitaxial lift-off process. Initially, α-Fe_2O_3 was chosen as the sacrificial layer for membrane detachment due to its compatibility with the BaM crystal structure. However, α-Fe_2O_3 proved problematic due to its slow etching rate, which led to inefficient lift-off even with strong acids, jeopardizing membrane quality. To address this, the study explored alternative materials and found that ZnO, with a similar crystal structure and a much faster dissolution rate, significantly enhanced the efficiency of the lift-off process. This transition to ZnO not only improved process efficiency but also underscored the critical role of material selection in optimizing epitaxial lift-off techniques. This work advances the fabrication methods for freestanding BaM membranes and highlights the practical application of material science principles in overcoming fabrication challenges.

UN-ThP-15 Exploring the Epoxidation of Isoprene on Copper-Based Catalysts*, **James Whitted**,* James Madison University*; M. Corbett,* Wilkes University*; A. Baber,* James Madison University

Isoprene (C_5H_8) is a common greenhouse gas that forms the infamous haze observed over the Blue Ridge Mountains. It contributes to a large portion of the planet's ozone formation, and therefore finding alternative value-added uses for isoprene is critical. Isoprene is a diene, and due to its molecular structure, has both allylic hydrogen and non-allylic hydrogen sides. It is therefore a model reactant molecule for studying selective epoxidation. Atomic oxygen on Cu(111) is known to enhance the epoxidation of propylene, which contains allylic hydrogens, while Ag(110) and Ag(111) with atomic oxygen encourages the epoxidation of ethylene, which does not have allylic hydrogens. This molecule is ideal to study epoxidation reactivity on a AgCu near surface alloy (NSA), specifically for its allylic hydrogen and non-allylic hydrogen sides, which mimic propylene and ethylene. Olefins have several different reaction pathways that can be isolated through specific reaction schemes. The major reaction pathway for isoprene on oxidized Cu(111) is combustion. Creating an NSA comprised of Ag atoms on Cu(111) is expected to produce a favorable surface to form an epoxide from isoprene, while also limiting the unwanted combustion pathway. Ultra-high vacuum temperature programmed desorption (UHV-TPD) spectra were gathered on clean and partially oxidized Cu(111) and Ag/Cu(111) after dosing isoprene. As the amount of oxygen dosed on Cu(111) increased, carbon dioxide yield also increased, indicating that the combustion pathway was in full effect. To minimize overoxidation of isoprene to CO_2 under UHV, Ag was deposited on Cu(111) via physical vapor deposition. Auger electron spectroscopy was used to determine Ag coverages on the surface, post-deposition. TPD results indicate that the combustion pathway was deterred in the presence of 1 ML of Ag/Cu. Future work will focus on potential coexisting products and the molecular geometry of isoprene adsorption and packing using scanning tunneling microscopy.

UN-ThP-16 Characterizing Next-Generation SRF Materials for Accelerator Infrastructure*, **Helena Lew-Kiedrowska**, V. Do, S. Willson,* University of Chicago*; C. Wang,* National Cheng Kung University, Taiwan*; L. Shpani, S. Seddon-Stettler, M. Liepe,* Cornell University*; S. Sibener,* University of Chicago

Superconducting radiofrequency (SRF) cavities are used to accelerate beams of charged particles in particle accelerators. The standard material for SRF cavities is Nb because it is the highest temperature elemental superconductor with a critical temperature (T_c) of 9.7 K.SRF performance can be further improved by growing a higher T_c metal alloy onto the Nb surface such as Nb_3Sn (T_c = 18.3 K) or by preventing the growth of a native oxide layer on Nb with capping layers of an inert metal such as Au. Previous studies have shown that anodization improves Sn incorporation for Nb_3Sn growth, and that Au capping achieves oxide passivation for Nb. In this work, we characterize anodized samples of Nb and electroplated Au on Nb samples using scanning electron microscopy and atomic force microscopy. Our results demonstrate how the underlying Nb substrate can affect metal growth on the surface: Au growth showed preferential binding in surface defects, and anodizing the Nb sample increased its surface roughness, which may explain increased Sn incorporation.

UN-ThP-17 Mitigating Hydrophobic Recovery of Oxygen Plasma-Treated PEEK*, **Nicholas Shows**, M. Mowatt, M. Hawker,* California State University, Fresno

Polyether ether ketone (PEEK) is a chemically inert and wear resistant thermoplastic polymer which exhibits similar elasticity and tensile properties to human cortical bone. These characteristics demonstrate why PEEK is used in orthopedic surgical procedures including cranioplasties, spinal cages, and hip arthroplasties. Despite favorable mechanical properties, PEEK is hydrophobic. Surface hydrophobicity decreases PEEK’s cytocompatibility, and therefore, osseointegration. Previous research demonstrates that hydrophilic surfaces exhibit greater cytocompatibility, resulting in more favorable osseointegration. Greater surface hydrophilicity can be achieved using radio frequency (RF) oxygen plasma treatments. PEEK films treated with RF oxygen plasma exhibit a contact angle nearly 50° lower than that of native PEEK. After oxygen plasma-modification, PEEK returns to its native hydrophobic state over time through hydrophobic recovery. A hydrophobic PEEK surface will not contain osseointegrate as well as the oxygen plasma-treated PEEK immediately after plasma treatment. Prior research suggests storing various plasma-treated PEEK films in water after treatment can lessen the extent of hydrophobic recovery. Oxygen plasma-treated PEEK exhibits optimized surface hydrophilicity immediately after treatment. Strategies to mitigate the hydrophobic recovery of RF oxygen plasma-treated PEEK remain unexplored.

This study examined the hydrophobic recovery of RF oxygen plasma-treated PEEK when stored in aqueous and ambient conditions. PEEK sheets were cut into individual films and sonicated to ensure a clean surface. PEEK films were subjected to plasma treatment in an inductively-coupled plasma reactor using an oxygen gas precursor. Optimized plasma parameters including power, pressure, and treatment times were selected based on previous literature. Plasma-modified PEEK films and untreated controls were then aged up to 30 days in ambient or aqueous conditions. Contact angle goniometry was used to analyze surface wettability of treated PEEK and untreated PEEK controls. RF oxygen plasma-treated PEEK exhibited an increasing contact angle over time in ambient conditions, indicating hydrophobic recovery occurred. RF oxygen plasma-treated PEEK did not return to its hydrophobic state when aged in aqueous conditions. Modification methods which lessen hydrophobic recovery have potential to improve the usability of PEEK in orthopedic surgical applications by improving its osseointegration.

UN-ThP-19 Deconvoluting Information-Rich Ga(I) X-Ray Adsorption Near-Edge Spectroscopy Features from First Principles*, **Grace Miller**,* Washington State University*; C. Huang,* University of California at Los Angeles*; S. Scott,* University of California Santa Barbara*; J. McEwen,* Washington State University

Due to the high demand of propylene, it is appealing to look at replacing Pt- and Cu-based catalysts for propane dehydrogenation. In this regard, an attractive alternative are Ga-based compounds. X-ray Adsorption Near-Edge Spectroscopy (XANES) contains information about the coordination environment and the oxidation state of Ga under reaction conditions. In our previous work, we deconvoluted the experimental features of Ga(III) compounds [1]. Since Ga(I) and Ga(III) compounds are both involved in propane dehydrogenation, we benchmark the spectral features of Ga(I) compounds in this work. We compare the calculations derived from structures based on *Li et al.* [2] to three additional Ga(I) structures $(Ga(Si(SiMe_3)_3)_{4,}(Ga(C(SiMe_3)_3)_{4,}$ $((Ga_8Br_8)_6NEt)$ to further deconvolute the XANES features. Based on the literature, the XANES features with higher intensities correspond to Ga(I) oxidation states while the XANES features with lower intensities correspond to Ga(III) oxidation states. Using the CASTEP code with a Perdew-Berkman Erzenhoff (PBE) functional, we simulate the XANES from first principles. We further compare the Ga(III) features of our compounds to what has been identified previously in the literature [1]. Interestingly, two bulk Ga(I) structures did not have the high intensity feature as was identified in the other Ga(I) compounds. The study is ongoing where we are quantifying interaction energy between Ga(I) cations within these structures, where our initial results indicate that the interaction energy between them is attractive.

UN-ThP-20 Characterization and Oxidation of Curved Metal Surfaces*, **Allison Kerr**, D. Killelea,* Loyola University Chicago

Due to the importance of oxide surfaces in heterogeneously catalyzed oxidation reactions, it is necessary to gain a fundamental understanding and behavior of oxygen on transition metal surfaces. Additionally, the atomic arrangement of the metal surface plays an important role in the behavior of the oxygen on the surface, which provides a need to study high defect density surfaces that are more akin to industrial catalysts. The research presented herein utilizes a curved rhodium crystal c-Rh(111) with two different well-defined defects on either side to conduct a systematic study of the influence of defect geometry on the kinetics and dynamics of different oxygen species present on the surface. Scanning tunneling microscopy (STM), low energy electron diffraction (LEED), temperature programmed desorption (TPD), and Meitner-Auger electron spectroscopy (MAES) will be used to look at the surface on an atomic scale and to observe what chemical species are on the surface after introducing oxygen into the vacuum environment.

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