Science History Institute

Chemistry · Engineering · Life Sciences

SCI America

Innovation Day Poster Session Guide

September 13, 2022

Online Poster Session, 9:00 AM – 10:00 AM

In-Person Poster Session, 10:15 AM – 11:15 AM

On Innovation Day emerging industry leaders celebrate today's innovations in the chemical industry and seek solutions for tomorrow's challenges. By taking early-career scientists out of the lab and giving them broader access to their colleagues and to the historical and social context of their research, Innovation Day supports a 21st-century chemical enterprise that addresses society's most pressing needs. Cohosted by the Society of Chemical Industry (SCI) and Science History Institute since 2004, Innovation Day 2022 will be a hybrid event held in person and online on September 13. In its 19th year of highlighting breakthroughs and achievement in innovation, our program continues to attract leading speakers and participation from across all sectors of the chemical enterprise.

Innovation Day 2022 features 18 posters. The themes of this year's event explore sustainability and digitization with particular focus on carbon capture and net zero goals, materials science, artificial intelligence for manufacturing, and artificial intelligence for materials discovery.

This Poster Session Guide is organized alphabetically by poster presenter last name. The Guide includes poster presenter name(s), company affiliation, and poster title and abstract for each poster. Please use this as a guide as you prepare to explore posters during the virtual or in-person poster sessions on September 13.

For full poster citations, please contact the poster presenter(s) during Innovation Day 2022.

Presenter Name: **Gregory Cleveland, Rebecca Siegelman**
Company: **DuPont**
Poster Title: **Aqueous Nitride Etch Technology for 3D NAND**
Abstract:
The NAND flash memory market is currently transitioning from 2D to 3D architectures in order to reduce the cost per bit. In fabricating 3D NAND structures, a key step involves the selective removal of silicon nitride from alternating paired layers of silicon nitride and silicon dioxide in high aspect ratio trenches. Traditional industrial solutions have utilized hot phosphoric acid (85%, 160 °C) as the primary wet etchant, but these formulations have significant limitations in 3D NAND applications regarding etch uniformity and byproduct redeposition. With growing demands in performance and sustainability, the need for disruptive new technologies has become pronounced. A global collaborative effort at DuPont aims to fulfill that need with novel chemistries that eliminate phosphoric acid from selective silicon nitride etchants in favor of predominantly aqueous formulations. This poster aims to highlight the drawbacks of current etching technologies and to provide clear motivations for DuPont's disruptive technologies.

Presenter Name: **Frank Cui**
Company: **DuPont Engineering Technology Center**
Poster Title: **Application of Electrochemical Techniques in Chemical Process Industry**
Abstract:
Electrochemical techniques such as Electrochemical Impedance Spectroscopy and Potentiodynamic Polarization are powerful tools to study material interfacial reactions. Chemical Process Industry handles a vast range of chemicals at various conditions at every steps of production process: from transportation, storage to reaction. Interaction (often time corrosion) between chemicals and their containing equipment is an important subject to study in order to ensure production success and safety. In many cases, electrochemical techniques could be employed to obtain critical information which would otherwise not available. This poster showcases several successfully application examples of these techniques in DuPont:
1.) Differentiating subtle corrosiveness between two chemical additives. This investigation enabled adoption of new additive with significant saving;
2.) In-situ evaluation of alloy corrosion resistance in a solid medium and this test protocol significantly shortened testing cycle and enabled development of basic data within a more practice time frame;
3.) Develop Integrity Operation Window (IOW) for anodic protection in a commercial acid application. This study was used as guidance for a new DuPont offering.

Presenter Name: **Paul Doll**
Company: **Dow Chemical Company**
Poster Title: **The Journey Towards Sustainable Coatings**
Abstract:
The term sustainability is frequently used to promote new products and technologies these days. However, many chemists and chemical engineers struggle to reduce this large nebulous concept into meaningful and actionable items. Examples will be provided that demonstrate a clear flow from Dow's mission statement to focused sustainable areas to newly developed coatings technologies. More durable coatings made with renewable feedstocks that efficiently use the materials and eliminate hazardous materials are leading the journey towards more sustainable coatings.

Presenter Name: **Di Du**
Company: **ExxonMobil Technology and Engineering Company**
Poster Title: **Machine Learning Assisted Discovery and Development of Microporous Materials**
Abstract:

Microporous materials play a crucial role in producing energy and energy products at scale. Material development and scale-up can greatly benefit from the advances in artificial intelligence, machine learning, and other technologies and therefore accelerate the materials workflow from lab bench to commercial scale. Two key questions need to be addressed including (1) what are the critical variables that impact the synthesis (2) and how the material properties can be controlled and optimized. This poster provides an overview of machine learning approaches and experimental techniques to build quantitative synthesis-property relationships (QSPR). These methods provide a highly efficient path to optimize synthesis parameters towards target(s) such as material purity, morphology and other physical and chemical properties, and enable us to speed up our materials workflow. Our workflow combines design of experiments (DoE), machine learning and deep learning, and high-throughput experimentation (HTE). We developed a DoE strategy to screen the key parameters for the material synthesis. The advantages of deploying DoE over experience-based trial and error approach is that it enables strategic exploration of multiple factors and their interactions simultaneously. We will discuss the DoE strategy customized for the use with HTE batch experiments. In order to build QSPR, we featurized the characterization data using machine learning and deep learning approaches. For example, we quantified crystal purity using peak deconvolution of powder XRD pattern. We used a deep learning model to calculate crystal size and aspect ratio from scanning electron microscopy (SEM). We also performed functional principal component analysis to ensure the surface area calculated from the linear region of Brunauer-Emmett-Teller (BET) adsorption curve selected using Rouquerol rule explains a substantial fraction of variance. We used feed-forward neural network models to summarize QSPR for extended investigation at different scales. We validated the accelerated workflow with a known material. Without referring to historical data, we used the workflow to systematically probe a large and complex synthesis parameter space and obtain small pure crystals of the material. The new workflow demonstrated a significant reduction in the number of experiments needed to meet the same goals as past experiments.

Presenter Name: **Mark Ewing**
Company: **Eastman Chemical Company**
Poster Title: **Data-Driven Experimentation for Optimizing Fiber Cut Length for NaiaTM Textile Yarn Applications**
Abstract:

For decades, scientists have used designed experiments as an efficient way to study relationships between multiple input and output variables. Advances in computing power have unlocked the modern field of optimal experiments, enabling advanced statistical analysis for complex experimental structures. This NaiaTM staple fiber cutting experiment is the first documented staggered-level experiment in industry. Real-world experimental designs often require constraints on randomization. Time, cost, or equipment limitations prevent some factors from being independently reset at frequent intervals. Staggered-level designs provide a flexible structure for experiments with more than one hard-to-change factor by allowing the hard-to-change factor levels to be reset at different points in time throughout the design. Careful and rigorous data-driven experimentation is critical for successful front-end innovation. Optimal experimental designs enable scientists to capture the best opportunities for product development and commercialization, advancing materials discovery.

Presenter Name: **Mark Ewing, Cameron Brown**
Company: **Eastman Chemical Company**
Poster Title: **AI/ML Assisted Design and Synthesis of Industrial Polyester Resins for BPA-NI Coating Applications**
Abstract:
The vast design space for polyester resins presents a tremendous challenge to innovation – how do I quickly identify and synthesize materials to solve challenges in novel applications? Leveraging a library of historic formulations and modern AI and Machine Learning techniques, Eastman has developed a digital solution to accelerate the materials and application discovery process. This poster shares how Eastman uses AI/ML to rapidly identify novel polyester resin formulations to address the growing global demand to replace BPA with highly functional alternatives.

Presenter Name: **Gabriela Faux**
Company: **DuPont**
Poster Title: **Dupont Tedlar® films sustainability benefits through its extended life cycle**
Abstract:
Dupont Tedlar® film is a polyvinyl fluoride film that provides long lasting surface protection to a variety of surfaces. Tedlar® films are used in many different industries, such as photovoltaics, aerospace, building and construction, healthcare, signage, and transportation. The films exhibit excellent chemical and solvent resistance, UV and weather stability, and are easily cleanable and formable. In addition, Tedlar® is mold and mildew resistant and has low toxicity and volatiles. These characteristics of Tedlar® films enable it to play a crucial role in sustainability through its extended life cycle in various applications, such as renewable energy, building/construction, transportation, and others. For example, Dupont Tedlar® has played an important role in photovoltaics panels since the 1980s with Tedlar® based backsheets increasing the lifetime of a solar panel beyond 20 years. A total of 835 million tonnes of CO_2 emissions has been avoided with the increase installation volume of photovoltaic panels with Tedlar® since 2004. This poster will explore the sustainability benefits of Tedlar® films in a variety of industries.

Presenter Name: **Ashish Jayaraman**
Company: **Dow Chemical Company**
Poster Title: **Characterization of Biofilm Growth on Acrylic Elastomeric Coatings with High Solar Reflectivity using an Accelerated Test Method**
Abstract:
Low T_g acrylic coatings with high solar reflectivity have been used to great effect as coatings on buildings with low slope roofs to increase the roof substrate service life and to lower the energy use of the structure. The growth of biofilms in ponded water areas on a coated roof is a significant issue affecting coating longevity where repeated wet-dry cycles of the biofilm result in premature failure of the coating. An accelerated test method using biofilm isolates from an exterior roof has been developed to quickly characterize biofilm growth in a laboratory setting as a function of time on elastomeric roof coating. Automated image analysis using CIELAB color space measurements was used to quantify color changes (ΔE^*) on the substrate that correlate to biofilm growth. The effect of the chemical composition of coating filler on biofilm growth in this accelerated test will also be discussed.

Presenter Name: **Jayashree Kalyanaraman**
Company: **ExxonMobil Technology and Engineering Company**
Poster Title: **Enabling Process Intensification with Proton Conducting Membrane Reactors for Steam Methane Reforming**
Abstract:
Rapidly increasing installation and adoption of renewable power – coupled with demands for more energy efficient process technologies – has kindled a development of process intensification strategies. Simultaneously there is renewed interest in hydrogen feedstocks for power generation and heating. Steam methane reforming is still a dominant approach to hydrogen production from fossil fuel feedstocks, but improvements (e.g. carbon capture) are needed to meet emissions benchmarks. One novel approach gaining momentum are electrically driven membrane reactors. Perovskite based electrolytic membranes provide an ideal platform by combining in-situ separation of hydrogen from carbon dioxide while driving the process with electrical energy (potentially green) thereby significantly reducing the overall carbon intensity of hydrogen production. This poster will specifically focus on the mechanism of transport within the solid oxide membranes and provide a process framework of how it can replace the conventional SMR process.

Presenter Name: **Jue Liang**
Company: **Dupont**
Poster Title: **Meeting the Challenge: Aqueous Digital Inks for the Future of Packaging and Textile**
Abstract:
Digital technologies are transforming the world and everyone's life since the new century. Printing industry is embracing the same trend. The attractiveness of digital printing over analog print is growing year after year with inks playing a strategic role in this process. Today digital printing is delivering unique benefits to brands, converters and end consumers including customization, personalization, cost-effective short runs, design flexibility and does not compromise on color brilliance. Another dimension that aqueous digital printing inks bring to packaging and textile printing is sustainability. Consumers, along with brand owners and retailers, are sensitive to the environmental impact. Brand owners and retailers are focused on lowering the environmental footprint and improving the sustainability of their products while keeping high level of printing quality and printing consistency. Aqueous pigment inks help provide a key component to address the sustainability demand of digital printing. For decades, DuPont Digital Printing has been on the cutting-edge of ink, dispersion and polymer technologies, empowering customers to achieve brilliant prints on a wide array of substrates for textile, paper and packaging applications. DuPont's belief is by combining its print technology experience (inks, dispersions, polymers) with that of the other value chain participants, solutions will be developed and that the digital transition in printing industry will increase in the coming years. Whether enabling the creation of fashionable clothing or vibrant packaging, DuPont Digital Printing is making the world a more beautiful place now and for generations to come with our technologies and products.

Presenter Name: **Alyssa M. Love**
Company: **ExxonMobil Technology & Engineering Company**
Poster Title: **Synthesis of High Activity and Low Cost Transition Metal Catalysts for Sustainable Reforming**
Abstract:
In industrial catalytic research there is a need for platform material synthesis strategies in order to adapt to shifting application needs. Here, we report synthesis strategies for the preparation of supported first-row transition metal catalysts due to their low cost and their potential utility in natural gas reforming. We

prepared supported Co, Ni, and Cu catalysts via a simple incipient wetness impregnation with an organic complexation agent incorporated in the metal precursor solution. This work was adapted from an approach to prepare well-dispersed noble metal catalysts on silica (Catalysis, 2022, 34, 102-157). We evaluated which transition metal precursor and organic molecule combinations were easily soluble in an aqueous medium and then impregnated these solutions onto oxide supports. While alkanolamine molecules, readily form a complex with Co and Cu carbonate precursors in water, Ni carbonate instead requires an acidic molecule like citric acid to dissolve. We evaluated the resultant metal dispersion through a combination of chemisorption and TEM. We developed a N2O chemisorption technique to quantitatively characterize Co and Cu dispersion with TGA-MS (whereas conventional volumetric H2 chemisorption works best for Ni) and compared these results with metal particle size evaluation via TEM.

Presenter Name: **Aaron Peters**
Company: **ExxonMobil Technology and Engineering Company**
Poster Title: **MOFs for CCS, Deep CCS, Direct Air Capture and Water Harvesting**
Abstract:
Global anthropogenic CO2 emissions now exceed 40 Gt/yr, ∼75% of which derive from the combustion of fossil fuels. In order to keep average surface temperatures well below 2 °C, preferably below 1.5 °C, of preindustrial values, as set forth by the Paris Agreement, integrated assessment model (IAM)scenarios have underscored the need for rapid decarbonization of the power generation sector. Although many 1.5 and 2 °C IAM scenarios project rapid scale-up of variable renewables by midcentury, the growing need to curb anthropogenic CO2 emissions has motivated the deployment of alternative low-carbon technologies such as carbon capture and sequestration in the near-term. Taking inspiration from the crystal structures of diamine-appended metal–organic frameworks (MOFs) exhibiting two-step cooperative CO2 adsorption, we report a family of robust tetraamine-functionalized frameworks that retain cooperativity, leading to the potential for exceptional efficiency in capturing CO2. This work details the use of amine-appended MOFs in CCS, Deep CCS, direct air capture (DAC), and water harvesting.

Presenter Name: **Trong Pham**
Company: **ExxonMobil Technology and Engineering Company**
Poster Title: **Zeolite design for next-generation MTO chemistries: EMM-68**
Abstract:
The zeolite-catalyzed methanol-to-olefin (MTO) reaction provides a sustainable route to produce light olefins such as ethene and propene from non-petroleum resources. The oligomerization of these light olefins into jet and diesel fuels is an active research area of commercial importance and vital to the decarbonization of heavy industrial applications. In traditional MTO processes, ethylene is predominantly produced by the commercial CHA (chabazite) zeolite catalyst. Ethylene is a much less active monomer than higher olefins (C3= & C4=) when undergoing oligomerization to produce fuels, and new catalytic materials are required to enable the selective production of these desirable molecules. Towards this end, a new aluminosilicate zeolite (EMM-68), has been discovered. EMM-68 with its 10 x 8 x 8 narrow pore apertures would exhibit a similar high selectivity to light olefins due to its diffusional properties, while the large cavity size of 8.0 x 9.4 x 7.7 Å—as compared to CHA (with a dimension ~ 8.4 x 7.5 x7.5 Å) — accommodates highly alkylated benzene intermediates that are suggested to be critical in producing C3= and C4= olefins.

Presenter Name: **John Quigley**
Company: **Eastman Chemical Company**
Poster Title: **Intelligent Material Design at Eastman via Six Sigma Tools**
Abstract:

Eastman's engineered solutions platform has built a tool that leverages QFD 1.0 principles to enable the application and product development teams to position ideal materials for a discrete set of customers needs. With our foundation of world class structure-property relationship understanding – and by leveraging machine learning & formulation expertise to build composition optimization framework that utilizes this new tool –Eastman will drive innovative material development framework to meet tomorrow's customer needs.

Presenter Name: **Karen Sanchez**
Company: **ExxonMobil Technology and Engineering Company**
Poster Title: **High-loft, ultra-soft nonwoven solutions**
Abstract:
Customer trends within the absorbent hygiene segment comprising of baby care, feminine care, and adult incontinence are driving a need for innovative products that deliver on comfort, security, and discreetness. ExxonMobil has a longstanding history in nonwoven application development and is a leader in nonwoven innovation. A recent demand by the absorbent hygiene market was the need for a new type of "cushiony" softness by means of a lofty nonwoven. Lofty nonwovens are spunbond nonwovens that have exceptional z-directional thickness. ExxonMobil delivered by developing a new polypropylene grade, Achieve™ Advanced PP3684, designed for tailored "loft" solutions. ExxonMobil's loft solution utilizes bico technology and a combination of three ExxonMobil products to meet specific market needs. By balancing the side-by-side ratio and weight loadings, countless opportunities have been unlocked for developing unique products with distinct hand feels. ExxonMobil has also developed new innovative methods for characterizing lofty nonwoven performance by measuring thickness, compressibility, and resilience.

Presenter Name: **Kevin Stevens**
Company: **ExxonMobil Technology & Engineering Company**
Poster Title: **Accelerated Development of Novel Polymers via Hybrid Modeling Approaches**
Abstract:
Traditional scale-up activities of new polymer families were focused on iterative, experimentally-focused approaches. Evolving market drivers and the need for new, higher performance materials to allow advanced polymer solutions necessitate faster time to market. Acceleration can be realized by using hybrid modeling approaches to supplement experimental data and enable early optimization. Adaptation of a hybrid modeling method to polymer structures enable fundamentally structured, and generalizable, and data driven predictions of polymer physical properties from a simulated polymer structure via a component-based approach. Further, inclusion of catalyst kinetics at different scales enables the prediction of polymer structure and, therefore, polymer properties, such that early process and product workflows are predominantly digital.

Presenter Name: **Yunsong Xie**
Company: **ExxonMobil Technology and Engineering Company**
Poster Title: **3D printing dashboard – an online hub bridges research, technology, and business**
Abstract:
3D printing allows for direct transformation of 3D digital data into a 3D object. It presents growing market opportunity for chemical companies to grow the polyolefin polymer sales. There have been significant progresses in developing a variety of 3D printing polyolefin materials in ExxonMobil research and technology. An Azure Cloud hosted dashboard was recently developed to bridge research and technology development with business. This dashboard enables our internal global users access the latest update of 3D printing capability. The dashboard content includes not only pictures and videos of the in-house 3D

printing capabilities, but also data visualization tools for the technical data of the developed 3D printed polyolefin materials. The dashboard also has the capability of tracking the user's activity on the website, thus enable learning loop for app improvement. Overall, this dashboard has provided and will continue to serve as a platform for research, technology, and business sectors to conveniently interact together for polyolefin 3D printing applications in ExxonMobil.

Presenter Name: **Ligeng Yin**
Company: **The Dow Chemical Company**
Poster Title: **High Biocarbon Content Si-acrylate Hybrid Film Formers for Skin and Sun Care**
Abstract:
Dow currently offers acrylates/polytrimethylsiloxymetacrylate copolymers as DOWSIL™ FA40xx Silicone Acrylate (xx = 01-04 & 12) solution polymers delivered in a variety of solvents for skin and sun care markets. Enabled by the Si-acrylate hybrid technology, these products offer excellent water and sebum repellency, wash-and rub-off resistance, flexibility, and low tackiness. As consumers become more conscious about sustainability and economic circularity, we strive to improve their biorenewability and thus reduce the reliability on fossil fuels. A variety of bioderived acrylate monomers have been successfully incorporated into the backbone, and the resulting polymer compositions contain up to 50% biobased carbon content. In combination with a green carrier such as bioethanol, the overall biocarbon content was improved to be up to 80%, with great potential to meet guidelines from both the ISO16128 standard and USDA BioPreferred® program. The impact of the bioderived acrylate monomers on the neat film and foundation formulations will also be discussed.