PURDUE UNIVERSITY

GSO

Program

Purdue ChE GSO presents
The 31st Annual
Davidson School of Chemical Engineering
Graduate Research Symposium
August 17-18, 2022

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Preface

It is with great pleasure that I welcome you to the 31st Annual Chemical Engineering Graduate Research Symposium hosted by the Purdue University Davidson School of Chemical Engineering. With our first in-person symposium since the start of the COVID-19 pandemic, we are proud to preserve and present this event along its long history of strengthening the relationships between our department and industry, your attendance and presence today continue this tradition. With your support, our senior graduate students benefit greatly from the industrial feedback they receive, become better prepared for the hiring process, and continue expanding their professional networks for a more fulfilling career path.

Furthermore, your financial contributions help to support the Graduate Student Organization's mission of building a flourishing and enriching community for our students. As we return to in-person research, presentations, and department involvement, we cannot stress the importance of a strong community enough. With community, our students can tackle the many challenges and adversity of a Ph.D. program during an era of great uncertainty. All of this is made possible by your generous support, we can host a variety of professional development, service, and social events. We serve our department's community by hosting professional and social events like seminar series, volleyball tournaments, and board game nights. And we serve our local community by hosting service events like volunteering for the after-school science program with local third graders, tree planting, and highway cleanups.

We hope you take this opportunity to listen to the oral presentations from our graduate students and help them with the important transition from academia to industry. We also encourage you to spend some at the poster session to become more familiar with the research of our rising graduate students as they continue to learn and grow along their unique Ph.D. and career paths.

I would like to personally extend my sincerest gratitude to all in attendance today. Our symposium could not be successful without your continued support, and it is greatly appreciated by the Graduate Student Organization, the graduate student body, and the department as a whole. We look forward to a continued partnership in the years to come and many more fulfilling symposia.

Montgomery Smith
President, Chemical Engineering Graduate Student Organization
2022-2023

Keynote Speaker

Gautam Kumar

Director and GM
Global Supply of Equipment and Materials
Intel Corporation

Gautam Kumar is a Director and General Manager in the Global Supply Chain Organization of Intel Corporation

Gautam began his career at Intel in 2007 as a Process Engineer within Intel's Portland Technology Development organization. His focus area was in Dielectric Thin Films where he first led the technology transfer of Intel's 45nm and 32nm nodes into high volume manufacturing. He was then appointed as the lead engineer in developing next generation low-k dielectric thin films for Intel's 14nm technology node where he led the invention of a novel dielectric stack that enabled the patterning pitches in the multi-pass patterning integration scheme. He was then appointed Engineering Manager responsible for the 14nm pilot line and process ramp.

Following the successful transfer of the 14nm technology node into high volume manufacturing, Gautam moved from Technology Development to Intel's Xeon Product Marketing group where he worked with Google, Microsoft, and Amazon Web Services in helping define their Cloud Compute infrastructure by optimizing Cooper Lake, Cascade Lake and Ice Lake Xeon processor power and performance to the customer's requirements. He was then appointed as the Chief of Staff within Intel's Xeon Strategy group where he led the business development plan for integrating Microsoft's Pluton Security IP on Intel's Silicon. He also led the Strategy definition for Intel's response to ARM's market share growth in the cloud and datacentre segment and Intel's end to end security strategy.

Gautam then took on his current role within Intel's Global Supply Chain organization as Director and GM where he leads the business, technology strategy and executive engagement for Intel's strategic collaboration with Lam Research Corporation. He also leads Intel India's Supply Chain business development organization responsible for Supply Chain systems, analytics, and ecosystem development.

Gautam received his BTech in Chemical Engineering from the Birla Institute of Technology and Science, India (2001) and his PhD in Chemical Engineering from Purdue University (2007).

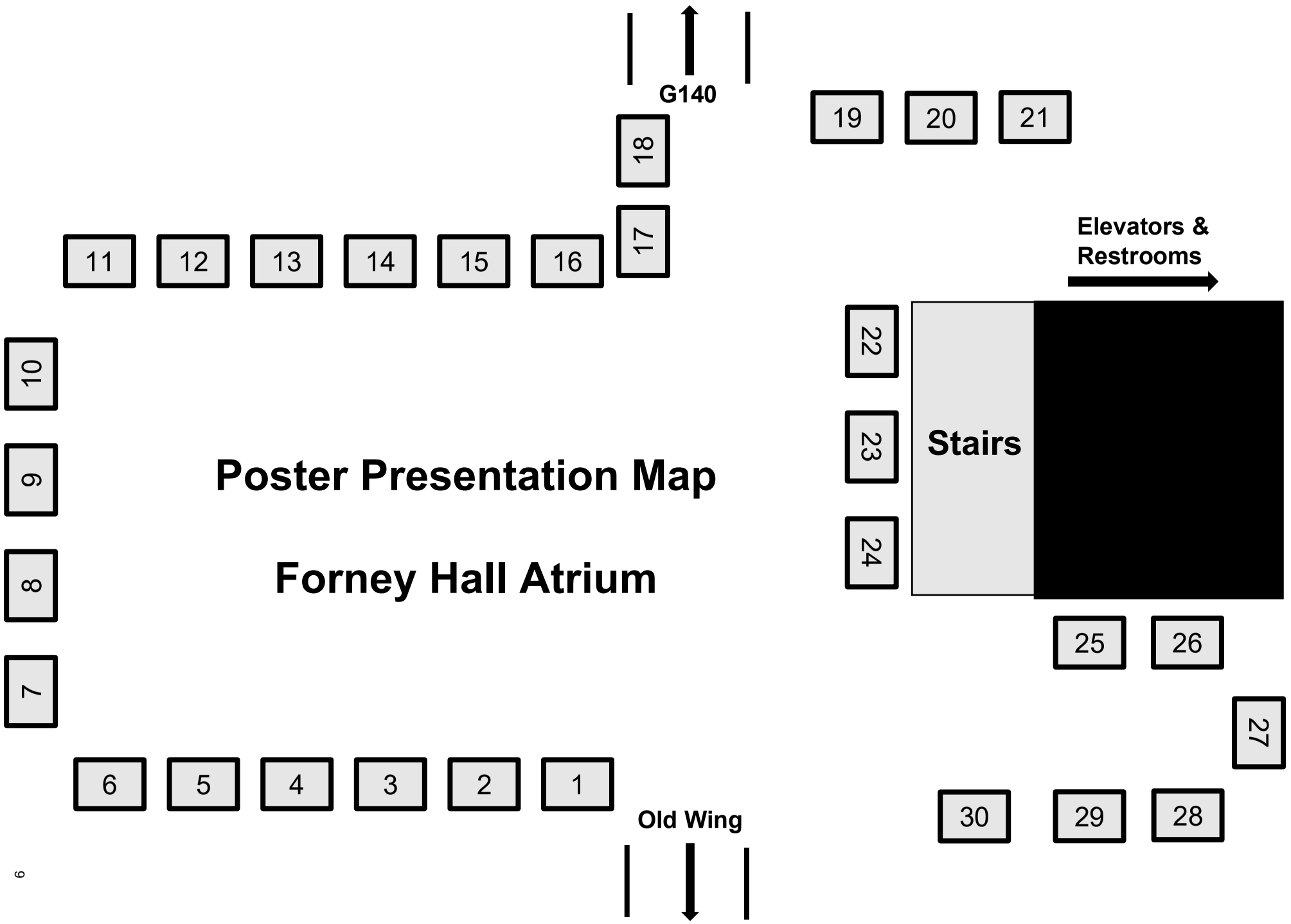
Schedule of Events

Thursday, August 18, 2022

8:30AM – 9:30AM	KEYNOTE ADDRESS DR. GAUTAM KUMAR DIRECTOR AND GM/INTEL CORPORATION *FRNY G140*
9:30AM – 12:05PM AND 2:25PM – 5:00PM	Student Research Seminars *Davidson School of Chemical Engineering* *FRNY G124* *FRNY B124*
12:05PM – 12:55PM	Lunch
12:55PM – 2:25PM	Poster Showcase Davidson School of Chemical Engineering *FRNY Atrium*

Poster #	Poster Title	Name(s) of Advisor(s)	Name(s) of Presenter(s)	Subject Area
1	Bioinspired adhesives and materials for tissue engineering applications	Julie Liu	Carly Battistoni Jessica Torres	Biotechnology
2	Metabolic modeling of inflammatory lipids in mammalian cells using cybernetic framework and information theory	Ramkrishna Doraiswami	Sana Khanum	Biotechnology
3	FOREVER Risk of Forever Chemicals	Chongli Yuan	Shichen Wu	Biotechnology
4	Developing an Empirical Model for Designing Tunable Collagen and Hyaluronic Acid Blended Hydrogels	Julie Liu	Paulina Babiak	Biotechnology
5	Engineering Cyanobacteria for Photosynthetic Production of Amino Acids	John Morgan	Melissa Marsing	Biotechnology
6	Spatiotemporal Signal Pathway Modulation Directed Human Heart Organoid for Cardiac Disease Modeling	Xiaoping Bao	Po-Yu Liang	Biotechnology
7	The effect of PLGA monomer sequence on the radiation-controlled release of drugs	You-Yeon Won	Sung-Ho Shin	Biotechnology
8	Effect of monomer sequences on glass transition temperature of poly(lactic-co-glycolic acid) copolymers	You-Yeon Won	Samruddhi Patil	Biotechnology
9	Dropwise additive manufacturing of pharmaceuticals	Gintaras Reklaitis Zoltan Nagy	Varun Sundarkumar	Pharmaceuticals
10	A Facile, Catchall Pathway for Carbon Impurity Minimization via Ligand Engineering of Colloidal Cu(In1-xGax)S2 Nanoparticles for Thin-Film Photovoltaics	Rakesh Agrawal	Daniel Hayes	Material Science
11	Using Computationally Generated Kinetic Data to Learn a Universal Stability Score	Brett Savoie	Veerupaksh Singla	Material Science
12	Towards a Hybrid MC/MD Method for Investigating SEI Degradation in Lithium-Ion Batteries	Brett Savoie	Dylan Gilley	Material Science
13	Automated Exploration of Radical and Ion-Containing Reaction Networks	Brett Savoie	Hsuan-Hao Hsu	Material Science
14	Developing Machine Learning Models for Automated Reaction Deduction	Brett Savoie	Tianfan Jin	Material Science
15	Evaluating Conjugated and Radical Conductive Polymers in Sensing and Spintronic Application Spaces	Bryan Boudouris	Hamas Tahir Aaron Woeppel	Material Science
16	Adhesion of Next Generation Energetic Materials	Stephen Beaudoin	Anne Serban	Material Science
17	Advances in Shortcut Modelling and Optimization of Heat Integrated Separation Processes	Rakesh Agrawal	Akash Nogaja	Process Intensification

18	Crystallization and Particle Technology Systems Engineering (CryPTSys) - Crystallization Group	Zoltan Nagy	Yash Barhate Inyoung Hur Monika Neal Montgomery Smith Wei-Lee Wu	Process Intensification
19	Model-Based Design and Monitoring of an Integrated Purification Process for Pharmaceutical Continuous Manufacturing	Zoltan Nagy	Inyoung Hur	Process Intensification
20	Upcycling Plastic Waste into Fuels, Waxes, and Other Valuable Products via Hydrothermal Processing	Linda Wang	Clayton Gentilcore	Energy
21	Solution-Processed Thin Film Semiconductors for Scalable, Low-Cost Manufacturing of Photovoltaic Devices	Rakesh Agrawal	Shubhanshu Agarwal Kiruba Catherine Vincent	Energy
22	Electrification and Decarbonization of Ethylene Production	Rakesh Agrawal	Edwin Rodriguez	Energy
23	Manufacturing of Electrified Chemical Processes in a microgrid	Can Li	Asha Ramanujam	Energy
24	Enhancing Capacity, Kinetics, and Thermal Safety of Lithium-ion Battery Graphite Anodes with a Conductive Polymer Binder	Vilas Pol	Daniel Gribble	Energy
25	First Principles Analysis of Oxidative Ethane Dehydrogenation on Iron Sulfide Catalysts Using Sulfur as a Soft Oxidant	Jeffrey Greeley	Anik Biswas	Catalysis and Reaction Engineering
26	Designing complex alloy catalysts with Density Functional Theory and machine learning	Jeffrey Greeley	Gaurav Deshmukh	Catalysis and Reaction Engineering
27	First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts	Jeff Greeley	Zuhal Cakir	Catalysis and Reaction Engineering
28	Micro-CT Scanning for Measuring Lyophilized Structures	Vivek Narsimhan Alina Alexeenko	Isaac Wheeler	Fluid Dynamics and Interfacial Phenomena
29	Dynamics of Multicomponent Vesicles in Viscous Fluids	Vivek Narsimhan	Anirudh Venkatesh	Fluid Dynamics and Interfacial Phenomena
30	Continuum and Molecular Studies of Interfacial flows and hydrodynamic singularities: drops, jets, and films of complex fluids in electric fields	Osman Basaran	Aaditya Joshi Sumit Kumar Xiao Liu Hansol Wee Evgeniy Boyko	Fluid Dynamics and Interfacial Phenomena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Student Research Seminar Schedule

Session A – FRNY G124

9:30 AM – 9:50 AM	**Consequences of Intracrystalline Diffusional Constraints for Propene Oligomerization over Brønsted Acid Zeolites** Elizabeth Bickel *Prof. Raj Gounder*
9:50 AM – 10:10 AM	**Tuning Active Site Distributions in Zeolite Catalysts for Regioselective Methylation of Toluene to para-Xylene** Sopuru Ezenwa *Prof. Raj Gounder*
10:15 AM – 10:35 AM	**Elucidating Effects of Potential, Hydrogen Peroxide, and Interlayer Interactions on Site Structure, Stability, and Activity of Fe-N-C Catalysts for Electrochemical O2 Reduction** Ankita Morankar *Prof. Jeff Greeley*
10:35 AM – 10:55 AM	**Elucidating Structure-Property Relationships at Metal-Metal Oxide Interfaces for Heterogeneous Catalysis** Kaustubh Sawant *Prof. Jeff Greeley*
11:05 AM – 11:25 AM	**Development of X-ray Emission Spectroscopy to Characterize the Electronic Structure of 5d Metal Catalysts** David Dean *Prof. Jeff Miller*
11:25 AM – 11:45 AM	**Influence of Bifunctional PtZn/SiO2 and H-ZSM-5 on the Rates and Selectivity of Propene Aromatization** Kurt Russell *Prof. Jeff Miller*
11:45 PM – 12:05 PM	**Upcycling Plastic Waste into Fuels, Waxes, and Other Valuable Products via Hydrothermal Processing** Clayton Gentilcore *Prof. Nien-Hwa Linda Wang*

Morning

Student Research Seminar Schedule

Session B – FRNY B124

9:30 AM – 9:50 AM	**Development of Polymer Lung Surfactant for Treatment of Acute Respiratory Distress Syndrome** Daniel Fesenmeier *Prof. You-Yeon Won*
9:50 AM – 10:10 AM	**Radioluminescent Nanoparticles for Multimodal Cancer Treatment** Kaustabh Sarkar *Prof. You-Yeon Won*
10:15 AM – 10:35 AM	**Combined Radiation-Induced Photodynamic Therapy and Immunotherapy Using Calcium Tungstate Nanoparticles, 5-Aminolevulinic Acid, and Epacadostat** Dhushyanth Viswanath *Prof. You-Yeon Won*
10:35 AM – 10:55 AM	**Live Cell Probes for Mitochondrial Epigenome** Han Zhao *Prof. Chongli Yuan*
11:05 AM – 11:25 AM	**High-throughput Transport Screening Platform through Collagen and Hyaluronic Acid Matrices** Paulina Babiak *Prof. Julie Liu*
11:25 AM – 11:45 AM	**Impact of Collagen II and III on Collagen I Hydrogel Polymerization** Carly Battistoni *Prof. Julie Liu*
11:45 PM – 12:05 PM	**The effect of crosslinkers on mussel- and elastin-inspired surgical lung sealing** Jessica Torres *Prof. Julie Liu*

Afternoon

Student Research Seminar Schedule

Session A – FRNY G124

2:25 PM – 2:45 PM	**Discovery of TMPRSS2 Inhibitors by Virtual Screening, and Identification of Dehydration-Sensitive Backbone Hydrogen Bonds Using a Novel Descriptor** Suraj Ugrani *Prof. Sangtae Kim*
2:45 PM – 3:05 PM	**Computational Investigation of The Kinetics and Thermodynamics of Crystal Nucleation** Pelin Bulutoglu *Prof. Doraiswami Ramkrishna*
3:10 PM – 3:30 PM	**Modernizing Continuous Pharmaceutical Tablet Manufacturing Processes via Model Predictive Control** Yan-Shu Huang *Profs. Gintaras Reklaitis and Zoltan Nagy*
3:30 PM – 3:50 PM	**Blend Homogeneity of Active Pharmaceutical Ingredient Blended by Feeder Blender System Producing Small Batches in Semi Continuous Mode** Sumit Kumar *Profs. Gintaras Reklaitis and Zoltan Nagy*
4:00 PM – 4:20 PM	**Controlled Partial Site Coverage of Pd Nanoparticles by Titanium Oxide Strong Metal-Support Interactions (SMSI)** Christian Breckner *Prof. Jeff Miller*
4:20 PM – 4:40 PM	**Novel Ligand Design of 2D Halide Perovskites through Molecular Dynamics and Machine Learning** Zih-Yu Lin *Prof. Brett Savoie*
4:40 PM – 5:00 PM	**Developmental Pb Exposure Increases AD Risk via Altered Intracellular Ca2+ Homeostasis in hiPSC Derived Cortical Neurons** Junkai Xie *Prof. Chongli Yuan*

Afternoon

Student Research Seminar Schedule

Session B – FRNY B124

2:25 PM – 2:45 PM	**Design Features for Charge Transport in Nonconjugated Radical Polymers** Ying Tan *Profs. Brett Savoie and Bryan Boudouris*
2:45 PM – 3:05 PM	**Charge Transport and Magnetism in Nitroxide Radical-Based Single Crystals** Zihao Liang *Prof. Bryan Boudouris*
3:10 PM – 3:30 PM	**Achieving High Thermoelectric Performance and Stability of Tin-based Halide Perovskites** Sheng-Ning Hsu *Profs. Bryan Boudouris and Letian Dou*
3:30 PM – 3:50 PM	**Molecular Design of Topochemical Polymer Single Crystals with Closed-Loop Recyclability** Zitang Wei *Prof. Letian Dou*
4:00 PM – 4:20 PM	**Complex Deformation Histories and Their Implications for Modeling Thermomechanical Behaviors of Glassy Polymers** Hosup Song *Prof. Jim Caruthers*
4:20 PM – 4:40 PM	**Effect of Initial Conditions on Promotion and Inhibition of Filament Breakup** Xiao Liu *Prof. Osman Basaran*
4:40 PM – 5:00 PM	**Impact of Interfacial Rheology on Droplet Dynamics** Natasha Singh *Prof. Vivek Narsimhan*


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Abstracts

Consequences of Diffusional Constraints in Brønsted Acid Zeolites for Propene Oligomerization Rates and Selectivity

Elizabeth Bickel

Prof. Rajamani Gounder

Brønsted acid zeolites catalyze propene oligomerization, an important reaction for upgrading light alkenes into fuel-range hydrocarbons. Propene oligomerization rates are proposed to depend numerous sample properties, including H^+-site density and distribution, and zeolite topology. Yet, consensus is lacking among literature reports, reflecting concurrent variation in active site and crystallite properties in many zeolite samples crystallized by conventional methods, disparate reaction conditions, and a dearth of mechanistic connections between oligomerization rates and sample properties.

Herein, we crystallize MFI samples with independently varied H^+-site density (H^+/u.c. = 0.3–5.7), distribution, and crystallite size (0.03–2.70 μm) to interrogate their independent effects on propene dimerization rates (7–630 kPa C_3H_6, 503 K). Dimerization rates decrease with time; pressure step-change experiments indicate that this deactivation predominantly reflects increasing intracrystalline diffusional constraints imposed by bulky alkenes accumulating within the zeolitic micropores. Intracrystalline diffusion limitations on propene oligomerization rates are further evidenced by the systematic decrease of rates with increasing crystallite size for samples of fixed Al content. Effectiveness factor formalisms reveal that dimerization rates are disproportionately lower for MFI samples of dilute Al content (Si/Al 250) compared to those of higher Al content (Si/Al 50) because H^+ density influences the composition of products accumulated within the zeolitic micropores during catalysis, and thereby the extent to which diffusional constraints influence rate. Sample properties that increase diffusional constraints (e.g., lower H^+/u.c., larger crystallite size) result in higher selectivities to oligomer (e.g., C_9) and β-scission products, reflecting the longer intracrystalline residence times of products formed in these materials. Different zeolite topologies (TON, FAU, *BEA) were also tested to probe the consequences of pore size and connectivity for oligomerization rates and selectivities. Overall, this work reveals the important role of diffusional constraints in H-zeolites generated by reaction products within the catalyst micropores for propene dimerization rates and product selectivity.

References:

[1] Mlinar, A. N., et al., J. Catal. 288, 65-73 (2012).

[2] Bernauer, M. et al. J. Catal. 344, 157–172 (2016).

[3] Sarazen, M. L., Doskocil, E. & Iglesia, E. ACS Catal. 6, 7059–7070 (2016).

[4] Nimlos, C. T., et al. Chem. Mater., 32, 9277-9298 (2020)

Tuning Active Site Distributions in Zeolite Catalysts for Regioselective Methylation of Toluene to para-Xylene

Sopuruchukwu Ezenwa

Prof. Rajamani Gounder

Toluene methylation to *para*-xylene (*p*-X), a high-value polymer precursor, involves a network of parallel and sequential reactions that affect the *p*-X yield.[1] Mobil Five (MFI) zeolites are crystalline aluminosilicates which contain a diversity of catalytically active Brønsted acid sites (H^+) associated with distinct aluminum (Al) locations and arrangements within varying sizes of microporous voids that confine reactive intermediates and transition states or at unconfined external surfaces.[2] The distribution of Al (and H^+) is influenced by the organic and inorganic structure directing agents (SDA) employed during zeolite synthesis. Previous design strategies for MFI catalysts focused on either modifying its diffusion properties to favor formation of faster diffusing *p*-X within the micropores or eliminating unselective external H^+.[1] Here, we apply synthetic methods to tune the active site distribution within MFI voids and demonstrate the consequences for regioselective toluene methylation to *p*-X under conditions free of influences of external acid sites, intracrystalline residence times, and reactor-bed residence times. MFI samples with fixed Al content (Si/Al~50) were synthesized with conventional and non-conventional SDAs. Initial xylenes formation rates (per H^+) were zero-order in dimethyl ether (DME) pressures (>25 kPa) and transitioned from a first-order to zero-order dependence in toluene pressures (0.2-8.8 kPa), which reflected increasing coverages of co-adsorbed toluene on DME-derived intermediates that subsequently react in a kinetically-relevant C-C formation step to form xylenes. On the suite of MFI prepared using conventional SDAs, the *p*-X/*o*-X ratio (~0.5) was consistent with kinetic control due to the stabilization of methylation transition states by inductive effects of methyl in *para* and *ortho* positions to added methyl. In contrast, MFI synthesized by non-conventional SDAs exhibited significantly higher *p*-X/*o*-X ratios (~3-7).

Further kinetic and mechanistic assessments on a series of aluminosilicates (TON, MFI, BEA, MCM41) with acid sites located within varying void sizes (0.53-3.0 nm) revealed that xylenes formation rate and isomer selectivity differences among MFI materials reflect effects of acid sites located within distinct MFI void sizes on the kinetically-relevant methylation transition states. Taken together with past reports[3] on how organic SDAs can bias the siting of Al within distinct zeolite voids, our findings indicate that the SDAs used to crystallize MFI result in different acid site distributions that influence kinetically-controlled rates and selectivities during toluene methylation to xylenes. Overall, our work provides fundamental insights that can guide practical catalyst design for targeted upgrading of chemical feedstocks to higher-value products.

References:

[1] Chakinala, N.; Chakinala, A. G. *Ind. Eng. Chem. Res.* **2021**, *60*, 5331

[2] Knott, B. C.; Nimlos, C. T.; et al. *Chem. Mater.* **2018**, *8*, 770

[3] Pinar, A. B., et al. *Chem. Mater.* **2013**, *25*, 3654

Elucidating In-situ Structure based Stability-Activity Insights for Fe-N-C Catalysts during O_2 Reduction

Ankita Morankar

Prof. Jeffrey Greeley

Fe-N-C (iron-nitrogen-carbon) electrocatalysts have emerged as promising economic alternatives to carry out oxygen reduction reaction (ORR) at cathodes in acidic media in hydrogen fuel cells compared to their precious group metal-based counterparts. However, the structure of sites responsible for ORR are not completely understood. FeN_xC moieties, formed from a pyrolytic synthesis procedure, have been proposed to drive ORR activity, however, they can exist in a multitude of configurations with variations possible in their nitrogen environments (pyridinic, pyrrolic), site location (in-plane, edge, intrapore, single graphene layer, multilayered graphitic stack), site clustering, and nitrogen coordination (FeN_x with x from 1-4). Further, the stability of this catalyst declines in an acidic environment, posing a formidable challenge for their adoption in commercial fuel cells.[1,2]

In this study, we derive atomistic scale insights on the equilibrium structure of active sites, and their corresponding intrinsic stability as well as their intrinsic activity. This is done for a comprehensive set of sites spanning the aforementioned structural variations, using first principles density functional theory. We track the in-situ structural evolution of active sites as a function of the applied voltage using ab-initio thermodynamic phase diagrams. High coverages of oxidizing intermediates form at increasing electrode potentials, and we rigorously enumerate these with a graph theory formalism.[3] In addition to co-adsorption effects at high coverages, we also explicitly account for stabilization effects due to solvation. We determine these using an in-house formalism inspired by simulated annealing conducted on hydrated models.

Our results indicate that hydroxyl or epoxy groups form on the Fe-N-C catalyst surface, resulting either from H_2O dissociation at high voltages, or from dissociation of the byproduct, $H_2O_{2(aq)}$. Amongst all sites, pyridinic FeN_4 sites present at the zigzag edges of graphene, in isolation or as clusters, exhibit the highest ORR activity. Carbon atoms neighboring them get over-oxidized, however, with hydroxy groups within 0.1 V of ORR. Hence, any high potential spikes during the fuel cell operation could reduce stability via active site restructuring. The propensity for over-oxidation is observed for all other site geometries as well, although sites in the bulk only over-oxidize when H_2O_2 byproducts are present. The results, in turn, point to active site oxidation with associated processes such as carbon/nitrogen corrosion, as important drivers of Fe-N-C activity loss during fuel cell operation.

References:

[1] S. Liu, et al., *Nature Energy*, 2022

[2] C. H. Choi, et al., *Angewandte Chemie International Edition*, 2015

[3] S. Deshpande, J. Greeley, *npj Computational Materials*, 2020

Elucidating Structure-Property Relationships at Metal-Metal Oxide Interfaces for Heterogeneous Catalysis

Kaustubh Sawant

Prof. Jeffrey Greeley

In heterogeneous catalysis, oxides are widely used as supports for transition metal nanoparticles. The oxide supports are known to interact with the nanoparticles in highly complex and non-intuitive ways that fundamentally alter the catalytic properties of the system. The strong metal support interaction (SMSI), wherein metal nanoparticles supported on oxides are believed to be partially covered by reduced, ultrathin oxide films, is among the best-known classes of oxide-metal interfacial interactions in heterogeneous catalysis[1]. In the current study, periodic density functional theory (DFT) calculations, along with surface science experiments in collaborators' groups, are carried out to systematically study the molecular-level underpinnings of these transformations.

As a starting point, we analyze the Pd/ZnO system. Since ZnO is an irreducible oxide, it provides a test of the traditional hypothesis that partial reduction of support cations is necessary to exhibit SMSI. In order to compare our calculations with surface science experiments, where the ultrathin oxide films are not in equilibrium with bulk species, we developed a mixed canonical – grand canonical phase diagram scheme. The scheme, when combined with exhaustive DFT calculations of different ultrathin ZnO_xH_y film structures and stoichiometries, permits direct comparison of the calculated free energies of disparate films. Although, the thin film models provide more well-defined conditions for studying SMSI, there are thermodynamic difference with the real SMSI system. These differences can be described by changing the thermodynamic ensemble used to analyze the DFT results and extrapolating to deduce the stability of films at realistic SMSI conditions. Using this formulation, we show that oxy-hydroxy films, which don't exist in bulk, may promote SMSI in irreducible oxides. This behavior is traced to both hydrogen incorporation in the films and strong stabilization of the films by the metal substrates. Secondly, we demonstrate that the formation energies of these films are related to the binding energies of isolated Zn and O atoms via linear scaling relationships. We exhibit the explanatory and predictive power of these relationships for several common ultrathin film systems, and further discuss how the SRs can lead to identification of easier-to-calculate descriptors to estimate the film formation energies of complex thin film oxides. As an example, we show that using just the Zn and O adsorption energies, it is possible to determine a comprehensive phase map for ZnO_xH_y film adsorption on disparate transition metal surfaces.

Finally, we elucidate the impact of overlayer oxide formation on CO oxidation reaction. We found that the graphite-like ZnO interacts weakly with Pt surface and barely affects the surface electronic properties. On the other hand, the honeycomb-like $Zn_6O_5H_5$ can contribute negative charge to the Pt atoms confined within the zinc hydroxy rings and tune the adsorption behavior of CO with little sacrifice of the total number of active sites. The formation of such ordered zinc hydroxide phase can serve as an effective way to tune the chemistry of metal surfaces. Ultimately, the goal is to provide design principles for metal nanoparticle catalyst coated with different surface oxides since these systems play a crucial role in industrially relevant catalysts.

Novel Non-Resonant X-ray Emission Spectroscopy to Characterize the Electronic Structure of 5d Metal Catalysts

David Dean

Prof. Jeffrey T. Miller

The future of sustainable energy and chemical conversion will rely on high-performance catalysts. Over the past century, characterization techniques have developed in parallel to catalyst materials to afford a more precise understanding of catalyst structure. [1] The correlation of catalyst structure and performance has expedited catalyst discovery and tuning.

X-ray spectroscopy is a powerful tool used to evaluate the geometric structure of catalysts. Specifically, X-ray absorption spectroscopy (XAS) and X-ray diffraction (XRD) are useful for obtaining information about local coordination, bond distances, and phase structure. Synchrotrons are powerful photon sources that generate the high flux of X-rays necessary to conduct XAS and XRD on catalyst materials. Synchrotrons have been increasingly employed, often in tandem with in-situ treatment systems, to study catalyst structure under realistic reaction conditions. [2] This work outlines the development of synchrotron non-resonant X-ray emission spectroscopy (NR-XES) as a new tool for catalyst characterization.

As part of the NSF Center for Innovative and Strategic Transformation of Alkane Resources (CISTAR), a series of metal alloy nano-catalysts are being developed for hydrocarbon conversion on an industrial scale. The design of these catalysts is based on both geometric and electronic considerations. Recent advances in synchrotron technology have enabled the development of NR-XES, which is an element-specific technique that probes weak electronic transitions to obtain information about the structure of valence electrons, which are involved in adsorbate binding as well as catalytic transformations. [3] This work aims to be the first application of in-situ NR-XES to 5d metal catalyst materials. This technique, conducted at the Brookhaven National Laboratory 8-ID beamline, has assessed changes in valence electron structure. The formation of Pt-Zn, Pt-Sn, Pt-Mn, and Pt-Cu alloys resulted in a narrowing of the d-band, with the most significant loss of electron density near the Fermi level. Additionally, decreasing Pt nanoparticle sizes yielded a shift of the d-band electrons to higher energy. Lastly, surface adsorption of oxygen shifted the Pt d-band to lower energy. The novel NR-XES characterization capability furnishes an understanding of the valence electron structure, which aims to accelerate the development of the next generation of high-performance catalyst materials for sustainable chemical and energy technologies.

References:

[1] Fechete, I., Wang, Y., Vedrine, J. C. The past, present, and future of heterogenous catalysis. *Catalysis Today* 189 2-27 (2012).

[2] de Groot, F. High-Resolution X-ray Emission and X-ray Absorption Spectroscopy. *Chem. Rev.* 101, 1779-1808 (2001).

[3] Glatzel, P., Sikora, M., Smolentsev, G., Fernandez-Garcia, M. Hard X-ray Photon-In Photon-Out Spectroscopy. *Catalysis Today* 145, 294-299 (2009).

Influence of Bifunctional PtZn/SiO2 and H-ZSM-5 on the Rates and Selectivity of Propene Aromatization

Christopher Russell

Jeff Miller

As light alkane resources have become more available due to technological developments including hydraulic fracturing, horizontal drilling, and the abundance of shale gas reserves, methods to convert these resources to aromatics has become increasingly desirable. One process for converting shale gas (especially ethane, propane, and butane) to benzene, toluene, and xylene (BTX) is through catalytic dehydrogenation followed by aromatization of the respective olefins (i.e. ethene, propene, and butene) [1]. Previous studies suggest that the use of a bifunctional dehydrogenation (e.g. Ga, Zn, or Pt) and acid catalyst (e.g. H-ZSM-5, SPA) increases the aromatization rate and selectivity to BTX. However, these studies compare catalysts at equivalent space velocity, or at equivalent propene conversion; they do not account for the reactive species that are formed as intermediates during olefin aromatization [2].

This study demonstrates the differences between BTX formation from propylene in the presence and absence of dehydrogenation catalysts (i.e., PtZn). Further, it indicates how propylene conversion is an inaccurate descriptor of the progress of the reaction, and when using a more complete description (i.e., conversion of all reactive species), the presence of the dehydrogenation catalyst does not significantly impact the selectivity to aromatics.

In this study, physical mixtures of H-ZSM-5 (Si/Al = 40) and PtZn/SiO_2 are compared to solely H-ZSM-5 for propene aromatization at 723 K - 823 K. During propene aromatization, a large number of products are formed: stable products (i.e., BTX, methane, and ethane) and reactive species (i.e., ethene, butenes, etc.). Reactive species will continue to react and form aromatic products, thus describing reaction progress in terms of conversion of all reactive species as opposed to solely propylene conversion is more accurate. When measuring reaction progress using propylene conversion, the presence of PtZn mixed with H-ZSM-5 suggests that the presence of PtZn significantly increases the selectivity to aromatics. However, when measuring the reaction progress using conversion of all reactive species, the selectivity to BTX is similar regardless of the presence of PtZn. While the selectivity to BTX is unaffected by the presence of PtZn, the other products' selectivity is changed. At 723 K, the other stable products are methane, ethane, and propane. At 823 K, propane becomes a reactive species, and only methane and ethane are the other stable products.

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Upcycling Plastic Waste into Fuels, Waxes, and Other Valuable Products via Hydrothermal Processing

Clayton Gentilcore

Prof. Nien-Hwa Linda Wang

Plastic waste quantities have exponentially increased in the past 60 years, but only 9% of these plastics were mechanically recycled and 12% were incinerated. The remaining 79% of plastic wastes, totaling over 6 billion tons, have accumulated in landfills and the oceans. These plastic wastes slowly degrade over time into microplastics and toxic chemicals that pollute the environment and pose severe risks to food and water supplies, human health, and life on the planet.[1-2] Conventional methods of plastic waste treatment, specifically mechanical recycling, incineration, and pyrolysis, have been ineffective in reducing plastic waste accumulation rates.[1]

Low-pressure hydrothermal processing (LP-HTP) has been invented by the Wang Research Group to convert polyolefin plastic wastes (HDPE, LDPE, PP) to gasoline and diesel fuels and other valuable products.[2] This process does not require the use of catalysts or costly fuel upgrading processes, and produces minimal char and polyaromatic hydrocarbons (<1 wt%). Preferred conversion conditions result in 87 wt% of polyolefin wastes converted to oils having carbon number distributions within the ranges of gasoline and diesel (C_4-C_{25}), with the remaining 13 wt% converted to light hydrocarbon gases (mainly C_3). The oils can be separated into high-quality gasoline and diesel fuels, and the energy produced from combusting the gases (5.7 MJ/(kg plastic)) is higher than that required for feedstock pretreatment (0.7 MJ/(kg plastic)), depolymerization by LP-HTP (1.5 MJ/(kg plastic)), and oil separation by distillation (2.2 MJ/(kg plastic)). This fuel production method, emitting 0.24 (kg CO_2)/(kg plastic) from gas combustion, is more energy efficient and environmentally friendly than fuel production from crude oil (46.4 MJ/(kg feed) and 0.77 (kg CO_2)/(kg feed)), resulting in 92% energy savings and 69% less GHG emissions. This method also has lower capital, operating, and overall production costs compared to crude oil refining into fuels.[2]

LP-HTP methods have the potential of annually converting up to 220 million tons of polyolefin waste into 190 million tons of fuels, saving up to 1.5 billion barrels of oil equivalent (BOE) and reducing GHG emissions compared to crude oil refining by up to 100 million tons of CO_2. LP-HTP methods can reduce plastic waste accumulation and pollution by providing financial incentives to increase plastic waste collection. These methods have the potential to transform the current linear path of crude oils to polyolefins to plastic wastes into a more sustainable and economical circular path of producing clean fuels, chemicals, and other products from polyolefin wastes.[2]

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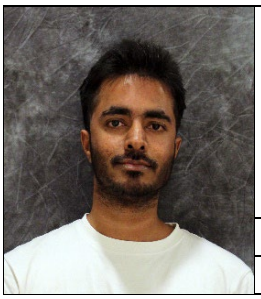

Discovery of TMPRSS2 inhibitors by molecular docking, and machine learning using a novel descriptor

Suraj Ugrani

Prof. Sangtae Kim

Repeated viral outbreaks in the past and the recent COVID-19 pandemic have highlighted the urgent necessity for a broad-spectrum antiviral. Host proteases implicated in the infection mechanism of multiple viruses are ideal targets for such drugs. The human Transmembrane Protease Serine Type 2 (TMPRSS2), which is used by several coronaviruses including SARS-CoV-2, has emerged as a favorable target for treatment of coronaviruses[1].

In this work, we perform virtual screening of small molecule protease inhibitors from the MEROPS database by molecular docking using UCSF DOCK to identify potential TMPRSS2 inhibitors. We also briefly describe our homology model of the protease used for docking in the early days of the pandemic, which was found to be in close agreement with the subsequently resolved crystal structure. Compounds with the highest docking scores are then analyzed for important interactions with the binding pocket. In addition, we employ a novel descriptor based on the concept of 'hydrogen bond-wrapping', which refers to the tendency of non-polar side chain groups to surround a protein's backbone hydrogen bonds[2]. By implementing machine learning models, which use the results from docking, we identify regions in the binding pocket which are most sensitive to dehydration, which could help guide the design of new inhibitors.

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Computational investigation of the kinetics and thermodynamics of crystal nucleation

Pelin Su Bulutoglu

Prof. Doraiswami Ramkrishna

Crystal nucleation is of fundamental importance for the modeling and control of many processes. Examples can be given from atmospheric sciences, biology, materials research, and the pharmaceutical industry. Despite its ubiquity, we do not have a complete understanding of crystal nucleation due to challenges in experiments that arise from the stochasticity of nucleation happening at the nanoscale. Direct observation of nucleation in experiments is still challenging and rare, which makes molecular simulations an invaluable asset in understanding nucleation. Classical nucleation theory (CNT) has been the prevalent theory to describe the mechanism of nucleation since its development in the early 20th century. CNT assumes that density and crystalline order increases simultaneously as the nucleus is formed and thus, the nucleus has an identical structure to its bulk crystal. This allows nucleation to be described by the change in a single nucleus size variable. However, nucleus size alone is not able to capture any structural changes in the cluster that arise due to non-classical mechanisms [1] or competing polymorphs [2].

This talk focuses on two cases where the inclusion of structure specific nucleus size coordinates provides additional thermodynamic and kinetic insight into crystal nucleation. First, we take an atomic-level look into the mechanism of NaCl nucleation from aqueous solution at elevated supersaturations. Two-dimensional free energy calculations as a function of structure-specific nucleus size coordinates reveal a thermodynamic preference for a non-classical mechanism through composite cluster formation. The computed free energy landscape agrees well with the composite cluster free energy model [3]. A switch in the mechanism from 1-step to 2-step is observed upon an increase in concentration. We propose that the shift in mechanism is the result of a change in stability ranking of the crystalline, amorphous and solution phases. Second, we investigate the competition between HCP and FCC structures in the Lennard-Jones fluid by calculating the free energy of the system as a function of polymorph specific nucleus size coordinates. The single saddle point on the free energy surface reveals that polymorph selection happens after the nucleation stage, and the critical cluster transforms into either HCP or FCC phase in the growth stage. We propose a population balance model that captures the nucleation, growth, and polymorphic transformations of a population of clusters in LJ nucleation from the melt. This multi-scale, first principles model can potentially predict the polymorphic outcome of a crystallization process and allow for a direct comparison to experiments.

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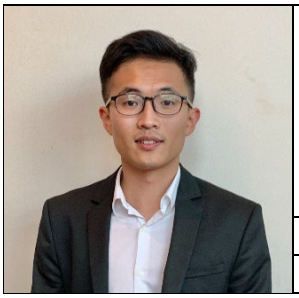

Modernizing Continuous Pharmaceutical Tablet Manufacturing Processes via Model Predictive Control

Yan-Shu Huang

Prof. Gintaras V. Reklaitis and Prof. Zoltan K. Nagy

Active control strategies are playing an essential role in modern pharmaceutical manufacturing. Instead of controlling the process input variables within tight ranges as practiced in traditional control approaches, a more flexible active control strategy has the potential to deal with process uncertainties and variations in raw material properties. Model predictive control (MPC) often serves as the preferred candidate for a centralized plant-wide control strategy. When there are many constraints on critical quality attributes (CQA) and strong process variable interactions exist in the multiple-input multiple-output (MIMO) system, MPC can demonstrate better capabilities in setpoint tracking and disturbance rejection compared to classical PID control. However, the implementation of MPC in pharmaceutical tablet manufacturing processes is still in infancy [1].

Under the concept of Quality-by-Control (QbC), a three-level hierarchical control structure can be applied to achieve effective setpoint tracking and disturbance rejection in the tablet manufacturing process through the development and implementation of a moving horizon estimation-based nonlinear model predictive control (MHE-NMPC) framework. When MHE is coupled with NMPC, historical data in the past time window together with real-time data from the sensor network enable model parameter updating and control. The adaptive model in the NMPC strategy compensates for process uncertainties, further reducing plant-model mismatch effects. The frequency and constraints of parameter updating in the MHE window should be determined cautiously to maintain control robustness when sensor measurements are degraded or unavailable. The practical applicability of the proposed MHE-NMPC framework is demonstrated via using a commercial scale tablet press, Natoli NP-400, to control tablet properties, where the nonlinear reduce-ordered mechanistic models used in the framework can predict the essential powder properties and provide physical interpretations.

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Achieving Blend Uniformity in pharmaceutical powders in batch, continuous and semi-continuous modes in different case studies

Sumit Kumar

Prof. Gintaras V. Reklaitis and Prof. Zoltan K. Nagy

In the pharmaceutical industry, solid dosages have multiple powder ingredients such as active pharmaceutical ingredients (API), excipients, lubricants etc. Mostly all the oral solid manufacturing processes start with the feeding of these ingredients followed by blending unit operation. Blending is a critical and essential unit operation in the manufacturing of all oral solid dosages. The objective of blending is to produce a homogenous mixture which is essential to ensure consistent dosage in the product[1]. Non-homogeneity in the product can be caused by material properties, blending process, blending time and even over blending. The challenge of achieving acceptable blend uniformity is much higher in low API drug loads. The objective of first case study is to achieve blend uniformity in a low API drug load product with six other excipients and determine the endpoint of blending. There needs to be a better understanding of how low concentration APIs (less than 0.5% w/w) can be homogeneously blended with other constituents.

Blend uniformity can be achieved by following a batch, continuous or semi-continuous mode of manufacturing. Blending was traditionally done in batch mode using various types of batch blenders that utilize convective transport and diffusive blending. With the emergence and acceptance of Continuous manufacturing, continuous batch blending has also picked up the pace and has its own merits and demerits[2]. Important challenges in continuous blending are to have a precise flow rate of the ingredients from the feeders throughout the run and to properly mix the material into a homogeneous run in a short residence time inside the blender. In second case study, we investigate an intermediate solution between batch blending and continuous blending – Semi-continuous blending providing small batches at a set frequency of time. Output from these small batches can be delivered downstream to both batch or continuous modes and have the flexibility of customizing the batch sizes. Important process parameters are varied to understand significance of each factor in achieving the right homogeneity[3]. The blend uniformity is then compared with the continuous feeding blending setup at Purdue pilot plant. The field of powder handling and blending is constantly innovating, and researchers from academia and industry are looking for improved, robust and effective integrated feeding blending solutions

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Controlled partial site coverage of Pd nanoparticles by strong metal-support interactions (SMSI)

Christian Breckner

Prof. Jeffrey T. Miller

Strong metal-support interactions (SMSI) is a phenomena that can occur in many metal supported on metal oxides catalysts. Recently, there has been increased interest in strong metal-support interaction (SMSI) based catalysts due to their ability to improve product selectivity, catalyst lifetime, and process performance in many reaction systems. Improvements on these key chemical processing properties are necessary as the world transitions to more efficient processes and alternative processes for liquid fuel and commodity chemical production.

SMSI was first observed for Pt/TiO_2 catalysts in the 1970's when reduction at 500 °C caused a near complete loss in CO uptake. STEM allowed researchers to fully understand why this happens: The TiO_2 species partially reduced to $TiO_{(2-x)}$ and covered the metal nanoparticles to near completion. Metal on SMSI oxide catalysts were simply not viable. Recent work looked at co-impregnated catalysts such as Pd and Ti on SiO_2 with hopes of reducing coverage. Coverages were effectively lowered while the advantageous properties remained. SMSI catalysts were studied for a wide array of chemical and some electrochemical processes; however, one major flaw persisted: the coverage levels were still above 70% which in many cases resulted in over-covered systems.

Motivated by the desire to advance SMSI catalysts, we showed that one can easily control coverage below 70% with the goal of providing a framework for which all SMSI catalysts can be synthesized to target a specific coverage level optimized for any reaction system. Using a combination of CO chemisorption, STEM, DRIFTS, propylene hydrogenation probe reactions, and XAS we show that SMSI coverage can be controlled by three different synthesis and pre-treatment methods: reducing the SMSI oxide loading to sufficiently low levels, using an intermediate oxidation step of varied temperature to partially remove coverage, and using an additional re-reduction step at varied temperatures to further induce coverage. The combination of these three methods allows for easily realizable coverage levels across the range of 0-85%.

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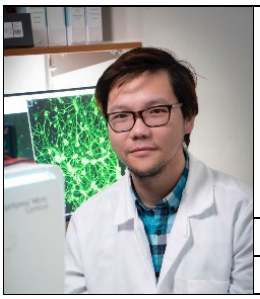
Novel Ligand Design of 2D Halide Perovskites through Molecular Dynamics and Machine Learning

Zih-Yu Lin

Prof. Brett M. Savoie

Organic-inorganic hybrid perovskite semiconductors are under investigation for many applications owing to their excellent optoelectronic properties and relatively simple processing. Two-dimensional (2D) halide perovskites are an attractive class of hybrid perovskites that have additional optoelectronic tunability due to their accommodation of relatively large organic ligands. Nevertheless, contemporary ligand design depends on either expensive trial-and-error testing of whether a ligand can be integrated within the lattice or conservative heuristics that unduly limit the scope of ligand chemistries.

Here, the structural determinants of ligand incorporation and perovskite stability are established by molecular dynamics (MD) simulations of over ten thousand perovskites, including an algorithmically generated set of prospective ligand chemistries and all previously reported experimental primary ammonium ligands based on C, H, O, S, and N. The simulation results show near-perfect predictions of true positive and negative examples drawn from the literature and reveal important ligand features to perovskite stability. Additionally, this large dataset is used to train machine learning classifiers capable of predicting the geometric stability of perovskite structures based solely on generalizable ligand features, thus providing an inexpensive tool for screening putative ligands. As a demonstration, the model was used to guide the selection of five new ligands that were successfully synthesized and incorporated into 2D perovskites. This work provides a new paradigm for future low-dimensional perovskite design.



Developmental Pb exposure increases AD risk via altered intracellular Ca^{2+} homeostasis in hiPSC derived cortical neurons

Junkai Xie

Prof. Chongli Yuan

Exposure to environmental chemicals such as lead (Pb) during vulnerable developmental periods can result in adverse health outcomes later in life. Human cohort studies have demonstrated a strong association between developmental Pb exposure and Alzheimer's Disease (AD) onset in later life which were further corroborated by findings from animal studies. The molecular pathway linking developmental Pb exposure and increased AD risk, however, remains elusive.

In this work, we used human iPSC derived cortical neurons as model system to study the effects of Pb exposure to developing and mature human cortical neurons. Neural progenitor cells (NPC) were exposed to low dose of Pb at 15 and 50 ppb for 48 h, differentiated into cortical neurons and assessed for maturity and AD-like pathogenesis. Although developmental Pb exposure does not seem to alter the differentiation process, we observed significantly altered neuronal morphology including neurite length and synapse density. Furthermore, mature neurons with Pb exposure showed significantly elevated intracellular calcium concentration, altered epigenetic landscapes and transcriptomic profile. Comparison of transcriptomic data between treated and unexposed cells revealed differentially expressed genes enriched in calcium-homeostasis regulating processes such as GRIN1 and CAMK2B which we further verified using immunofluorescence. Developmental Pb exposure also leads to elevated phosphorylated tau, neurofibrillary tau and Aβ42 along with other AD transcriptomic markers.

Collectively, our findings provide an evidence base for calcium dysregulation caused by developmental Pb exposure as a plausible molecular mechanism accounting for increased AD risk in populations with developmental Pb exposure.

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Effect of micelle size on the surface-mechanical behavior of a Polymer Lung Surfactant formulation

Daniel Fesenmeier

Prof. You-Yeon Won

If not properly managed, acute lung injuries, either through direct or indirect causes, have the potential to present serious risk for many patients worldwide. One of the mechanisms for the transition from direct lung injury to the more serious acute respiratory distress syndrome (ARDS) is the deactivation of the native lung surfactant, which stabilizes alveoli by lowering the high air-water surface tension, by injury-induced infiltrates to the alveolar space. Currently, there are no surfactant replacement therapies which are used to treat/prevent ARDS. To this end, our research group has shown that using a synthetic polymer lung surfactant has the potential to be an effective therapeutic for the treatment and prevention of ARDS [1].

To properly design the polymer lung surfactant, an in depth understanding of the factors influencing the surface-mechanical properties of the formulation is needed. The current formulation is composed of polystyrene-block-poly(ethylene glycol) (PS-PEG) which exists as kinetically “frozen” micelles in water. Due to the non-equilibrium nature of the PS-PEG “frozen” micelles, the final size of the micelles will change based upon changes in the formulation pathway. Therefore, we explored the effects of changing the micelle spherical size on the resulting micellar Langmuir film’s surface-mechanical properties.

The findings demonstrated the reduction in micelle aggregation number results in the subsequent monolayer having higher compressibility moduli and bending stiffnesses and collapsing at lower surface pressures [2]. The collapse pressure correlated with the appearance of out-of-plane wrinkle structures detected by Brewster angle microscopy (BAM). The increase of collapse pressure and onset of wrinkling of the larger micelles with thicker PEG coronas, indicate larger micelles form a more stable film at high surface pressure which is more desirable for the lung surfactant application. Finally, analysis of Brewster angle microscopy (BAM) images of out-of-plane wrinkle structures which formed upon monolayer collapse indicates the presence of continuous 1 nm thick PEG layer which allows micelle monolayers to bend under high compression.

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Radioluminescent nanoparticles for multimodal cancer treatment

Kaustabh Sarkar

Prof. You-Yeon Won

Head and neck squamous cell carcinomas (HNSCCs) are the 8th most common cancer in the United States predominantly affecting people over 65 years of age [1]. Current therapies for HNSCC include surgical resection, chemotherapy (CT), and radiotherapy (RT). For locally advanced HNSCC, the CT-RT combination ("chemoradiation") has been shown to be more effective than CT or RT alone and is the current standard of care [2]. Intratumoral (IT) chemotherapy based chemoradiation has the potential to overcome the limitations of conventional systemic CT-RT that severely affects a patient's quality of life. For realization of maximum benefits from IT CT-RT, our team has developed a radiation-controlled drug release nanoparticle formulation (paclitaxel and $CaWO_4$ nanoparticles co-encapsulated within a capsule formed by poly(ethylene glycol)-poly (lactic acid), named "PEG-PLA/CWO/PTX NP"). The formulation provides controlled release of anti- cancer drug Paclitaxel (PTX) from the formulation when irradiated with X-rays. The formulation is localized within the tumor for at least a month and the therapeutic efficacy in immune-deficient NRG mice xenograft models has been established in our previous publications [3].

The present work examines the effects of stereochemical structures of PTX on the efficacy of the PEG-PLA/CWO/PTX nanoparticle formulation. Stereochemical differences in two different Paclitaxel samples were identified and characterized using 1D and 2D nuclear magnetic resonance, Raman spectroscopy and circular dichroism studies. The differences in paclitaxel structures lead to significant differences in the *in vitro* and *in vivo* efficacy of the formulation. The two different paclitaxel show similar performance when used as a free drug with solvents used during clinical administration of CT. However, these subtle stereochemical differences significantly influence the release kinetics of PTX from the PEG-PLA/CWO/PTX formulation when irradiated with high energy X-rays. The different release profiles consequently manifest as different pharmacokinetic profiles of intratumoral PTX concentration in murine xenograft models. PEG-PLA/CWO/PTX formulations made with the two different PTX stereoisomers show significantly different efficacies in survival studies conducted in mice xenograft models. In conclusion, the present study demonstrates that differences in the stereochemical structures of an active drug like PTX might not be a parameter affecting the efficacy of treatment when used as a free drug but can significantly affect the efficacy when encapsulated in a nanomedicine platform.

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Combined Radiation-Induced Photodynamic Therapy and Immunotherapy Using Calcium Tungstate Nanoparticles, 5-Aminolevulinic Acid, and Epacadostat

Dhushyanth Viswanath

Prof. You-Yeon Won

Head and neck squamous cell carcinoma (HNSCC) is the 7th most common cancer worldwide with a 5-year survival rate of around 50%. It is predominantly diagnosed at the locally advanced stage, for which chemotherapy-radiotherapy combination is the primary form of treatment. However, development of resistance to these treatments results in high rates of cancer recurrence and unfavorable prognosis. Therefore, there is need for alternative treatment modalities that use different mechanisms of action.

Photodynamic therapy (PDT) is one such option that has shown promise in achieving complete responses in patients with residual or recurrent HNSCC following conventional RT. The combination of RT and PDT (RT-PDT) has demonstrated improved outcomes for a multitude of cancers, with their synergism further bolstered when the two therapies are applied concurrently rather than sequentially. However, conventional concurrent RT-PDT is limited in three important ways; (1) an optical device is required to deliver light to the site of PDT; (2) conventional PDT is limited to surface tumors due to the small penetration depth of visible light in human tissue; (3) it is highly localized and cannot treat metastasis.

This talk will discuss our recent work on a new concurrent RT-PDT method that addresses the limitations of current RT-PDT approaches for treatment of HNSCC. This method uses a new RT-to-PDT transducer, namely, radio-luminescent $CaWO_4$ (CWO) nanoparticles (NPs) encapsulated within micellar self-assemblies formed by poly(ethylene glycol)-poly(lactic acid) (PEG-PLA) block copolymers. These NPs are used in combination with 5-aminolevulinic acid (ALA), an FDA-approved water-soluble prodrug that causes preferential accumulation of an endogenous photosensitizer, protoporphyrin IX (PPIX), in cancer cells. Under ionizing radiation, CWO NPs emit UV-A/blue light, which activates PPIX. A confocal microscopy study suggests that the radio-luminescence energy transfer process potentiates a type-II photodynamic reaction which converts molecular oxygen into cytotoxic reactive oxygen species (ROS). *In vitro* clonogenic cell survival assays confirmed that concurrent PDT indeed significantly enhance the cell kill effects of X-rays. Ongoing studies are exploring the possibility of combining RT-PDT with immune inhibition blockade immunotherapy (IT) using Epacadostat (IDOi) *in vivo*. The hypothesis is that IDO inhibition coupled with localized cell death due to RT-PDT promotes T cell growth and maturation within the tumor microenvironment, resulting in systemic anti-tumor immune responses. This work will serve as the foundation for future studies evaluating the clinical translatability of this technology.

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Live cell probe for mitochondrial epigenome

Han Zhao

Prof. Chongli Yuan

Mitochondria, as the center of energy production, play an important role in cell homeostasis by regulating the cellular metabolism and mediating the cellular response to stress. As a mini cell, a mitochondrion is composed of its own membrane, DNA, and core protein machinery. The functional role of mitochondria is partially encoded by its own DNA (mtDNA). Epigenetic enzymes including DNA methyltransferases (DNMTs) has been found to colocalize with mitochondria[1-2], suggesting the role of epigenetic regulation of mtDNA. Epigenetic changes such as DNA and histone methylation, that are most abundant in nucleus, have been increasingly recognized to play a significant role in homeostasis and stress response. The current approaches focus on individual organelles, while neglecting the crosstalk between organelles. The cross-talking between the metabolome and the epigenome has attracted significant attention in recent years but with a major focus on how metabolism contributes to epigenomic changes. Few studies have focused on how epigenetic modifications may alter the mitochondrial composition and activity. Moreover, the understanding of regulatory role of mitochondrial epigenome was hindered by lack of tools to track mtDNA methylation in real time. Previous research on mitochondria has been largely focused on the mitochondrial structure and activity which motivate the development of a series of structures and activity probing tools.

To fill this knowledge gap, we designed a novel probe targeting methylated CpGs of mtDNA. We demonstrated the capability of our probe to reveal the spatial distribution of methylated mtDNA using super resolution microscopy. Our probe enables the ability to capture mtDNA methylation changes at a single-cell level. Couple with our previous probe targeting nucleus DNA methylation[3], we were also able to track single-cell mtDNA and nuclear DNA methylation simultaneously and discovered the unsynchronized dynamics of the nucleus and mitochondria. In summary, our tool offers a unique opportunity to understand the epigenetic regulation of mtDNA and its dynamic response to the microenvironment and cellular changes.

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High Throughput Platform for Macromolecular Transport

Paulina Babiak

Prof. Julie C. Liu

The expansion of mAb treatments available resulted in a need for advancement in administration routes. Subcutaneous administration is less invasive; requires shorter clinic times, which results in a significant improvement in patient's quality of life; improves patient compliance; and reduces cost to the healthcare system. The injected biotherapeutic, however, needs to traverse complex structures of the subcutis and the extracellular matrix (ECM) before it is absorbed by the lymphatic system to have an active effect. The ECM is largely composed of collagen, a fibrous protein, and hyaluronic acid (HA), and anionic polysaccharide. The high viscosity of HA is believed to act as a barrier for therapeutic transport. Transwell macromolecular recovery assay is a promising method to study transport of macromolecules through biological barriers. The Transwell inserts are permeable support devices which utilize permeable membrane which allows transport of macromolecules while trapping larger components (such as cells and fibrillar components of the extracellular matrix). In this work, we study the transport of a panel of macromolecules through tissue models composed of collagen and HA. Set of molecules was chosen to include Lysozyme (Lys, a small positive molecule), beta-lactoglobulin (BLg, a negative molecule), Dextran at 20 kDa (Dex, a linear molecule), bovine serum albumin (BSA; large negative molecule), and Bovine IgG (a large molecule which resembles therapeutic monoclonal antibodies in size).

Recovery of five model molecules through collagen at 4 mg/mL were performed demonstrated collagen matrix acts as size sorter. In these curves, the ranking for recovery after 48 hours is Lys>BLg~Dex>BSA>IgG. This ranking is directly related to the Hydrodynamic radii of the molecules, with Lys being the smallest molecule at 1.9 nm, followed by BLg at 3.5 nm, Dex at 3.2 nm, BSA at 4.1 nm and IgG at 5 nm. As control, recovery through HA at 20 mg/mL (1500 kDa) was tested. The ranking for recovery at 48 hours changed to BSA>BLg>IgG>Dex>Lys. BSA is the most negative molecule tested, thus the matrix composed of solely HA (a negative polysaccharide) likely repels BSA, and thus increased recovery is observed. Lysozyme on the other hand is the most positive molecule, which likely experiences attractive electrostatic forces which slow down its recovery. To compare the contributions of both collagen and HA simultaneously, hydrogels composed of collagen at 4 mg/mL and HA at 0.5, 2, 4, and 8 mg/L were tested. The ranking for recovery after 48 hours in ColHA gels was same as the Col-only gels, suggesting mass transport through the ColHA matrices is size dominated. However, addition of HA in the matrices slowed down the recovery of the molecules.

Inconclusion, collagen and HA play pivotal role in macromolecular transport. Collagen provides a tortuosity barrier while HA inhibits to the transport through its viscous properties. While free HA matrix recovery is governed primarily by electrostatic forces, recovery in ColHA matrices is a function of mainly the Col microstructure, meanwhile HA inhibits recovery.

Impact of Collagen II and III on Collagen I Hydrogel Polymerization

Carly Battistoni

Prof. Julie Liu

The extracellular matrix (ECM) confers structure to tissues and provides mechanical and biochemical signals to cells. Collagen (col) is the most abundant protein in the body and the main structural component of the ECM. Most tissues are composed of a combination of different collagen types. Blended col hydrogels have been studied, including col I/II hydrogels for cartilage tissue engineering[1] and col I/III hydrogels for cardiac[2] and vocal tissue engineering[3]. The addition of col II and III for these applications improved biological responses which highlights the importance of chemical cues blended col hydrogels provide. These blended gels exhibit different properties compared to collagen I gels alone.

To understand tissue physiology better, this work studies the polymerization kinetics of blended col hydrogels. Polymerization kinetics determine how the microstructure of gels forms. The microstructure of hydrogels then impacts gel properties such as mechanical, degradation, and transport. Additionally, polymerization temperature (25, 30, and 37 °C) was used to create tunable gel properties.

Col II dramatically slowed the polymerization of the gels, whereas collagen III largely impacts the rate of polymerization during the growth phase. At higher temperatures, all gels formed small fibrils and resulted in the lowest moduli; at lower temperatures (25 °C), larger fibrils were observed. Interestingly, the addition of col III introduced void spaces into the gels not observed in col I alone or col I/II gels. Col I/III also resulted in the stiffest gels and col I/II the weakest. Preliminary degradation and molecular transport studies on col I/II and col I showed that col I/II alters the degradation profile and slows dextran release out of the gels. Blended gels can be used to study drug delivery through different tissue types. Higher fidelity matrices can be created through the inclusion of additional ECM components or cells.

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The effect of crosslinkers on mussel- and elastin-inspired surgical lung sealing

Jessica Torres

Prof. Julie C. Liu

After lung resections, sutures and staples are used to close lung tissue, but these techniques result in air leakages in ~50% of all cases [1]. Surgical sealants can supplement sutures and staples to prevent air leaks, but no available sealants are adhesive enough, elastic enough to allow normal lung expansion, and stable over time. We developed bioinspired protein-based sealants that combine adhesion from L-3,4-Dihydroxyphenylalanine (DOPA) residues native to mussel adhesive proteins with the mechanical properties of elastin. These proteins are cytocompatible, provide the strongest bonds between substrates of any rationally designed protein when submerged in water, and can be easily applied underwater because they coacervate in physiological conditions.

We examined the burst pressure adhesion, swelling properties, and elastic moduli of the adhesive formulations when crosslinked with iron nitrate, (hydroxymethyl)phosphonium chloride (THPC), or sodium periodate to tune the adhesive and mechanical properties of our protein adhesive. The formulations had elastic moduli (3-9 kPa) similar to that of lung tissue (1-5 kPa) [2] and exhibited minimal volumetric change at equilibrium within three days of application. We measured the burst pressure strengths of our formulations with each different crosslinker. Upon application, all unmodified protein formulations failed to create a seal across the substrate boundary, whereas the DOPA-modified protein mixed with iron and periodate attained average burst pressures of 29 and 47 kPa, respectively. Tisseel, a commercially available surgical sealant, had a burst pressure strength of 1.3 kPa. Thus, the two most promising formulations had adhesion strengths significantly greater than the commercial standard.

The elastin-based DOPA-modified protein adhesives showed promise for biomedical applications including lung sealants. We demonstrated the tunability of mechanical properties of the material through various crosslinking schemes to match the stiffness of soft tissues and quickly volumetrically equilibrate. Furthermore, we found DOPA-modified elastin mixed with periodate and iron formulations to be promising for lung sealant application due to their high burst pressures and elasticity.

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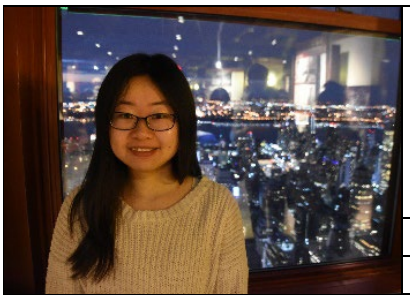

Design Features for Charge Transport in Nonconjugated Radical Polymers

Ying Tan

Prof. Bryan Boudouris and Prof. Brett Savoie

Conducting polymers based on open-shell radical moieties exhibit potentially advantageous processing, stability, and optical attributes compared with conventional doped conjugated polymers. Despite their ascendance, reported radical conductors have been based almost exclusively on the (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) radical, which raises fundamental questions regarding the ultimate limits of charge transport in these materials and whether some of the deficiencies exhibited by contemporary materials are due to the choice of radical chemistry.

To address these questions, we have performed a density functional theory (DFT) study of the charge transfer characteristics of a broad range of open-shell chemistries relevant to radical conductors, including p-type, n-type, and ambipolar open-shell chemistries. We observe that, far from being representative, TEMPO exhibits anomalously high reorganization energies due to strong spin localization. This, in turn, limits charge transfer in TEMPO relative to more delocalized radicals. By comprehensively mapping the dependence of charge transfer on radical-radical orientation, we have also identified a large mismatch between the conformations that are favored by intermolecular interactions and the conformations that maximize charge transport in all the open-shell chemistries studied. These findings suggest that significant opportunities exist to exploit directing interactions to promote charge transport.

Further, we have established the relationship between the fundamental molecular design and intramolecular charge transport behavior in radical polymers, in the first quantum chemical study of a set of radical polymers composed of systematically varied components, including backbone units, open-shell chemistries, and spacing units between the backbone and the radical groups. For each radical polymer with hundreds of atoms and large orientational variability, comprehensive conformer sampling was implemented, and analysis of interacting radical networks was performed on the conformational ensemble of low-energy structures. Complementary metrics based on graph-based resistor theories were used to analyze charge transport in these systems. We observe that no universally optimal linker or backbone chemistry exists; rather, the best linker and backbone chemistry are strongly influenced by the specific details of the radical. Spacers can sometimes improve the global connectivity but may also lead to trap formation. This framework for rationalizing the interplay of designable components augers enormous opportunities for further improving this class of open-shell macromolecules.

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Charge transport and magnetism in nitroxide radical-based single crystals

Zihao Liang

Prof. Bryan W. Boudouris

Nonconjugated radical polymers and small molecules are employed as conducting materials in multiple organic electronic devices, including electrolyte-supported devices and solid-state electronic devices, because of their charge transport and redox-active open-shell properties.[1] In fact, macromolecules with nonconjugated backbones and stable radical pendent groups can have impressive charge transport capabilities (i.e., thin film conductivities of ~20 S m^{-1}) if proper molecular design principles are employed.[2] Despite the success of nonconjugated radical polymers as solid-state charge conductors, the charge transport properties of nonconjugated open-shell small molecules have received less attention despite the fact that studying small molecule systems can facilitate the development of macromolecular radical conductors.

Furthermore, the unpaired electrons on these materials provide a means by which to respond to magnetic fields, making these materials promising candidates for organic magnets. Through proper molecular designs, strong antiferromagnetic and ferromagnetic ordering can be achieved. However, early work on the magnetic properties of nonconjugated radical polymers have only showed weak magnetic interactions among the open-shell sites because the distance between these sites in nonconjugated polymers is too far to have enough interactions. Therefore, new chemistries are needed to control the topology of open-shell sites into a strongly magnetically interacting network.

Motivated by the need to develop open-shell small molecule materials, we quantify the electrical conductivity and magnetic properties in organic radical single crystals. Through proper molecular engineering of functional groups, we synthesized and crystallized a nitroxide radical-based material that has a single-crystal electrical conductivity of ~3 S m^{-1}, which is one of the highest values for nonconjugated organic materials reported to date. Furthermore, we manipulate the molecular packing of the nitroxide radical molecules in the single crystals by introducing alkyl chains to the molecular structures. As a result, strong antiferromagnetic ordering is obtained in the crystals with a Neel temperature of 40 K. In conclusion, new open-shell materials are developed with excellent charge transport capabilities and strong magnetic properties. This effort provides clear insights into designing the next-generation radical conductors and magnetic materials.

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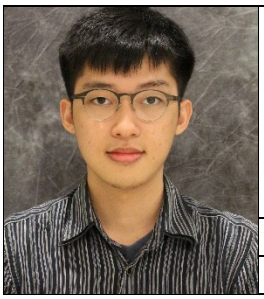

Achieving High Thermoelectric Performance and Stability of Tin-based Halide Perovskites

Sheng-Ning Hsu

Prof. Bryan W. Boudouris and Prof. Letian Dou

Halide perovskites have received much interest in optoelectronic applications thanks to their promising light absorption and photoluminescence features, long carrier lifetime and diffusion length. In addition, their solution-processability allows for low-cost, low-temperature, and large-area manufacturing. Thus, many efforts have focused on generating high-performance perovskite-based photovoltaics, light-emitting diodes, and photodetectors. Currently, commercialization of halide perovskites is hampered by their intrinsic instability under exposure to light and moisture, but two-dimensional (2D) halide perovskites are a possible replacement given their ability to overcome this critical limitation. By partially replacing the monovalent cations with relatively bulky organic ligands, halide perovskites are sliced into 2D layers sandwiched by the bulky ligands, and these ligands act as passivation layers that enhance the overall stability of the materials. Furthermore, the chemistry associated with the ligands opens new opportunities for tuning their end-use properties. However, this effort only scratched the surface of numerous applications of 2D perovskites that go well beyond solar energy conversion.

Thermoelectric (TE) devices are solid-state devices that interconvert electrical energy and thermal energy, and due to their compact structure, TE devices are used in waste heat harvesting and cooling electronic components. The maximum efficiency of a TE device is limited by the dimensionless material figure-of-merit, $ZT = \frac{S^2\sigma}{\kappa}T$.[15] Here σ, S, κ and T are the electrical conductivity, Seebeck coefficient, the thermal conductivity, and absolute temperature, respectively. With advanced instrumentation, we are able to characterize the ZT of thin film samples with high throughput.

Sn-based halide perovskites are promising for thermoelectric (TE) device applications because of their high electrical conductivity as well as the low thermal conductivity associated with their soft lattices. However, conventional three-dimensional Sn-based perovskites are not stable under typical TE device operating conditions. Here, we apply two strategies to improve the stability of the Sn-based perovskites for thermoelectric energy conversion. Firstly, we incorporated bulky conjugated ligands and form stable 2D halide perovskites. We demonstrate a thin film with a large power factor of 5.42 (average) and 7.07 (champion) $\mu W\ m^{-1}\ K^{-2}$ at 343 K with an electrical conductivity of 5.07 $S\ cm^{-1}$, and a Seebeck coefficient of 118.1 $\mu V\ K^{-1}$. Combined with the thermal conductivity of 0.124 $W\ m^{-1}\ K^{-1}$, the thin film is estimated to have ZT ~ 0.02. Importantly, these thin films show excellent operational stability (i.e., for over 100 hours) at 313 K. Secondly, we fabricate 3D tin-based perovskites with improved stability by alloying Sn and Pb, which in turn enhance the hole mobilities. These works suggest that the halide perovskites are a promising platform for thermoelectric energy conversion applications.

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Molecular Design of Topochemical Polymer Single Crystals with Closed-Loop Recyclability

Zitang Wei

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Commercial polymer production is a major driver of projected petroleum consumption and environmental pollution, yet energy-intensive and poorly selective scission of the ubiquitous C-C bonds in contemporary commercial polymers pose tremendous challenges to recycling and upcycling. From a fundamental chemistry perspective, the C-C bonds in conventional polymers are too strong to break at desired conditions without side reactions. Moreover, creating dynamic and reversible C-C bonds in a polymer remain a grant challenge in polymer science and engineering.

We propose that a truly reversible C-C bond between monomers can be realized by precisely elongating the bond using topochemical polymerizations (TCPs). TCPs have attracted considerable attention over traditional solution-phase polymerization because of the solvent- and catalyst-free conditions, simultaneously offering highly regulated products with high yield. TCPs can produce high molecular weight polymers without tedious purifications. Here, we demonstrate a topochemical approach for creating elongated C-C bonds with a bond length of 1.57~1.63 Å between repeating units in the solid state (v.s. 1.54 Å in conventional polymers) with decreased bond dissociation energies. Elongated bonds were introduced between the repeat units of 7 polymers from bis(indendione) derivatives (BIT). In all cases, the materials exhibit rapid depolymerization via breakage of the elongated bond within a desirable temperature range (140~150 °C). Furthermore, the topochemically prepared highly crystalline polymers are processable via ultra-sonication, meanwhile maintaining high depolymerization yield. Additionally, varying functional groups on the side chains can introduce different types of intermolecular interactions that significantly influence photochemical reactivities and polymer elastic modulus responses.

Based on current progress, we have established the complete circular economy of synthesis processing-application-recycling-resynthesis via the never-before-used polymer single crystals. The basic design rules also suggest that a large chemical space of tensile-strained polymers potentially exists. Clearly, a new chapter of polymer research has been opened and many opportunities will arise.

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Complex deformation histories and their implications for modeling thermomechanical behaviors of glassy polymers

Hosup Song

Dr. James M. Caruthers

In applications a key feature of polymeric glasses (i.e., plastics) is their mechanical stability under various conditions. The challenge here is that, unlike in case of materials in an equilibrated state such as metals or rubbers, behavior of the polymeric glasses depends on their entire thermomechanical history. As a result, there is no unique stress-strain curve that characterizes a material at a given temperature below Tg. The shape of the curve changes dramatically depending on the history the material has been subjected to. Numerous phenomenological models exist that curve fit the stress strain behavior of polymeric glasses; however, the "parameters" of these models have to be changed for each new thermomechanical history rendering them non-predictive. Then there are a few constitutive models that claim to have captured the true physics behind the glassy behavior. However, our analysis shows that these models still predict the response in case of a limited set of basic thermomechanical histories but fail qualitatively in case of more complex histories. Clearly a sufficiently rich set of experiments is sorely needed that can be used for validating current and future constitutive models. Creation of such a canonical data set is the primary goal of this project.

A striking feature of the response of a polymer glass to constant strain rate deformation is yield followed by softening known as the stress overshoot. The magnitude of the stress overshoot is sensitive to the thermomechanical history. In this research we carry out a large suite of multi-step deformation experiments where the last step is the constant strain rate loading during which the stress overshoot is observed. In this we systematically explore the effect of varying previous steps on the final stress overshoot magnitude. The previous steps include combination of creep, stress relaxation and constant strain rate deformations. A technical challenge in performing multi-step deformation protocols is to avoid a brittle failure of the specimen during large deformations. We use a custom synthesized copolymer that has higher ductility than conventional polymeric materials; we are able to achieve 60% strain in uniaxial extension without failure. A custom-built setup allows for monitoring not just axial but also lateral strain, which in turn allows for evaluating the Poisson ratio and the specific volume of the material as a function of the deformation.

We have identified a specific four-step deformation experiment comprising: (1) the constant strain rate loading, (2) partial unloading to a specified stress, (3) creep under that stress and (4) resumption of the constant strain rate loading, for which all existing literature models give qualitatively wrong predictions. A novel constitutive model being developed in our group that correctly predicts the four-step deformation experiment will be discussed.

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Effect of Initial Conditions on Promotion and Inhibition of Breakup during Filament Contraction

Xiao Liu

Prof. Osman A. Basaran

Liquid filaments surrounded by a gas arise in nature and applications, including ink-jet printing, DNA micro-arraying, paint spraying, spray drying, crop spraying, and metallic coating. As filaments contract, they either retract into spheres or disintegrate to form numerous droplets. In most previous studies, the filament's initial shape at time $t = 0$ has been idealized as a perfect cylinder capped off at both ends by identical hemispheres (radii R) and the fluid within which is at rest. [1]-[4] Motivated by the fact that in experiments and applications the filament fluid is often not quiescent at $t = 0$, the effect of a nonzero initial velocity profile is examined for Newtonian filaments. The variation of contraction velocity in time is obtained for different initial velocity conditions. A comprehensive phase diagram is presented in the space of L_0 (initial aspect ratio) and $v_{z,max}$ (initial tip velocity) for filaments of intermediate Ohnesorge number $Oh \equiv \mu/\sqrt{\rho\gamma R}$ (density ρ, viscosity μ, and surface tension γ) that delineates regions of the parameter space where breakup occurs from those where filaments contract to spheres without breakup.[5]

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Impact of Interfacial Rheology on Droplet Dynamics

Natasha Singh

Prof. Vivek Narsimhan

In recent years, understanding the dynamics of complex interfacial architectures between two immiscible fluids has gained the attention of many researchers. Membrane modifiers (for instance, surface-active agents or surfactants) are often added to emulsions to tailor them for applications in industry and bioscience. Polymer blends, vesicles, capsules, and lipid bilayers are some examples of fluid particles with complex interfaces, i.e., interfaces whose mechanics cannot be described solely by surface tension. From the modeling point of view, these complex fluid particles can be viewed as liquid droplets with a viscoelastic membrane of an adsorbed layer of surfactants, polymers, and proteins to capture the mechanics of the system. By understanding the detailed dynamics of simpler processes (breakup, deformation, sedimentation and coalescence), one can develop quantitative guidelines on how to process multiphase fluids with a wide range of complicated, surface-active species.

Droplet interfaces embedded with certain low molecular-weight surfactants and proteins exhibit predominantly viscous responses. Eicosanol (a fatty alcohol), hexadecanol (a low molecular weight surfactant), and protein β-casein are some of the examples of surface-active agents that form highly viscous membranes, giving rise to surface shear and dilational viscosity. Here, we examine the dynamics of droplets with such viscous interfaces.

In this work, we perform boundary-integral simulations to explore the effect of surface viscosity and surfactant transport on droplet breakup and relaxation in an extensional flow under the Stokes flow regime. We model the surface rheology of the droplet using the Boussinesq–Scriven constitutive relationship for a Newtonian interface. We incorporate the effect of surfactant transport by solving the time-dependent convection-diffusion equation and consider a nonlinear equation of state (Langmuir adsorption isotherm) to correlate the interfacial tension with the changes in surfactant concentration. We observe that the surface shear/dilational viscosity increases/decreases the critical capillary number beyond which the droplet becomes unstable and breaks apart by reducing/increasing the droplet deformation at a given capillary number compared to a droplet without interfacial viscosity. We present the relative importance of surface shear and dilational viscosity on droplet stability based on their measured values reported in experimental studies on surfactants, lipid bilayers, and proteins. We also discuss the impact of surface viscosity and surfactant transport on the relaxation of an initially extended droplet in a quiescent external fluid.

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Resumés

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EDUCATION

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PhD in Chemical Engineering
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Research Topic: High-Throughput In Vitro Platforms for Biotherapeutic Screening
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Columbia University, New York, NY **May 2019**
Bachelor of Science in Chemical Engineering
Academic Honors: Columbia University ASP Academic Achievement Award (Engineering), Columbia University ASP Leadership Award (Engineering), Sheldon E. Isakoff Scholarship, Columbia University Dean's List (Fall 2015, Spring 2016, Fall 2016, Fall 2018, Spring 2019)
Activities and Societies: Engineers Without Borders (Water Project Lead), Hong Kong University of Science and Technology Study Abroad (Spring 2017)

CAREER OBJECTIVE

Highly motivated PhD student seeking to develop biologically inspired materials at a post-doctoral or industry position.

SKILLS

Scanning Electron Cryo-microscopy	Confocal Microscopy
Immunostaining	Enzyme-linked immunoassay (ELISA)
Shear Rheology	Mammalian Cell Culture
Bacterial Cell Culture	Cell Extraction from Tissues
Protein Expression and Purification	Genetic Cloning

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Jan 2020 – Present**

- Engineered in vitro collagen and hyaluronic acid-based tissue models to improve current understanding of fundamental mechanics of the auto-injection process and improving drug bioavailability
- Studied DOPA modified elastin-like polypeptides for surgical adhesive application
- Mentored undergraduates

Undergraduate Researcher, Columbia University **Sept 2017 – May 2019**

- Genetically engineered caspase-3, expressed and purified enzyme variants, and evaluated phase behavior and protease activity of engineered caspase-3 enzymes
- Mentored an undergraduate student by introducing him to laboratory techniques and preparing him for an individual research project
- Mentored a high school student from an underrepresented community. Provided lessons on biology and experimental techniques, prepared detailed protocols with visual aids

Paulina M. Babiak

PUBLICATIONS AND PRESENTATIONS

1. **Babiak, P.M**., Hakim, M., Xu, Q., Torres, J., Buno, K., Bilionis, I., Solorio, L., and Liu, J.C., "Developing an Empirical Model for Designing Tunable Collagen and Hyaluronic Acid Blended Hydrogels," MRS Spring Meeting, Honolulu, HI, May 2022
2. **Babiak, P.M.,** Hakim, M., Xu, Q., Torres, J., Holt, W., Buno, K., Bilionis, I., Solorio, L., Liu., J.C. "Rational Design of Collagen and Hyaluronic Acid Hydrogels for Subcutaneous In Vitro Tissue Environments" AIChE, Boston, MA, 2021
3. **Babiak, P.M.,** Hakim, M., Holt, W., Xu, Q., Torres, J., Buno, K., Bilionis, I., Solorio, L., Liu., J.C. "Rational Design of Collagen and Hyaluronic Acid Hydrogels for Subcutaneous In Vitro Tissue Environments" (Manuscript in preparation)
4. **Babiak, P.M.,** Sanjuan, L., Ahmadzadegan, A., Hakim, M., Xu, Q., Vlachos, P., Solorio, L., Liu, J.C., "High Throughput Platform for Macromolecular Transport through Tunable Collagen and Hyaluronan Hydrogels for Therapeutic Monoclonal Screening" (Manuscript in preparation)
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6. Torres, J.E., Meng, F., Buno, K., **Babiak, P.M.,** Madduri, S., Solorio, L., Yeo, Y., Liu, J.C. "In Vitro Biologics Recovery Tissue Platform with Collagen and Crosslinking Hyaluronic Acid Hydrogels" (In preparation)
7. Xu, Q., Torres, J.E., Hakim, **M., Babiak**, P.M., Pal, P., Battistoni, C.M., Nguyen, M., Panitch, A., Solorio, L., Liu, J.C. "Collagen and hyaluronic acid-based hydrogels and their biomedical applications" Materials Science and Engineering: R: Reports. 146, 100641, (2021)

AWARDS AND HONORS

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EDUCATION

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PhD in Chemical Engineering | GPA: 3.65/4.0
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Honors Bachelor of Science in Chemical & Biomolecular Engineering | GPA: 3.58/4.0
Academic Honors: Degree with Distinction
Senior Thesis: *Simulating and Predicting Protein-Protein Interactions of Monoclonal Antibodies via Coarse-Grained Molecular Simulations*
Advisor: Christopher J. Roberts

SKILLS

Mammalian Cell Culture

- Human and rabbit MSCs, 3T3s; cytocompatibility; gel encapsulation; fixing and embedding

Colorimetric & fluorescent assays
ELISA
Confocal & widefield microscopy
RNA isolation
Rheology
Compression testing
Immunofluorescent staining
Cryotome & vibratome

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug 2018 – Present**

- Investigating the chondrogenic and chondroprotective capacity of various extracellular matrix molecules when incorporated into a collagen I/II blend scaffold with mesenchymal stem cells for cartilage tissue engineering
- Exploring influence of inflammatory environments on mesenchymal stem cell chondrogenic differentiation capacity
- Evaluating the impact of collagen II or III to a collagen I hydrogel on the polymerization kinetics of the system and resulting microstructure and mechanical and transport properties
- Mentoring two undergraduate researchers
- Cell Culture Lab Manager: maintains cell culture equipment and liquid nitrogen and CO_2 levels, training all new lab members on proper cell culture techniques and etiquette

Undergraduate Researcher, University of Delaware **Jan 2016 – May 2018**

- Studied protein solution viscosity of mAbs using multiple particle tracking microrheology to evaluate the feasibility of intravenous administration *(co-advised by Dr. Eric Furst)*
- Employed computer simulations to predict high concentration protein-protein interactions based on low concentration B_{22} data which was then compared to experimental excess Rayleigh ratio to assess the robustness of the model that aims to determine the plausibility of high concentration formulation

Quality Control Intern, Ultra Tab Laboratories **Jun 2015 – Aug 2015**

- Tested raw materials with various techniques, such as FT-IR and UV-Vis spectroscopy, to verify they were within USP specifications; developed spreadsheets to consolidate and analyze data
- Analyzed stability samples on products that were tested every 3, 6, 9, 12, and 24 months using HPLC for an assay of potency and stability

Carly M. Battistoni

AWARDS AND HONORS

- Estus H. and Vashti L. Magoon Award for Excellence in Teaching (College of Engineering, Purdue University) **2022**
- Leslie Bottorff Fellowship (Biomedical Engineering, Purdue University) **2019 – 2021**
- Ross Fellowship (Chemical Engineering, Purdue University) **2018**
- Chemical Engineering Alumni Laboratory Award (University of Delaware) **2018**
- Walter Silowka Chemical Engineering Scholarship (University of Delaware) **2017**

LEADERSHIP & TEACHING EXPERIENCE

Vice President & Treasurer Graduate Student Organization **2020 – 2021**

- Assisted President in overseeing organization
- Led information sessions and panels for prospective students virtually during COVID-19
- Managed organization funds (~$21k) and reimbursements

First-Year Representative Graduate Student Organization **2019 – 2020**

- Organized mentor-mentee program for incoming first-year students (~20 students)
- Helped ease the transition into graduate school via communication early in the summer and through organization of events such as an ice cream social and board game night

Chemical Engineering Calculations, Graduate TA **Fall 2019 & Spring 2021**

- Held weekly office hours help students on homework and graded exams (~155 students and ~60 students)

Undergraduate Chemical Engineering Laboratory, Undergraduate TA **Spring 2018**

- Assisted graduate teaching assistants in undergraduate laboratory (~50 students)

Computer and Informational Sciences, Undergraduate TA **Fall 2015**

- Ran lab section for an introductory MATLAB course (~30 students)

PUBLICATIONS AND PRESENTATIONS

1. *Sundar, S., ***Battistoni, C.,** *McNulty, R. *et al.* An agent-based model to investigate microbial initiation of Alzheimer's via the olfactory system. *Theoretical Biology and Medical Modelling* 17, 5, (**2020**)
2. Lin, C., **Battistoni, C. M**., Liu, J. C. "Redox-Responsive Hydrogels with Decoupled Initial Stiffness and Degradation" *Biomacromolecules.* 22 (12) *5270-5280,* (**2021**)
3. Xu, Q., Torres, J.E., Hakim, M., Babiak, P.M., Pal, P., **Battistoni, C.M.**, Nyugen, M., Panitch, A., Solorio, L., Liu, J.C. "Collagen and hyaluronic acid-based hydrogels and their biomedical applications" *Materials Science and Engineering: R: Reports.* 146, 100641, (**2021**)
4. Kilmer, C. E., **Battistoni, C. M.**, Cox, A., Breur, G. J., Panitch, A., Liu, J. C. "Collagen Type I and II Blend Hydrogel with Autologous Mesenchymal Stem Cells as a Scaffold for Articular Cartilage Defect Repair." *ACS Biomaterials Science and Engineering* 6 (6), *3464-3476,* (**2020**)
5. **Battistoni, C.M.**, Babiak, P.M., Cahya, L., Minnich, J., Athreya, R., Panitch, A., and Liu, J.C., Influence of Polymerization Conditions on Collagen I, II, and III Blend Hydrogels, Materials Research Society Spring Meeting, Honolulu, HI, May 2022, *(Poster Presentation)*
6. Lin, C.Y., **Battistoni, C.M.**, and Liu, J.C., Redox-Responsive Hydrogels with Decoupled Initial Stiffness and Degradation, Society for Biomaterials Annual Meeting, Baltimore, MD, 2022, *(Poster Presentation)*
7. **Battistoni, C.M.**, Liu, J. C., Kilmer, C.E., Durkes, A., Breur, G., Panitch, A. Collagen Type I and II Blend Hydrogels with Mesenchymal Stem Cells As Scaffolds for Articular Cartilage Defect Repair, American Institute of Chemical Engineers Annual Meeting, Orlando, FL, 2019 (*Oral Presentation*)

Elizabeth Bickel

2435 Neil Armstrong Drive #16, West Lafayette, IN, 47906
(615)-239-4632
bickele@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **Expected Dec. 2022**
Ph.D. in Chemical Engineering
Advisors: Prof. Rajamani Gounder, Prof. Fabio Ribeiro
Research Topic: Alkene oligomerization catalyzed by Brønsted acid zeolites and zeolite synthesis
Activities and Societies: CISTAR Student Leadership Council, AIChE, ACS

Tennessee Technological University, Cookeville, TN **May 2017**
B.S. Chemical Engineering | GPA: *3.9/4.0*
Academic Honors: *in cursu honorum*, and *distinction in the major*
Activities and Societies: Tau Beta Pi, Omega Chi Epsilon, AIChE

CAREER OBJECTIVE

A PhD candidate seeking a postdoctoral position in chemical engineering in the area of catalysis.

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2017 – Present**

- Developed experimental protocols and performed experiments to investigate influences of intracrystalline diffusion and active site proximity for oligomerization reactions of light olefins within zeolite catalysts.
- Investigated influences of synthesis compositions on crystallite size and active site distribution in different zeolite topologies.
- Characterized zeolite samples with techniques to assess crystallinity (micropore volume measurements, X-ray diffraction), quantify active sites (temperature programed desorption), and probe active site distribution (ion-exchange methods, elemental analysis), and crystallite size distribution (scanning electron microscopy, dynamic light scattering).

Undergraduate Research Assistant, Tennessee Tech University **Jan. 2015 – May 2017**

- Studied interactions between electron donor/electron acceptor materials in photovoltaic thin films using techniques such as fluorimetry and UV visible spectroscopy.
- Analyzed neutron scattering data to assess concentration gradients in photovoltaic thin films.

Undergraduate Research Assistant, Oak Ridge National Lab **Summer 2016, Summer 2017**

- Synthesized and characterized metal oxide supported catalysts with different dispersions of noble metals.
- Performed kinetic measurements for 2-propanol conversion and methane conversion reactions on perovskite and metal oxide supported noble metal catalysts

PUBLICATIONS

1. **Bickel, E. E.**, Hoffman, A., Lee, S., Snider, H. E., Nimlos, C. T., Zamiechowski, N. K., Hibbitts, D., Gounder, R., "Altering the Arrangement of Framework Al Atoms in MEL Zeolites Using

Mixtures of Tetrabutylammonium and Sodium Structure-Directing Agents." *Chemistry of Materials*, 2022, *in press*

2. **Bickel, E. E.**, Nimlos, C. T., Gounder, R., "Developing Quantitative Synthesis-Structure-Function Relations for Framework Aluminum Arrangement Effects in Zeolite Acid Catalysis." *Journal of Catalysis*, 2021, 399, 75-85
3. Vernuccio, S. **Bickel E. E**., Gounder, R. Broadbelt L.J. "Propene Oligomerization on Beta Zeolites: Development of a Microkinetic Model and Experimental Validation." *Journal of Catalysis*, 2021, 395, 302-314.
4. Polo Garzon, F., Blum, T., Bao, Z., Wang, K., Fung, V., Huang, Z., **Bickel, E. E.**, Jiang, D., Chi, M., Wu, Z., "In Situ Strong Metal–Support Interaction (SMSI) Affects Catalytic Alcohol Conversion." *ACS Catalysis*, 2021, 11, 14, 1938-1945.
5. Vernuccio, S. **Bickel E. E**., Gounder, R. Broadbelt L.J. "Microkinetic Model of Propylene Oligomerization on Bronsted Acidic Zeolites at Low Conversion." *ACS Catalysis*, 2019, 9, 10, 8996-9008.
6. Polo Garzon, F., Fung, V., Liu, X., Hood, Z., **Bickel, E. E.**, Bai, L., Tian, H. Foo, G., Chi, M., Jiang, D., Wu, Z. "Understanding the Impact of Surface Reconstruction of Perovskite Catalysts on CH_4 Activation and Combustion.", *ACS Catalysis*, 2018, 8, 11, 10306-10315
7. Polo Garzon, F., Yang, S., Fung, V., Foo, G. **Bickel, E. E.**, Chisholm, M., Jiang, D. Wu, Z., "Controlling Reaction Selectivity through the Surface Termination of Perovskite Catalysts." *Angewandte Chemie*, 2017, 56, 9820-9824.

AWARDS AND HONORS

CATL Division-ChemCatBio Graduate Student Travel Award, ACS Spring Meeting	2022
Ryland Travel Grant, Purdue University	2022
Top Poster Presentation Prize, Catalysis Club of Chicago Young Scientist Symposium	2022
Marcy and Bob Ziek Student Travel Award, Purdue University	2021
Outstanding Graduate Mentor Award, Purdue SURF, Purdue University	2021
Third Place, Perfect Pitch Competition, CISTAR Biannual Meeting, Virtual Conference	2020
Phillips 66 Fellowship, CISTAR, Purdue University	2019
Ross Fellowship, Purdue University	2017
Derryberry Award, Tennessee Technological University	2017
Rising Renaissance Engineering Spectrum Award, Tennessee Technological University	2017
Outstanding Senior Award, Tennessee Technological University	2017
Third Place Oral Presentation, AIChE Southern Regional Conference	2017
Outstanding Senior Award, Tennessee Technological University	2016
Captain William Lafayette Anderson Scholarship Endowment for Chemical Engineering	2016
3rd Place, Materials Science and Engineering I, AIChE National Poster Competition	2015
Dr. John C. McGee and Family Endowment Scholarship, TTU	2015
Don Nichols/I. C. Thomasson Scholarship Endowment, TTU	2014
Wallace S. and Margaret H. Prescott Scholarship Endowment, TTU	2014
Academic Merit Scholarship, Middle Tennessee State University	2013

LEADERSHIP AND OUTREACH

Research mentor for six undergraduate students and one high school student	2018–2022
CISTAR Student Leadership Council, Education and Outreach Coordinator	2019–2020
Tau Beta Pi Engineering Joint Council Representative	2016–2017
American Institute of Chemical Engineers TTU Chapter President	2015-2016
Engineering a Future Summer Camp, Activity Director	2015

Christian Breckner

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EDUCATION

Purdue University, West Lafayette, IN **Expected Jul. 2023**
PhD in Chemical Engineering | GPA: 3.5/4.0
Advisor: Jeffrey T. Miller
Research Topic: Catalysis
Activities and Societies: AIChE, CCC, CISTAR

University Of Wisconsin, Madison, WI **May 2019**
B.S. Chemical Engineering| GPA: 3.6/4.0
Activities and Societies: AIChE, SCIENCountErs, FASTrack

CAREER OBJECTIVE

I am motivated by the need for our world to transition from traditional energy resources to a diverse energy profile including alternative sources. This, combined with improved process efficiencies and new process developments, is key for transitioning to lower emission loads for chemical processing and production. I want to focus on catalyst development and optimization as catalysts are key tools used in all chemical processes and production.

SKILLS

XAS Characterization

- I have learned to analyze materials using XANES and EXAFS on bulk materials, single sites, single metal and alloyed nanoparticles, and complexing agents

MATLAB	Chemisorption
Aspen	DRIFTS
Catalyst Synthesis	STEM
Collaborative	Time management

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2019 – Present**

- Advanced fundamental understanding of SMSI phenomena in catalysts
- Characterized and tested single site catalysts for liquid fuel production from ethylene
- Collaborated with research groups collecting and analyzing XAS for catalyst characterization

Undergraduate Researcher, University of Wisconsin **Sept. 2017 – May 2019**

- Modified and tested E. coli for production of methyl ketones
- Helped develop techniques for CRISPR-Cas9 utilization
- Tested catalysts for production of liquid fuels additives sourced from ethanol

Christian Breckner

PUBLICATIONS AND PRESENTATIONS

1. **Breckner, C. J.**; Zhu, K.; Wang, M.; Zhang, G.; Li, C. W.; Miller, J. T.; "Controlled partial site coverage of Pd nanoparticles by titanium oxide strong metal-support interactions (SMSI)," Pre-print.
2. Yan, Q.; Simmons, T. R.; Cordell, W. T.; Lozada, N. J. H.; **Breckner, C. J.**; Chen, X.; Jindra, M. A.; Pfleger, B. F.; "Metabolic engineering of β-oxidation to leverage thioesterases for production of 2-heptanone, 2-nonanone and 2-undecanone," *Metabolic Engineering*, 61, 335-343 (2020).
3. Ma, R.; Gao, J.; Dean, D.; **Breckner, C.**; Liang, K.; Zhou, B.; Miller, J.; Zou, G.; "Insights into the Nature of Selective Nickel Sites on Ni/Al_2O_3 Catalysts for Propane Dehydrogenation," *ACS Catalysis*, Submitted 2022.
4. Zelinsky, R.; Dean, D. P.; **Breckner, C. J.**; Miller, J. T.; Epling, W. S.; "Pd/BEA Hydrocarbon Traps: Effect of Hydrothermal Aging on Trapping Properties and Pd Speciation," *Applied Catalysis B: Environmental*, Submitted 2022.
5. Khivanstev, K.; Pham, H.; Engelhard, M. H.; Aleksandrov, H. A.; Li, X. H.; Tian, J.; Koleva, I. Z.; Wei, X.; Sun, Y.; Tran, P.; Graham, T. R.; Jiang, D.; Dean, D. P.; **Breckner, C. J.**; Miller, J. T.; Vayssilov, G. N.; Szanyi, J.; Datye, A.; Wang, Y.; "Transforming CeO_2 nanoparticles into Ce^{+3} ions on alumina significantly enhances catalytic activity," *Science*, Submitted 2022.

AWARDS AND HONORS

Valedictorian, La Crosse Logan High School	2015
William F. Vilas Merit Scholarship	2015-2019
Bill Hoyt Great People Scholarship	2016
CISTAR Dow Course Ind. Rxn. Eng. Certificate	2022

Pelin Su Bulutoglu

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(979)-587-4585
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EDUCATION

Purdue University, West Lafayette, IN **Expected Dec. 2022**
PhD in Chemical Engineering | GPA: 3.8/4.0
Advisor: Prof. Doraiswami Ramkrishna
Research Topic: Computational investigation of the kinetics and thermodynamics of crystal nucleation

Bogazici University **Jul. 2017**
MSc in Chemical Engineering | GPA: 4.0/4.0
Advisor: Prof. Ahmet Kerim Avci
Research Topic: Catalytic dry reforming of glycerol to produce synthesis gas

Bogazici University **Jan. 2015**
BSc in Chemical Engineering | GPA: 3.1/4.0

CAREER OBJECTIVE

I am a chemical engineer experienced in molecular modeling with a focus on nucleation kinetics and mechanisms, looking for a full-time opportunity in the pharmaceutical industry, particularly for computer-aided discovery and/or formulation development roles

SKILLS

Molecular simulations

- Proficiency in MD softwares LAMMPS and GROMACS, visualization tools (VMD), analysis tools (PLUMED), Monte Carlo simulations, Hybrid MC/MD, free energy calculation methods

Experience in HPC
Python
MATLAB
Numerical methods
Stochastic methods
Reaction engineering
Shell scripting

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Jan. 2018 – Present**

- Molecular simulations of nucleation and polymorph selection in crystallization processes
- Simulations of externally applied electric fields for solid-state transformations in crystals
- Population balance modeling of (i) an agitated filter dryer – dynamic property extraction from experimental data, (ii) crystallization – growth and polymorphic transition rate extraction from simulated data

Process R&D Intern, AbbVie **Jun. 2021 – Aug. 2021**

Developed a high performance, parallelized, multi-functional in silico tool that

- predicts solubility and other thermophysical properties of drug candidates in organic solvents,
- employs elements from both first principles and data-based methods, and
- is deployed through a user-friendly, interactive web interface, allowing ease of access for teams across the organization

Pelin Su Bulutoglu

Research Assistant, Bogazici University **Jan. 2015 – Jul. 2017**

- Member of Catalyst Technology and Reaction Engineering Laboratory
- Simulation and experiments of catalytic synthesis gas production via reforming reactions in microchannels
- Transient modelling of the isomerization reactor operating in the Izmir Refinery of Turkish Petroleum Refineries, Co.

PUBLICATIONS AND PRESENTATIONS

Publications:

1. **Bulutoglu, P.S.**, Wang, S., Boukerche, M., Nere, N.K., Corti, D.S. and Ramkrishna, D., 2022. An investigation of the kinetics and thermodynamics of NaCl nucleation through composite clusters. PNAS Nexus.
2. **Bulutoglu, P.S.**, Parks, C., Nere, N.K., Bordawekar, S. and Ramkrishna, D., 2019. Exploring New Crystal Structures of Glycine via Electric Field-Induced Structural Transformations with Molecular Dynamics Simulations. Processes, 7(5), p.268.
3. **Bulutoglu, P.S.**, Say, Z., Bac, S., Ozensoy, E. and Avci, A.K., 2018. Dry reforming of glycerol over Rh-based ceria and zirconia catalysts: New insights on catalyst activity and stability. Applied Catalysis A: General, 564, pp.157-171.
4. **Bulutoglu, P.S.**, Koc, S. and Avci, A.K., 2016. Simulation of exhaust gas reforming of natural gas in a microchannel reactor. International Journal of Hydrogen Energy, 41(19), pp.8184-8192.

Conference Presentations:

1. **Bulutoglu, P.S.** "An investigation of the composite cluster mechanism of aqueous NaCl nucleation at elevated concentrations", STMS Series, June 17th, 2022
2. **Bulutoglu, P.S.**, Wang, S., Boukerche,M., Nere, N.K., Ramkrishna, D. "An investigation of the kinetics and thermodynamics of nucleation through composite cluster formation", AIChE 2021, November 7-11, Boston, MA.
3. **Bulutoglu, P.S.**, Nere, N.K., Bordawekar, S., Ramkrishna, D. "A Multidimensional free energy approach for polymorph selection in crystallization of glycine from solution", AIChE Annual Meeting, November 10-15, 2019, Orlando, FL.
4. **Bulutoglu, P.S.**, Avci, A.K., "Catalytic CO2 reforming of glycerol for hydrogen production", HYPOTHESIS XII, June 28-30, 2017, Syracuse, Italy
5. **Bulutoglu, P.S.**, Koc, S., Avci, A.K., "Simulation of exhaust gas reforming of natural gas in a microchannel reactor", 7th International Exergy, Energy and Environment Symposium, 27-30 April 2015, Valenciennes, France.

AWARDS AND HONORS

Bilsland Fellowship, Purdue University Graduate School	2021
Estus H. and Vashti L. Magoon Award for Excellence in Teaching	2021
Best poster award, 29th Annual Purdue Chemical Engineering GSO Symposium	2020
1st place in the "National Student Design Contest" organized under the 11th National Chemical Engineering Conference, Eskisehir, Turkey. Subject: Methanol production from synthesis gas obtained via coal gasification	2015

David Dean

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(331)-330-5773
dean49@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **August 2019 – Expected May 2023**
Ph.D. in Chemical Engineering | GPA: 3.61/4.0
Advisor: Jeffrey T. Miller
Research Focus: Development of New Synchrotron X-ray Techniques for Catalyst Materials

University of Texas at Austin, TX **August 2015 – May 2019**
B.S. in Chemical Engineering | GPA: 3.65/4.0
Research Focus: Estimating Octane Number for High Molecular Weight Hydrocarbons

OBJECTIVE

Highly analytical and results-oriented role, achieving industry leading advancements, which builds on previous successes in a Research Scientist position. Available beginning May 2023.

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **January 2020 – Present**

- Davidson School of Chemical Engineering, Miller Group
- Synthesize and characterize nano-catalyst materials for hydrocarbon conversion as part of the NSF Center of Innovative and Strategic Transformation of Alkane Resources (CISTAR).
- Discovery of novel catalyst materials for dehydrogenation and oligomerization.
- Develop new synchrotron X-ray spectroscopy characterization for catalyst materials at Brookhaven National Laboratory and Argonne National Laboratory.
- Provide synchrotron X-ray spectroscopy expertise for groups from several other universities.
- Devise strategies to mitigate catalyst deactivation for dehydrogenation catalysts.

Undergraduate Research Assistant, University of Texas at Austin **April 2019 – August 2019**

- McKetta Department of Chemical Engineering, Allen Group
- Computational work to estimate octane number for high molecular weight hydrocarbons.

Solvay Chemical: Research Intern, The Woodlands, TX **May 2018 – August 2018**

- Oil and Gas Chemical Additives Research Laboratory, Armstrong Group and Sun Group
- Armstrong Group: Analyzed the prevention of biocides binding to shale using chelating agents.
- Sun Group: Built and commissioned a new testing system for the development of new corrosion inhibitor chemical formulations.

LyondellBasell: Process Engineer Co-op, Clinton, IA **August 2017 – December 2017**

- Olefins unit (1.3 billion lb/year ethylene)
- Engineer solutions for priority process hazard analysis (PHA) action items and oversee the management of change (MOC) for each.

Solvay Chemical: Process Engineer Intern, Pasadena, TX **May 2017 – August 2017**

- Ethoxylation batch plant (140 million lb/year surfactants)
- Executed 6 new product introductions successfully in consultation with company R&D.
- Wrote EPA Spill Prevention Control and Countermeasures (SPCC) plan for the facility.

Solvay Chemical: Process Engineer Intern, Pasadena, TX **May 2016 – August 2016**

- Ethoxylation batch plant (140 million lb/year surfactants)
- Assisted with construction of new Delta V DCS control system and OSI PI historian.
- Strategize solutions for loop reactor performance issues.

David Dean

PUBLICATIONS

First Author Publications

Ganesh, H. S.; **Dean, D. P.**; Vernuccio, S.; Edgar, T. F.; Baldea, M.; Broadbelt, L. J.; Stadtherr, M. A.; Allen, D. T. Product Value Modeling for a Natural Gas Liquid to Liquid Transportation Fuel Process. *Ind. Eng. Chem. Res.* 59, 3109-3119 (**2020**).

Seemakurthi, R. R.; Deshpande, S.; **Dean, D. P.**; Muhlenkamp, J. A.; Alcala, R. N.; Jeffries, A. L.; Clarke, R. J.; Chavan, I. S.; Senyk, J.; Xu, Y.; Serban, A.; O'Brien, C. P.; Datye, A. K.; Hicks, J. C.; Miller, J. T.; Greeley, J. An Algorithmic High Throughput Framework Driven by Mechanistic Insights and Graph-Theory Based Methods for Identification of Selective Propane Dehydrogenation Catalysts. *Submitted to Nature Catalysis, 2022.*

Additional Publications

Zelinsky, R.; **Dean, D. P.**; Breckner, C. J.; Marino, S.; Miller, J. T.; Epling, W. S. Pd/BEA Hydrocarbon Traps: Effect of Hydrothermal Aging on Trapping Properties and Pd Speciation. *Submitted to Applied Catalysis B: Environmental, 2022.*

Krishna, S. H.; Jones, C. B.; Wang, Y.; **Dean, D. P.**; Miller, J. T.; Schneider, W. F.; Gounder, R. Influence of Framework Al Density in Chabazite Zeolites on Copper Ion Mobility and Reactivity During NOx Selective Catalytic Reduction with NH3. *Submitted to Nature Catalysis, 2022.*

Ma, R.; Gao, J.; Kou, J.; **Dean, D. P.**; Breckner, C. J.; Liang, K.; Zhou, B.; Miller, J. T.; Zou, G. Insights into the Nature of Selective Nickel Sites on Ni/Al2O3 Catalysts for Propane Dehydrogenation. *Submitted to ACS Catalysis, 2022.*

Khivantsev, K.; Pham, H.; Engelhard, M. H.; Aleksandrov, H. A.; Li, X. S.; Tian, J.; Koleva, I. Z.; Wei, X.; Sun, Y.; Tran, P.; Graham, T. R.; Jiang, D.; **Dean, D. P.**; Breckner, C. J.; Miller, J. T.; Vayssilov, G. N.; Szanyi, J.; Datye, A. K.; Wang, Y. Transforming CeO2 Nanoparticles into Ce+3 Ions on Alumina Significantly Enhances Catalytic Activity. *Submitted to Science, 2022.*

ACTIVITIES

CISTAR/Purdue Undergraduate Mentorship Programs	2020-Present
Davidson School of Chemical Engineering Safety Committee	2020-2022
Graduate Student Organization: Safety Officer	2020-2022
Growing Intercultural Global Energy Leaders (GIGEL) Program	2022-Present
Food Finders Food Bank Volunteer (Lafayette, IN)	2020-Present
American Institute of Chemical Engineers	2015-Present
UT Austin Omega Chi Epsilon (OXE) Honors Society	2016-2019
UT Austin Student Engineering Council	2016-2018
Purdue Intramural Basketball Champions	2022

AWARDS AND HONORS

Davidson School of Chemical Engineering Safety Award	2021
Purdue University Ross Fellowship	2019-2020
Graduated Cockrell School of Engineering with Honors	2019
1st place Cockrell School of Engineering Design for the Future Competition	2016

SKILLS

Synchrotron X-ray Absorption Spectroscopy	OSIsoft PI
Synchrotron X-ray Diffraction	MS Office
Emerson Delta V DCS	MatLab, BASIC
AspenTech IP21	AutoCAD

SOPURUCHUKWU A. EZENWA

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EDUCATION

Purdue University, West Lafayette, IN **Expected May 2023**
PhD in Chemical Engineering | GPA: 3.95/4.00
Advisor: Rajamani Gounder
Research Topic: Influence of Active Site Distribution in Acid Zeolite on Arene Conversion Catalysis

Tufts University, Medford, MA **May 2018**
BSc in Chemical Engineering | GPA: 3.83/4.0
Academic Honors: *summa cum laude, with highest thesis honors*

CAREER OBJECTIVE

Apply my diverse background knowledge and expertise to understand, conceptualize, and design complex systems that tackle some key challenges in sustainable chemical and energy production.

SKILLS

Catalyst synthesis, characterization and kinetics studies in flow and batch reactor

GC-MS	MATLAB
FTIR N_2	JMP
UV-Vis	CasaXPS
Temperature Programmed Techniques (TPX)	Design-Expert
Argon Physisorption	Aspen Plus
SEM-EDX	Microsoft Project

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Oct. 2018 – Present**

- Synthesize and characterize zeolites and molecular sieve-based catalysts that have potential to advance the current landscape of fuel and chemical production from hydrocarbons resources
- Conduct kinetic and mechanistic studies to elucidate influence of active site and structural properties of Brønsted acid zeolites on arene transformation rates, selectivity and deactivation
- Investigate safety practices and develop tools to promote safer cultures in chemical labs

Undergraduate Research Assistant, Tufts University **Mar. 2016 – July 2018**

- Combined experimental and computational methods to probe selective alkane oxidation on bulk and supported metal oxides to guidance for the design of highly efficient catalysts
- Designed automated lab-scale packed bed reactor system for kinetic and mechanistic studies

PUBLICATIONS (Corresponding author*; Co-first author and equal contribution†)

1. **Ezenwa, S.**, Jan, D.-Y., Gounder, R.* Tailoring Active Site Distributions in Zeolite Catalysts for Regioselective Toluene Methylation to *para*-Xylene. *Manuscript in preparation*
2. **Ezenwa, S.**,† Talpade, A. D.,† Ghanekar, P., Joshi, R., Devaraj, J., Ribeiro, F. H., Mentzer, R.* Toward Improved Safety Culture in Academic and Industrial Chemical Laboratories: An Assessment and Recommendation of Best Practices, *ACS Chem. Health Saf.* **2022**, *29*, 202-213.
3. Annamalai, L.,† **Ezenwa**, **S.**,† Dang, Y., Tan, H., Suib, S. L.,* Deshlahra, P.* Comparison of Structural and Catalytic Properties of Monometallic Mo and V Oxides and M1 Phase Mixed Oxides for Oxidative Dehydrogenation, *Catalysis Today*, **2021,** *368*, 28-45

4. Talpade, A. D.,† Ghanekar, P.,† **Ezenwa, S.**, Joshi, R., Kravitz, S., Tunga, A., Devaraj, J., Ribeiro, F. H., Mentzer, R.* Promoting a Safe Laboratory Environment Using the Reactive Hazard Evaluation and Analysis Compilation Tool, *ACS Chem. Health Saf.* **2021**, *28*, 134–143.
5. Annamalai, L.,† Liu, Y.,† **Ezenwa**, **S.**, Dang, Y., Suib, S. L., Deshlahra, P.* Influence of Tight Confinement on Selective Oxidative Dehydrogenation of Ethane on MoVTeNb Mixed Oxide, *ACS Catalysis*, **2018**, 8, 7051-7067.

PRESENTATIONS (*Most Recent***)**

1. ACS Green Chemistry Summer School, Golden, CO, *Designing Catalysts for Regioselective Methylation of Toluene to para-Xylene and Promoting Safer Practices in Research Labs*, July 15-22, 2022, Poster
2. North American Catalysis Society Meeting, New York, NY, *Kinetic and mechanistic assessments of the influence of active site distribution in MFI zeolites on toluene methylation catalysis*, May 22-27, 2022, Oral
3. P2SAC Spring Conference, Virtual, *Demonstration of Reactive Hazards Evaluation & Analysis Compilation Tool (RHEACT)*, May 9-12, 2022, Oral
4. AIChE Midwest Regional Conference, Virtual, *Towards Safer Practices in Academic and Industrial Chemical Laboratories*, March 1-2, 2022, Oral

AWARDS AND HONORS

Advancing Science Conference Grant (*NOBCChE*)	*2022*
Bill Murray CISTAR Fellowship (*Purdue*)	*2022*
ACS Summer School on Green Chemistry & Sustainable Energy, Class of 2022 (*ACS*)	*2022*
Richard J. Kokes Award (*NACS*)	*2022*
BCA/Affiliate/Fellows Scholarship Award (*NSBE)*	*2022*
Best Poster Award in Catalysis and Reaction Engineering at ChE GSO Symposium (*Purdue*)	*2021*
Highest Thesis Honors in Undergraduate Research (*Tufts*)	*2018*
Donald A. Cowdery Memorial Scholarship Award (*Tufts*)	*2018*
Oliver Chapman Leadership Award (*Tufts*)	*2018*
Tau Beta Pi Engineering Honors	*2017*
Collegiate Initiative Scholarship (*NSBE Boston*)	*2017*
Gemma Cifarelli Memorial Scholarship Award (*Tufts*)	*2017*
ChBE Undergraduate Summer Research Scholarship Award (*Tufts*)	*2016*
Microsoft Diversity Scholarship	*2016*
Board of Corporate Affiliates Scholarship Award (*NSBE*)	*2015*
Henry J. Leir Scholarship (*Tufts*)	*2015, 2017*

OUTREACH, LEADERSHIP AND SERVICE

STEM Outreach Volunteer, **various K-12 schools, IN, MA**	*08/16 – present*
Technical Sessions Committee and Poster Reviewer, **2022 NOBCChE Conference**	*05/22 – present*
Engineering Design Package Safety Reviewer, **2022 AIChE ChemE-Car Competition**	*04/22 – present*
Institutional Representative & Symposium Committee, **Catalysis Club of Chicago**	*10/21 – present*
Vice-President Education, **Boiler Talks Toastmasters Club**	*12/20 – present*
Grad Chair; Past Membership Chair, **NSBE – Purdue Chapter**	*08/21 – present*
Social Director, Mentorship Program Chair, **Nigerian Student Association at Purdue**	*04/20 – 05/21*
Vice-President, Programs Chair, **NSBE – Tufts Chapter**	*04/15 – 04/17*
President, **Tufts African Student Organization (ASO)**	*05/15 – 05/16*

TEACHING EXPERIENCE *Teaching Assistant*: Advanced Chemical Reaction Engineering (*Purdue*), Process Dynamics and Control (*Purdue*), Design and Analysis of Experiments (*Tufts*); *Head Tutor*: General, Physical and Organic Chemistry, Calculus 1–3 (*Tufts)*

EXTRACURRICULARS: Soccer, Ultimate Frisbee, Flag Football, Squash, Disc golf

Daniel Fesenmeier

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EDUCATION

Purdue University, West Lafayette, IN **Expected May 2023**

PhD in Chemical Engineering | GPA: 3.55/4.0
Advisor: You-Yeon Won
Research Topic: Development of synthetic polymer lung surfactant for treatment of respiratory distress syndrome
Activities and Societies: American Physical Society, Graduate Student Organization- Purdue Graduate Student Government Representative

Undergraduate Institution **May. 2018**

Bachelor of Science: Chemical Engineering | GPA: 3.98/4.0
Academic Honors: Honors Program, Trustees' Merit Scholarship, Deans List
Activities and Societies: Omega Chi Epsilon Chemical Engineering Honors Society, College Mentor for Kids, Phi Sigma Kappa Fraternity

CAREER OBJECTIVE

Result-oriented individual with superb collaborative and technical communication skills seeking for a research position aimed at developing next generation of materials.

SKILLS

Interfacial phenomena of colloidal polymer systems

- Extensive experience with surface pressure-area isotherms, Brewster angle microscopy, liquid X-ray scattering, NMR relaxometry to understand interfacial behavior of surface-active polymers

Polymer synthesis	Origin Lab
Polymer characterization (GPC/SEC/NMR)	Python
Nanoparticle Formulation	Colloidal Characterizations (TEM,DLS)
Microfluidics	Technical Writing/Communication

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Jan. 2019 – Present**

- Investigated factors influencing surface-mechanical behavior of colloidal polymer nanoparticles for use as synthetic lung surfactant
- Designed and evaluated studies of efficacy of polymer lung surfactant in mouse models of direct lung injury
- Investigated delivery of polymer lung surfactant to mouse lungs via pharyngeal administration
- Developed method for polymer nanoparticle formulation which allows for superior control over size characteristics
- Mentored multiple undergraduate researchers
- Teaching assistant for Heat & Mass Transfer and Chemical Engineering Unit Operations Laboratory

Air Force Research Laboratory, Wright Patterson Air Force Base **May. 2017 – May. 2018**

Daniel Fesenmeier

PUBLICATIONS, PATENTS, AND PRESENTATIONS

1. **Daniel J. Fesenmeier**, Madathilparambil V. Suresh, Seyoung Kim, Krishnan Raghavendran, You-Yeon Won, ″Polymer Lung Surfactant Therapy Reduces Lung Injury and Inflammation in Mouse Models of Direct Lung Injury″, submitted, 2022.
2. **Daniel J. Fesenmeier**, Sungwan Park, Seyoung Kim, You-Yeon Won. "The Effect of Size Properties and End/Linking Group Chemistry on the Surface Mechanical Properties of Water Spread PS-PEG Micelles on the Water Surface." Bulletin of the American Physical Society March Meeting (2022).
3. **Daniel J. Fesenmeier**, Sungwan Park, Seyoung Kim, You-Yeon Won, ″Surface Mechanical Behavior of Water-Spread Poly(styrene)-Poly(ethylene glycol) (PS-PEG) Micelles at the Air-Water Interface: Effect of Micelle Size and Polymer End/Linking Group Chemistry″, Journal of Colloid and Interface Science 617, 764-777, 2022 (DOI: 10.1016/j.jcis.2022.03.008).
4. Seyoung Kim, **Daniel J. Fesenmeier**, Sungwan Park, Sandra E. Torregrosa-Allen, Bennett D. Elzey, You-Yeon Won, ″Pulmonary Pharmacokinetics of Polymer Lung Surfactants Following Pharyngeal Administration in Mice″, Biomacromolecules 23(6), 2471-2484, 2022 (DOI: 10.1021/acs.biomac.2c00221).
5. Won, Y.-Y. and **D.J. Fesenmeier**, Formulation of Monodisperse Kinetically Frozen Polymer Micelles via Equilibration-Nanoprecipitation, p.P.U.S. Patent, Editor. 2021

AWARDS AND HONORS

Ross Assistantship 2018

Clayton C. Gentilcore

101 Andrew Place, Apt. 211, West Lafayette, IN, 47906
(412) 443-1945
cgentilc@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **Expected May 2023**
PhD in Chemical Engineering | GPA: 3.52/4.00
Advisor: Dr. Nien-Hwa Linda Wang
Research Topic: Conversion of Plastic Waste into Useful Products
Activities and Societies:

Chemical Engineering Graduate Student Organization (ChE GSO) **May 2019 – May 2020**
Student Advocacy Officer

- Communicated with graduate students throughout the year to acquire input on improvements to ChE GSO and how ChE GSO may more effectively represent graduate student interests
- Served as a ChE GSO representative for the Engineering Graduate Student Advisory Committee (GSAC)

University of Illinois at Urbana-Champaign, IL **May 2018**
B.S. in Chemical Engineering with Honors | GPA: 3.59/4.00
Activities and Societies:

Omega Chi Epsilon Chemical Engineering National Honor Society **Dec. 2016 – May 2018**
Student Space Systems **Sept. 2016 – Dec. 2017**
Project Manager – Liquid V1 – Cooling

- Researched and aided design of cooling system for liquid rocket engine in Propulsion Department
- Supported designs and research through simulation programs and rocket propulsion analysis software

The What You Will Shakespeare Company **Sept. 2014 – May 2016**

- Acted in 6 productions while playing a key role in stage management and assisting in directing

SKILLS

Design and assembly of lab-scale reaction and separation systems including automation

- Automation of systems through LabVIEW

Chemical analysis by GC-TCD/FID, GC×GC-FID, GC-MS, HPLC, LC-MS, SEM-EDS, XRD

- Utilized to identify chemical products following experiments

Equipment design using Python programming
Kinetic modeling using MATLAB programming
Process simulation using Aspen Plus
Proficient in Microsoft Word, PowerPoint, Excel

Clayton C. Gentilcore

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2018 – Present**

- Conducting research within the Davidson School of Chemical Engineering while supervised by Dr. Nien-Hwa Linda Wang, Maxine Spencer Nichols Professor of Chemical Engineering
- Researching recovery of valuable products from plastic waste
- Acting laboratory safety officer (April 2019 – Present)

Undergraduate Researcher, University of Texas at Austin **Jun. 2017 – Aug. 2017**

- Conducted research within the Department of Petroleum and Geosystems Engineering while supervised by Prof. Kishore Mohanty and Dr. Himanshu Sharma as part of Summer Undergraduate Research Internship
- Performed phase behavior experiments and bulk foam tests to identify surfactants and stabilization agents that enhance oil recovery at various salinities

Undergraduate Researcher, University of Pittsburgh School of Medicine May 2016 – Jul. 2016

- Conducted research at within the Renal-Electrolyte Division of the Department of Medicine while supervised by Dr. Ossama Kashlan as part of Summer Undergraduate Research Program
- Studied the phylogenetic history of ENaC (epithelial sodium channel) and effects of SIN-1 and other nitrosylating agents on ENaC

TEACHING EXPERIENCE

Graduate Teaching Assistant, Purdue University Aug. 2019 – Dec. 2019; Jan. 2021 – May 2021

- Assisted teaching in courses surrounding Chemical Reaction Engineering (CHE 348) and Design of Staged Separation Processes (CHE 306) in Fall 2019 and Spring 2021, respectively

PUBLICATIONS AND PRESENTATIONS

1. Jin, K., Vozka, P., **Gentilcore, C.**, Kilaz, G., & Wang, N. H. L. (2021). Low-pressure hydrothermal processing of mixed polyolefin wastes into clean fuels. *Fuel, 294*, 120505. (Published)
2. Wang, X. P., Balchak, D. M., **Gentilcore, C.**, Clark, N. L., & Kashlan, O. B. (2022). Activation by cleavage of the epithelial Na+ channel α and γ subunits independently coevolved with the vertebrate terrestrial migration. *Elife*, *11*. (Preprint 2020; Published 2022)
3. Kashlan, O. B., Wang, X. P., Balchak, D. M., **Gentilcore, C.**, & Clark, N. L. (2020). The Terrestrial Migration of Vertebrates Drove the Evolution of ENaC Activation by Cleavage α. *The FASEB Journal*, *34*(S1), 1-1. (Published Abstract)
4. Kashlan, O. B., Balchak, D. M., **Gentilcore, C.**, & Clark, N. L. (2018). Cleavage of ENaC α and γ subunits evolved with the terrestrial migration. *The FASEB Journal*, *32*, 624-16. (Published Abstract)

SHENG-NING HSU

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EDUCATION

Purdue University, West Lafayette, IN **Expected Mar. 2023**
PhD in Chemical Engineering | GPA: 3.90/4.0
Advisor: Bryan W. Boudouris and Letian Dou

National Taiwan University **Jun. 2016**
B.S. in Chemical Engineering | GPA: 3.93/4.3 | Rank 21/108
Academic Honors: Presidential Award in Fall 2015
Activities and Societies: Aiki-Taich Club Founder and President

CAREER OBJECTIVE

I anticipate myself to gain experience and required skills in the semiconductor industry as an engineer or a R&D scientist. I'd also like to further develop my communication skills, a broader view on the industry, and other management skills to become a leader of the team.

SKILLS

Electrical Properties Characterization

- Characterize electrical properties of newly developed materials in the form the resistors or FETs at varying temperatures and magnetic fields
- Design and fabricate circuits to assist my measurements
- High-throughput experiments achieved by integrating instruments using LabView and instrumentation
- Lake Shore Cryotronics cryogenic magnetic probe station CRX-VF, Keithley 2450 SMU and 4200-SCS, Stanford Research System SR850 lock-in amplifier

Device Fabrication and Optimization

- Fabricating van der Pauw devices and 3ω devices for thermoelectric properties evaluation
- Spin coater, thermal evaporator, spray-coater, ultrasonic spray-coater, glove box

Electron-beam lithography
Nuclear Magnetic Resonance (NMR)
Thermogravimetric analyzer (TGA)
Atomic force microscopy (AFM)
Mass spectrometer (Mass Spec)
Function generator
MATLAB
ChemDraw
Autodesk EAGLE (PCB layout)
Ortep-3
LTSpice
Phenyl galvinoxyl radical synthesis
Carbodiimide coupling
Condensation polymerization
Column chromatography
Soxhlet extraction
Soldering
Fourier transform infrared spectroscopy (FTIR)
Size exclusion chromatography (SEC)
Profilometer
Optical and photoluminescent microscope
X-ray crystallography (XRD)
Hall effect Measurements
OriginLab
MestReNova
ShelXle
Mercury
Photoshop/Illustrator
Boc protection/deprotection
Stille coupling
Oxidative polymerization
Liquid-liquid extraction
Schelnk line

SHENG-NING HSU

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Dec. 2018 – Present**

- Synthesis of Bulky Ligands for 2D Halide Perovskites Featuring Stable Open-shell Ligands
- High-Performance Lead-Free 2D Halide Perovskites for Thermoelectric Applications
- 2D Halide Perovskite Field-Effect Transistors and Transistor Memories
- Magnetoresistance and Charge Transport Mechanism of Open-Shell Single Crystals

Research Assistant, National Taiwan University **Nov. 2017 – Aug. 2018**

- Low-k Adhesive Composites for High-Frequency Flexible Printed Circuit Boards

Undergraduate Researcher, National Taiwan University **Feb. 2015 – Aug. 2016**

- Low Voltage OFET with Ultrasonic Spray-Coated PVA-PMAA films as Gate Dielectric

PUBLICATIONS AND PRESENTATIONS

1. **Sheng-Ning Hsu**, Bryan W. Boudouris, and Letian Dou, "Thermoelectric Performance of Two-Dimensional Halide Perovskites Featuring Conjugated Ligands", *MRS Spring Meeting & Exhibit* **2022** *Session EQ05.11.06: Devices, Stability Sustainability I*
2. Shuyang Zhang, Maren Pink, Tobias Junghoefer, Wenchao Zhao, **Sheng-Ning Hsu**, Suchada Rajca, Arrigo Calzolari, Bryan W. Boudouris*****, Maria Benedetta Casu*****, and Andrzej Rajca,***** "High-Spin (S = 1) Blatter-Based Diradical with Robust Stability and Electrical Conductivity", *J. Am. Chem. Soc.* **2022**, 144, 13, 6059-6070
3. **Sheng-Ning Hsu**, Bryan W. Boudouris, and Letian Dou, "Thermoelectric Performance of Two-Dimensional Halide Perovskites Featuring Conjugated Ligands", *APS March Meeting* **2022** *Session F69: 2D Metal Halide Perovskites*
4. Ying Tan, **Sheng-Ning Hsu**, Hamas Tahir, Letian Dou, Brett M. Savoie, and Bryan W. Boudouris,* "Electronic and Spintronic Open-Shell Macromolecules, Quo Vadis?", *J. Am. Chem. Soc.* **2022**, 144, 2, 626-647
5. Wenchao Zhao, **Sheng-Ning Hsu**, Bryan W. Boudouris, and Letian Dou,***** "Two-Dimensional Organic Semiconductor-Incorporated Perovskite (OSiP) Electronics", *ACS Appl. Electron. Mater.* **2021**, 3, 12, 5155-5164
6. **Sheng-Ning Hsu**, Wenchao Zhao, Yao Gao, Akriti, Mauricio Segovia, Xianfan Xu, Bryan W. Boudouris,[*] and Letian Dou,[*] "Thermoelectric Performance of Lead-Free Two-Dimensional Halide Perovskites Featuring Conjugated Ligands", *Nano Lett.* **2021**, 21, 18, 7839-7844
7. **Sheng-Ning Hsu**, Wenchao Zhao, Yao Gao, Bryan W. Boudouris,[*] and Letian Dou,[*] "Thermoelectric Performance of 2D Halide Perovskites Featuring Conjugated Ligands", *APS March Meeting Poster* **2021**
8. Wenchao Zhao, Yao Gao, **Sheng-Ning Hsu**, Letian Dou,[*] and Bryan W. Boudouris,[*] "Highly efficient and stable flexible perovskite field-effect transistors", *APS March Meeting Poster* **2021**
9. Ke Ma, **Sheng-Ning Hsu**, Yao Gao, Zitang Wei, Linrui Jin, Blake P Finkenauer, Libai Huang, Bryan Boudouris,[*] Jianguo Mei,[*] and Letian Dou,[*] "Organic Cation Engineering for Vertical Charge Transport in Lead-Free Perovskite Quantum Wells", *Small Sci.* **2021**, 2000024
10. Yao Gao, Zitang Wei, **Sheng-Ning Hsu**, Bryan W. Boudouris,[*] and Letian Dou,[*] "Two-dimensional halide perovskites featuring semiconducting organic building blocks", *Mater. Chem. Front.*, **2020**, 4, 3400-3418
11. Yan-Cheng Lin, Chi-Haw Chiang, Chih-Cheng Kuo, **Sheng-Ning Hsu**, Tomoya Higashihara, Mitsuru Ueda, Wen-Chang Chen,[*] "A compatible and crosslinked poly(2-allyl-6-methylphenol-co-2,6-dimethylphenol)/polystyrene blend for insulating adhesive film at high frequency", *J. Appl. Polym. Sci.* **2019**, 136, 47828
12. Chien-Chung Shih, Mercedes Wu, **Sheng-Ning Hsu**, Li-Che Hsu, Chao-Wei Huang, Jeun-Yan Lam and Wen-Chang Chen,[*] "A robust, air-stable and recyclable hydrogel toward stretchable electronic device applications", *Macromol. Mater. Eng.* **2018**,1800282

AWARDS AND HONORS

Purdue College of Engineering Travel Grant **Feb. 2022**

Ryland Travel Grant **Feb. 2022**

Yan-Shu Huang

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(765)-701-7985
huan1289@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **Expected Aug. 2023**
Ph. D. in Chemical Engineering | GPA: 3.7/4.0
Advisor: Gintaras V. Reklaitis, Zoltan K. Nagy
Research Topic: Advanced process control in continuous pharmaceutical tablet manufacturing

National Taiwan University **Jun. 2017**
B.S. in Chemical Engineering | GPA: 4.14/4.30 | Rank: 3/118
Academic Honors: Summa Cum Laude

CAREER OBJECTIVE

Motivated chemical engineering graduate with strong background of process system engineering. Seeking to join the pharmaceutical industry as a senior engineer keen to apply my knowledge of process control, automation, machine learning and data integration into practice.

SKILLS

Python (Nmupy, Pandas, Scikit-learn, PyTorch)	Model predictive control
Matlab	Mechanistic model
DeltaV	Machine learning
OSISoft PI	PAT tools (NIR, Raman, Eyecon, ECVT)
Data communication (OPC, Ethernet/IP)	LIW feeders, roller compactor, tablet press

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2018 – Present**

- Implemented advanced process control in an integrated continuous tablet manufacturing process to improve the CQAs better than traditional recipe-based control strategy
- Investigated PAT tools to enable real-time monitoring of particle mass flow rate, particle size distribution, and API concentration.
- Applied machine learning-based hybrid model to predict ribbon properties and granule size distribution in the continuous dry granulation process
- Integrated all the process and product data to the distributed control system, and applied real-time optimization to make plant-wide decision
- Initiated research topics and designed experiment process; consolidated collaboration projects involving the FDA, NSF, five universities in the US and the UK

Graduate Teaching Assistant, Purdue University

- ChE 450 Design and Analysis of Process Systems
- ChE 697 Statistical Methods in Chemical Engineering

LEADERSHIP ACTIVITIES

- Graduate Mentor of Summer Undergraduate Research Fellowship (SURF) Program
- Treasurer of Taiwanese Graduate Student Organization at Purdue (ILTC)
- President of ILTC Badminton Club

Yan-Shu Huang

AWARDS AND HONORS

Eastman travel grant	**2021**
Emery travel grant	**2020**
MOST Undergraduate Fellowship, Ministry of Science and Technology, Taiwan	**2016 – 2017**

PUBLICATIONS AND PRESENTATIONS

1. **Huang, Y.-S**, Medina-Gonzalez, S., Straiton, B., Keller, J., Marashdeh, Q., Gonzalez, M., Nagy, Z. K., Reklaitis, G. V., "Real-time Monitoring of Powder Mass Flowrates for Plant-wide Control of a Continuous Direct Compaction Tablet Manufacturing Process", Journal of Pharmaceutical Sciences **2022**, 111(1), 69-81.
2. **Huang, Y.-S**, Sheriff, M. Z., Bachawala, S., Gonzalez, M., Nagy, Z. K., Reklaitis, G. V., "Evaluation of a combined MHE-NMPC Approach to Handle Plant-Model Mismatch in a Rotary Tablet Press", Processes **2021**, 9, 1612.
3. **Huang, Y.-S.**, Sheriff, M. Z., Bachawala S., Gonzalez, M., Nagy, Z. K., Reklaitis, G. V., "MHE-based NMPC of a continuous direct compaction tablet manufacturing process under plant-model mismatch", PSE **2021+**, Kyoto, Japan, June 2022.
4. **Huang, Y.-S.**, Sheriff, M. Z., Bachawala, S., Gonzalez, M., Nagy, Z. K., Reklaitis, G. V., "Adaptive Nonlinear Model Predictive Control of a Continuous Direct Compaction Tablet Manufacturing Process", Paper 185g, AIChE Annual Meeting **2021**, Boston, MA, November 2021.
5. **Huang, Y.-S.**, Medina-González, S., Bachawala, S., Bommireddy, Y., Gonzalez, M., Nagy, Z. K., Reklaitis, G. V., "Real-Time Monitoring of Powder Mass Flowrates for MPC/PID Control of a Continuous Direct Compaction Tablet Manufacturing Process", Paper 407c, AIChE Annual Meeting **2020**, San Francisco, CA, November 2020 (virtual).
6. **Huang, Y.-S.**, Ganesh, S., Marashdeh, Q., Zuccarelli, C., Nagy, Z. K., & Reklaitis, G. V., "Investigation of Electric Capacitance-Based and X-Ray-Based Sensors for Real-Time Mass Flow Rate Monitoring in Continuous Tablet Manufacturing", Paper 509g, AIChE Annual Meeting **2019**, Orlando, FL, November 2019.
7. Su, C. Y., Yang, A. C., Jiang, J. S., Yang, Z. H., **Huang, Y.-S.**, Kang, D. Y., Hua, C. C., "Properties of single-walled aluminosilicate nanotube/poly (vinyl alcohol) aqueous dispersions", The Journal of Physical Chemistry B **2018**, 122(1), 380-391.
8. Sheriff, M. Z., **Huang, Y.-S.**, Bachawala, S., Gonzalez, M., Nagy, Z. K., Reklaitis, G. V., "A Hierarchical Approach to Monitoring Control Performance and Plant-Model Mismatch", ESCAPE **2022**, Toulouse, France, June 2022.
9. Lagare, R., Acevedo, A. C., Araujo, M., Young, K., **Huang, Y.-S.**, Sheriff, M. Z., Nagy, Z. K., Reklaitis, G.V., "Development of virtual sensor for real-time prediction of granule flow properties", ESCAPE **2022**, Toulouse, France, June 2022
10. Rossi, F., **Huang, Y.-S.**, Kumar, S., Lagare, R., Mockus, L., Reklaitis, G. V.,"A General Strategy for Quantification of the Uncertainty on a Hybrid Model's Uncertainty Estimates", Paper 415f, AIChE Annual Meeting **2021**, Boston, MA, November 2021.
11. Medina-González, **Huang, Y.-S.**, Bachawala, S., Bommireddy, Y., Gonzalez, M., Reklaitis, G. V., Nagy, Z. K., "A NMPC Strategy Applied to a Continuous Direct Compaction Tablet Manufacturing", Paper 716b, AIChE Annual Meeting **2020**, San Francisco, CA, November 2020 (virtual).
12. Medina-González, **Huang, Y.-S.**, Bachawala, S., Bommireddy, Y., Gonzalez, M., Reklaitis, G. V., Nagy, Z. K., "Tablet Manufacturing Characterization: Lubricant blend Integration", Paper 744g, AIChE Annual Meeting **2020**, San Francisco, CA, November 2020 (virtual).

Sumit Kumar

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EDUCATION

Purdue University, West Lafayette, IN **Expected May. 2023**

PhD in Chemical Engineering | GPA: 3.4/4.0

Advisors: Professor Gintaras Reklaitis and Professor Zoltan Nagy

Research Topic: Applying PAT in the manufacturing of oral solid dosages and achieving blend uniformity of API in pharmaceutical blends

Purdue University, West Lafayette, IN **May. 2020**

MS in Chemical Engineering | GPA: 3.4/4.0

HBTI Kanpur, India **May. 2012**

B.Tech in Chemical Engineering | GPA: 75.5/100

Academic Honors: Passed with Distinction

Activities and Societies: Coordinator for cultural events and part of the soccer team

CAREER OBJECTIVE

I have 10 years of working experience in pharmaceutical product development of APIs and Oral solids. I have worked on API product development from feasibility, optimization and trial & validation stages and have led the team (as Process Engineering Expert) in the development & scale up of APIs and OSDs from Lab scale to plant scale. I am final-year PhD candidate at Purdue University under Prof. Gintaras Reklaitis and Prof. Zoltan Nagy. I aspire to be a leader in the pharmaceutical industry and impart all my learnings to make healthcare affordable to all.

CERTIFICATIONS

Applied Management Principles | Krannert School of Management **Fall. 2020**

Six Sigma Black Belt | American Society for Quality (ASQ) **Spring 2016**

Digital transformation, Digital Strategy, Data Analytics for Business Professionals, **Fall 2021**
Foundations of Industry 4.0, Introductions to Digital Twins, IoT Foundations | **LinkedIn Learning**

SKILLS

- Good understanding and exposure to product development, process engineering, PAT & QbD related activities at R&D and execution at manufacturing plant in the pharmaceutical industry
- Hands-on experience in Statistical software such as Design Expert and Minitab for DOE
- Statistical modelling of processes using PCA and PLS
- Proper understanding of six sigma tools and concepts, and ability to draw proper inferences
- Ability to lead a team, handle multiple projects and collaborate with cross-functional teams
- Strong analytical skills, communication & presentation skills and decision-making skills
- Leadership qualities, ability to motivate team members and get the work done

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Mon. Year – Present**

- Implementing NIR and Raman spectroscopy for real-time API concentration measurement using PLS models at feed frame of tablet press
- Achieving Blend uniformity of API in the feeding blending system in semi-continuous and continuous manner

- Setting up and working in the continuous manufacturing pilot plant at Purdue University utilizing direct compaction, dry granulation and wet granulation lines.

Dr Reddy's Laboratories Ltd, IPDO R&D, INDIA **July 2012 - Present**

PROCESS DEVELOPMENT SPECIALIST – OSD | Key responsibilities include:

- Assessing the unit operations in oral solid dosages manufacturing
- Optimizing the processes at lab scale and scaling up processes to plant scale
- Implementing PAT during process development and developing statistical models
- Mentoring and guiding Process Engineers and evaluating their performances
- Investigating failures, performing root cause analysis and identifying corrective actions

PROCESS ENGINEERING EXPERT – API

- Working on Process optimization, scale-up, equipment mapping and technology transfer
- Identifying and implementing new technology in the early development phase
- Working with cross-functional teams such as R&D, analytical, Quality Control, Quality Assurance, Project management and manufacturing
- Implementing Quality by Design, preparing Design of Experiments, utilizing statistical packages such as Minitab, Excel, Design Expert and ensuring proper implementation of cGMP practices

PROCESS ENGINEERING SCIENTIST

- Working on crystallization, reactions, mixing, filtration and drying
- Estimating hazard potential and ensuring safe and robust scale-up of processes
- Planning and performing experiments
- Performing powder screening to evaluate the Minimum Ignition Energy, Minimum Ignition Temperature, Bulk Powder Resistivity, DSC and Reaction Calorimetry

PUBLICATIONS AND PRESENTATIONS

1. Considerations in Raman spectroscopy for real-time API concentration measurement at tablet press
2. AICHE 2020: Real-Time Process Monitoring in Continuous Manufacturing of Oral Solid Dosages using Raman Process Analytical Technology
3. IFPAC 2019: Continuous Pharmaceutical Manufacturing equipment and sensor integration

AWARDS AND HONORS

- Was graded stellar amongst the top performers in the team in Dr Reddy's Labs
- Got National top 1 percent in National Standard Examination in Physics, NSEP 2006-07
- Got 99 percent marks in physics in AISSCE, 2007
- Got All India Rank 23 in 7th Junior Mathematics Olympiad in high school

Zihao Liang

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EDUCATION

Purdue University, West Lafayette, IN **Expected Aug. 2023**
PhD in Chemical Engineering | GPA: 3.41/4.0
Advisor: Prof. Bryan W. Boudouris
Research Topic: Charge-conducting polymers and organic small molecules

The University of Akron, Akron, OH **May. 2018**
M.S. in Polymer Science | GPA: 3.95/4.0
Advisor: Prof. Tianbo Liu
Research Topic: Self-assembly behaviors of macroions in solutions

East China University of Science and Technology (ECUST), Shanghai, China **July. 2017**
B.S. in Polymer Materials and Engineering | GPA: 3.60/4.0
Academic Honors: Scholarship for Comprehensive Curriculum Behavior
Activities and Societies: Associate President of Psychology Club

CAREER OBJECTIVE

Motivated team player seeking a Process Engineer position with an innovative employer in the semiconductor industry. Skillful at polymer and organic molecule synthesis and surface analysis.

RESEARCH EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2018 – Present**

- Developed radical polymers and small molecules to improve charge conducting capabilities. As a result, these conducting materials provided state-of-art performance in electric conductivity and thermo-mechanical processibility, which had major implications in electrochemical sensing, organic transistors, and flexible batteries.
- Created novel photoresist systems for 3D printing processes that provided micro/nanoscale features. More specifically, this resulted in rapid, continuous fabrication techniques to create complex 3D structures with sub-micron resolutions. This interdisciplinary work required a collaboration between chemical and mechanical engineers at Purdue University.
- Incorporated blended semiconducting polymers into organic electrochemical transistors which achieved state-of-art performance and response kinetics. These enhanced properties increased the preciseness and robustness of the mixed conducting systems (i.e., transporting electrons and ions).

Graduate Research Assistant, The University of Akron **Aug. 2016 – May. 2018**

- Manipulated self-assembled supramolecular structures through controlling net charge on host-guest complexes. This resulted in reliable approaches to accurately tune the intermolecular distances on the assemblies in nanoscale.
- Controlled fluorescence emissions in metal-organic cages through intra/intermolecular interactions, which lead to novel strategies to precisely adjust emission wavelengths and intensity of fluorophores.

Zihao Liang

SKILLS

Highlighted Skills

- 7+ years of experience of synthesis and purification of organic polymers and small molecules
- 2+ years of experience of polymer thin film and organic small molecule electronic device research

Other Laboratory Skills

NMR, MS, GPC	UV/vis, fluorescence spectroscopy
XRD, XPS	DSC, TGA
SEM, TEM, AFM, profilometry	e-beam lithography, thermal evaporation
Spin coater, vacuum probe station	electrochemical impedance spectroscopy

PUBLICATIONS AND PRESENTATIONS

1. Kim, H. J.; Perera, K.; **Liang, Z.**; Bowen, B.; Mei, J.; Boudouris, B. W. Radical Polymer-Based Organic Electrochemical Transistors. ***ACS Macro Letters 2022, 11(2), 243-250.***
2. Somers, P.; **Liang, Z.**; Johnson, J. E.; Boudouris, B. W.; Pan, L.; Xu X. Rapid, Continuous Projection Multi-Photon 3D Printing Enabled by Spatiotemporal Focusing of Femtosecond Pulses. ***Light: Science & Applications 2021, 10(1), 1-11.***
3. Chi, T.; Akkiraju S.; **Liang Z.**; Tan, Y.; Kim, H. J.; Zhao, X.; Savoie, B. M.; Boudouris, B. W. Design of an n-type Low Glass Transition Temperature Radical Polymer. ***Polymer Chemistry 2021, 12(10), 1448-1457.***
4. Chi, T.; Somers, P.; Wilcox, D. A.; Schuman, A. J.; Johnson, J. E.; **Liang, Z.**; Pan, L.; Xu, X.; Boudouris, B. W. Substituted Thioxanthone-Based Photoinitiators for Efficient Two-Photon Direct Laser Writing Polymerization with Two-Color Resolution. ***ACS Applied Polymer Materials 2021, 3(3), 1426-1435.***
5. Li, H.; Xie, T. -Z.; **Liang, Z.**; Shen, Y.; Sun, X.; Yang, Y.; Liu, T. Adjusting Emission Wavelength by Tuning the Intermolecular Distance in Charge-Regulated Supramolecular Assemblies. ***J. Phys. Chem. C 2019, 123, 37, 23280-23286.***
6. Li, H.; Xie, T. -Z.; **Liang, Z.**; Dahal, D.; Shen, Y.; Sun, X.; Yang, Y.; Pang, Y.; Liu, T. Conformational Change Due to Intramolecular Hydrophobic Interaction Leads to Large Blue-Shifted Emission from Single Molecular Cage Solutions. ***Chem. Commun. 2019, 55, 330-333.***
7. Li, H.; Wang, R.; Hong, Y.; **Liang, Z.**; Shen, Y.; Miyoshi, T.; Liu, T. Tuning the Inter-Cage Distance in Charge-Regulated Blackberry-Type Assemblies via Host-Guest Chemistry. ***Chem. Eur. J. 2019, 25, 16288–16293.***
8. **Liang, Z.**; Akkiraju, S.; Kim, H. J.; Liu, K.; Chi, T.; Boudouris, B. W. Design of n-type Radical Polymers and Their Utilization as Solid-State Conductors. Presented at ***APS March Meeting 2022***, Chicago, IL, March 16, 2022
9. **Liang, Z.**; Chi, T.; Akkiraju, S.; Tan, Y.; Savoie, B. M.; Boudouris, B. W. A Non-Conjugated Polymer with Flexible Backbones Bearing Spin-Delocalized Pendant Radical Groups. Presented at ***APS March Meeting 2021***, Online, March 17, 2021

AWARDS AND HONORS

Scholarship for Comprehensive Curriculum Behavior, Third Prize, ECUST, Shanghai 2016
Scholarship for Comprehensive Curriculum Behavior, Second Prize, ECUST, Shanghai 2014, 2015

LEADERSHIP ROLES AND TEACHING EXPERIENCE

Safety Officer, Boudouris Research Group 2021 - Present
Undergraduate Mentor, Boudouris Research Group 2022 - Present
Teaching Assistant, ChE, Purdue University (Design of Staged Separation Processes) 2019, 2021

Zih-Yu Lin

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www.linkedin.com/in/zih-yu-lin

EDUCATION

Purdue University, West Lafayette, IN **Expected May 2023**
PhD in Chemical Engineering
Advisor: Brett M. Savoie
Research Topic: Molecular dynamics and machine learning on Perovskite applications

MITx, Remote **Expected Oct. 2022**
Micro Master in Statistics and Data Science

National Taiwan University, Taipei, Taiwan **June 2019**
Bachelor of Science in Chemical Engineering

CAREER OBJECTIVE

Ph.D. candidate, and published researcher with four years' experience seeks new and challenging projects to apply diverse skillset and culminated expertise in chemical engineering, statistics, data science, machine learning, and molecular dynamics.

SKILLS

Python
SQL
C++
Bash
Matlab

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2019 – Present**
Research Assistant to Prof. Brett M. Savoie and Prof. Letian Dou

- Utilizing machine learning to design organic materials for 2D perovskite LEDs
- Utilizing molecular dynamics, kinetic Monte Carlo, and quantum calculations to investigate various properties of 2D/semi-2D perovskite LEDs
- Developing topology automated framework and its polarizable extension for atomic potentials in molecular dynamics simulations

The Data Mine, Purdue University **Aug. 2021 – May 2022**
Graduate Data Science Researcher with Viasat Inc.

- Working with Viasat Inc. on a super-resolution project to understand and implement the latest deep-learning model for image super-resolution and video frame interpolation

Molecular Engineering Laboratory, National Taiwan University **July 2017 – June 2019**
Undergraduate Researcher to Prof. Shiang-Tai Lin and Prof. David T. Wu

- Utilized molecular-dynamics simulations to provide molecular insights into methane hydrate (flammable ice) and hydrate-related properties

Zih-Yu Lin

PUBLICATIONS AND PRESENTATIONS

Journal Articles:

1. **Zih-Yu Lin**, Jiaonan Sun, Stephen B. Shiring, Yao Gao, Letian Dou, Brett M. Savoie, "Synthetic Design Rules for Two-Dimensional Halide Perovskites Gleaned from Thousands of Simulated Structures," Nature, 2022, submitted
2. Kang Wang, **Zih-Yu Lin**, Zihan Zhang, et al., "Suppressing Phase Disproportionation in Quasi-2D Perovskite Light-Emitting Diodes," Nature Photonics, 2022, under review
3. Akriti, **Zih-Yu Lin**, Jee Yung Park, Hanjun Yang, Brett M. Savoie, Letian Dou, "Anion Diffusion in Two-Dimensional Halide Perovskites", APL Materials, 2022, 10, 040903
4. Akriti†, Shuchen Zhang†, **Zih-Yu Lin**†, Enzheng Shi, Blake P. Finkenauer, Yao Gao, Alan J. Pistone, Ke Ma, Brett M. Savoie, Letian Dou, "Quantifying Anionic Diffusion in Two-Dimensional Halide Perovskites Lateral Heterostructures," Adv. Mater. 2021, 2105183 († contributed equally)
5. Bunjoon Seo, **Zih-Yu Lin**, Qiyuan Zhao, Michael A. Webb, Brett M. Savoie, "Topology Automated Force-Field Interactions (TAFFI): A Framework for Developing Transferable Force-Fields," J. Chem. Inf. Model. 2021, 61, 10, 5013–5027
6. **Zih-Yu Lin**, David T. Wu, Shiang-Tai Lin, "Equilibrium and Transport Properties of Methane at the Methane-Water Interface with the Presence of SDS," Phys. Chem. C 2018, 122, 51, 29259–29267

Conference Presentations:

1. **Zih-Yu Lin**, Stephen Shiring, Jiaonan Sun, Letian Dou, Brett M. Savoie, "Novel Ligand Design of 2D Halide Perovskites Through Molecular Dynamics and Machine Learning Model", Oral Presentation at ACS Spring Meeting, San Diego, US, Mar. 2022
2. **Zih-Yu Lin**, Akriti, Shuchen Zhang, Letian Dou, Brett M. Savoie, "Molecular Modeling of Halide Diffusion in 2D Organic-Inorganic Hybrid Perovskites", Oral Presentation at AIChE Annual Meeting, Boston, US, Nov. 2021

Xiao Liu

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(612)-803-4182
xiao207@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **Expected August 2023**
Ph.D. in Chemical Engineering | GPA: 3.88/4.00
Advisor: Prof. Osman Basaran
Thesis: Filament generated droplets during drop breakup, sheet rupture, and drop impact
Activities and Societies: Chemical Engineering Graduate Student Organization, American Physical Society (APS)

University of Minnesota – Twin Cities **May 2018**
B.Ch.E. in Chemical Engineering | GPA: 3.60/4.00

CAREER OBJECTIVE

Ph.D. candidate in Chemical Engineering with 5 years of research experience in computational and experimental fluid mechanics. Seeking a position as a research engineer in chemical industry, to leverage research skills to solve business relevant problems in R&D.

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant **August 2018 – Present**
Davidson School of Chemical Engineering, Purdue University
Research Objectives: Study the dynamics of free surface flows subject to non-quiescent initial flow field and/or with complex rheology and the stability of contracting filaments and films using Finite Element Method (FEM) based computational techniques and experimental techniques
Major Contributions:

- Introduced a new dimensionless parameter to characterize the dynamics of contracting filaments
- Analyzed the effect of initial conditions on filament contraction
- Developed an FEM algorithm for simulating viscoelastic free surface flows
- Conducted detailed experimental study for Corteva Agriscience to characterize various fluids for targeted drop delivery
- Developed an object detection code for droplets generated during drop impact within images from a high-speed camera

Ph.D. Intern **May 2022 – August 2022**
The Dow Chemical Company, Lake Jackson, TX

- Established a robust spray characterization and scale-up capability
- Obtained droplet size distributions for various nozzles
- Developed a new tool to improve data processing efficiency

Undergraduate Research Assistant **May 2017 – June 2018**
Department of Chemical Engineering and Materials Science, University of Minnesota - Twin Cities

- Developed criteria for distinguishing different regimes of morphologies of explosion-induced granular cratering
- Studied the dynamics of explosion-induced granular cratering via particle image velocimetry
- Designed a three-dimensional setup to mimic impact-induced cratering in granular media

Xiao Liu

PUBLICATIONS

1. **X. Liu**, B. Wagoner, H. Wee, and O. Basaran, "Effect of initial conditions on promotion and inhibition of breakup during filament contraction," AIChE Journal, 68 (2), e17491 (2022)
2. T. Liu, B. Cao, **X. Liu**, T.-P. Sun, and X. Cheng, "Explosion cratering in 3D granular media," Soft Matter, 16 (5), 1323-1332 (2020)
3. M. Gao, **X. Liu**, L. Vanin, T.-P. Sun, L. Gordillo, and X. Cheng, "Dynamics and scaling of explosion cratering in granular media," AIChE Journal, 64 (8), 2972-2981 (2018)
4. **X. Liu**, B. Wagoner, and O. Basaran, "Contraction velocity of viscoelastic filaments," *to be submitted to Physical Review Fluids*

PRESENTATIONS

1. **X. Liu**, B. Wagoner, O. Basaran. "Contraction dynamics of viscoelastic filaments." 74th Annual APS-DFD, Phoenix, AZ (2021)
2. **X. Liu**, H. Wee, C. Anthony, B. Wagoner, P. Kamat, O. Basaran. "Effect of ICs on dynamics of contracting filaments." 72nd Annual APS-DFD, Seattle, WA (2019)
3. B. Wagoner, C. Anthony, P. Kamat, V. Garg, S. Thete, H. Wee, **X. Liu**, O. Basaran. "Simulation, visualization, and analysis of drop breakup and coalescence in ink jet printing and drop based fabrication." Printing for Fabrication, San Francisco, CA (2019)

AWARDS AND HONORS

Eastman Travel Grant - Purdue University 2021
School of Chemical Engineering Travel Grant - Purdue University 2019

SKILLS

Programming:
Python
Fortran
MATLAB

Algorithms:
ALE Finite Element Method
Elliptic Mesh Generation
Finite Difference
Linear Solvers (Banded, Frontal, Multifrontal)

Languages:
English
Mandarin

Operating Systems:
Linux
MacOS
Windows

Laboratory:
Laser diffraction analysis
High-speed imaging
Soldering
Spectroscopy analysis (NMR, IR)
Chromatography
Compound synthesis

Applications and Packages:
Tecplot
ImageJ
Origin
Simulink
Aspen
ChemDraw
LaTeX
MS office suite

EXTRACURRICULAR ACTIVITIES

Graduate Student Organization Co-Curricular Chair **May 2019 – May 2020**
Davidson School of Chemical Engineering, Purdue University

- Organized hybrid social/professional development events, including Future Faculty seminars, Truth and Beauty seminars, and Future Faculty Lunches
- Coordinated poster sessions of multiple symposiums
- Initiated a new yearly seminar - Future Postdoc seminars

Ankita Morankar

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www.linkedin.com/in/ankitamorankar

EDUCATION

Purdue University, West Lafayette, IN **Expected Aug 2023**
PhD in Chemical Engineering | GPA: 3.86/4.0
Advisor: Professor Jeffrey Greeley
Research Topic: Modeling electrochemical reactions at the atomistic scale using first principles density functional theory calculations and molecular dynamics for clean energy applications
Activities: Volunteer, Murdock Science Club

Institute of Chemical Technology, Mumbai, India **May 2018**
Bachelor of Chemical Engineering | GPA: 9.23/10.0 | Rank: 9 (class of 76)
Activities: Outreach Co-ordinator, IIChE Student Chapter's Vortex in collaboration with C.R.Y.

CAREER OBJECTIVE

I'm interested in developing technological solutions to problems pertaining to the generation and storage of energy through the application of computational tools including quantum chemistry calculations, molecular dynamics, and data science. I'm also passionate about communicating science through outreach and mentorship programs.

SKILLS

Density Functional Theory	Molecular Dynamics
Electrochemistry	Graph Theory
Python	Bash
VASP	IQMOL
MATLAB	ASPEN

RESEARCH EXPERIENCE

Graduate Research Assistant, Purdue University **Aug 2018 – Present**

- developed in-situ structural insights and activity-stability descriptors to provide design principles for synthesis of active, durable Fe-N-C catalysts for O_2 electroreduction in fuel cells
- developed theory predicting solvation stabilization of reaction intermediates
- provided in-situ atomistic insight into cyclic voltammetry for O_2 evolution in electrolyzers
- developing theoretical model depicting electrochemical double layer in alkaline conditions for accurate kinetic barrier evaluations in carbon dioxide reduction in electrolyzers

Graduate Research Mentor **Oct 2020 – May 2022**

- trained an undergraduate student in theory on density functional theory, electrochemistry along with coding with bash and python
- guided her on a research project that led her to winning the 2nd Best Poster Prize in the Chemical Reaction Engineering Division at 2021 AIChE Annual Meeting
- mentored her through grad school applications, she currently is a student in UCSB

Research Intern, **Indian Institute of Technology Bombay, India** **May 2016– June 2016**
Advisor: Professor Sanjay Mahajani

- investigated cross-aldol condensation reaction for synthesis of 3-methyl-pent-3-en-2-one, an intermediate in perfumeries in autoclave batch reactors
- studied reproducibility and sensitivity of catalyst loading, precursor ratios, temperature, internal and external mass transfer to conversion and selectivity

Ankita Morankar

WORK EXPERIENCE

Industrial Intern, Hikal, Mumbai, India **May 2017 – July 2017**

- trained on-site in the production, effluent treatment, and plant utilities departments
- performed techno-economic analysis for synthesis of Thiabendazole, an active ingredient in agricultural chemicals from its raw materials

PUBLICATIONS

1. **Morankar A.**, Deshpande S., Zeng Z., Atanassov P., Greeley J., A first principles analysis to understand potential dependent surface configurations for Fe-N-C catalysts (in preparation)
2. **Morankar A.**, Deshpande S., Greeley J., Effects of overoxidation on the ORR activity of NPGM catalysts (in preparation)
3. **Morankar A.*,** Chun H.*, Zeng Z., and Greeley J., A first principles approach of solvation energy calculations for aqueous-phase reaction adsorbates using ab-initio molecular dynamic simulations (in preparation) (*equal contribution)
4. Rao S., **Morankar A.**, Verma H., and Goswami P., Emerging Photovoltaics: Organic, Copper Zinc Tin Sulfide, and Perovskite-Based Solar Cells, Journal of Applied Chemistry, Volume 2016 (2016)

SELECT PRESENTATIONS

Upcoming: 2022 Fuel Cells Gordon Research Conference (Smithfield, RI)
Elucidating Effects of Potential, Hydrogen Peroxide, and Interlayer Interactions on Site Structure, Stability, and Activity of Fe-N-C Catalysts for Oxygen Reduction

Other: 2022 ACS Fall (Chicago, IL)
2022 NAM (New York, NY)
2022 CCC (virtual)
2021 AIChE Annual Meeting (Boston, MA)
2020 AIChE Annual meeting (virtual)
2019 SUNCAT (San Jose, CA)

PATENTS

Morankar A., Harmalkar A., Chheda S., Reddy R., Shah P., "Process for nutrient recovery from human urine and utilization of treated urine" (Provisional Patent) **Mar 2018**

AWARDS AND HONORS

Ryland Travel Grant, Purdue University **Feb 2022**
Ambuja Cement Best Home Paper Award, ICT Mumbai (similar to senior design project) **Apr 2018**
2nd Prize, Biotechnology Entrepreneurship Student Team Competition, (pan-India) **Feb 2018**
2nd Prize, Chemical Engineer of the Year (IIChE Student Chapter's Vortex) **Oct 2017**
2nd Prize, Industry Defined Problem (IIChE Student Chapter's Vortex) **Oct 2017**
National Talent Search Scholar, NCERT, Gov. of India (pan-India) **Jun 2010 - May 2018**

LEADERSHIP EXPERIENCES

Graduate Teaching Assistant

Senior Design & Analysis of Process Systems (CHE 450) (class of 160 students) **Jan 2021**

- taught ASPEN, designed tests, and provided help with senior design projects

Chemical Engineering Thermodynamics (CHE 211) (class of 90 students) **Aug 2019**

- conducted office hours and recitation, prepared homework solutions and graded tests

Lab Data Safety Manager **May 2021 - Present**

- developed backup and data maintenance protocols, and conducted monthly meetings

EXTRACURRICULAR ACTIVITIES

Ping pong, Yoga, Painting, Dancing

Christopher (Kurt) Russell

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EDUCATION

Purdue University, West Lafayette, IN **May 2023**
PhD in Chemical Engineering, Advisor: Jeff Miller
Research Topic: Impact of (De)hydrogenation Catalysts on Olefin Aromatization on H-ZSM-5

Stanford University **Jun. 2018**
M.S. in Environmental Engineering, Atmosphere & Energy

Georgia Institute of Technology **May 2015**
B.S. in Chemical and Biomolecular Engineering

RESEARCH AND WORK EXPERIENCE

Purdue University, West Lafayette, IN **Aug 2018 – present**
Graduate Research Assistant

- Research the effects of combining hydrogenation catalysts (i.e., Ga, PtZn) and hydrogen with zeolites on the reactivity and product distribution of olefin reactions
- Characterize catalysts using *in situ* and *in operando* X-ray Absorption Spectroscopy and X-ray Diffraction at the Advanced Photon Source, Argonne National Labs
- Synthesize and characterize metal nanoparticles and isolated single sites on SiO_2 and Al_2O_3
- Developed SOPs, experimental methods, scheduling, and operational startup/shut down of the laboratory and performed maintenance and reconstruction of lab scale reactors
- Led laboratory experiments, problem solving sessions, and office hours as Teaching Assistant for undergraduate level Mass and Momentum Transfer and Chemical Reaction Engineering (~150 students/class)

University of Wyoming, Laramie, WY **Jul 2017 – Aug 2017, Jul 2018 – Aug 2018**
Graduate Research Assistant (Advisor: Maohong Fan)

- Explored CO2 uptake in inorganic carbonate solutions and developed thermodynamic data for absorption equilibria and carbonate/bicarbonate/CO2 phase equilibria under industrially relevant conditions
- Explored carbon nanotubes' impact on desorption of CO2 from MEA
- Provide technical and grammatical edits on scientific communication (papers, presentations, and theses)

Stanford University, Stanford, CA **Jan 2018 – Jun 2018**
Graduate Teaching Assistant (Instructor: Mark Jacobson)

- Air Pollution/Global Warming (~60 students): Taught students (via office hours and assisting in lecture) the history of global warming and air pollution science
- Air Pollution Modeling (~15 students): Assisted students in building regional or global weather models and understanding concepts to make computational modeling more efficient

Schlumberger, Odessa, TX **Jul 2015 – Aug 2016**
Integrated Fluids and Solids Engineer

- Saved clients >$200,000 by reducing dilution costs for drilling fluid
- Helped reduce maintenance cost by up to 90% and prevented non-productive time by performing preventative maintenance
- Ensured proper documentation by field staff and communicated daily performance of employees to clientele

Christopher (Kurt) Russell

Georgia Institute of Technology (Atlanta, GA)

Research Assistant: Atmospheric Trace Contaminants Lab **Summers 2012 – 2014**

- Conducted ion chromatography and organic/elemental carbon analyses on particulate matter
- Instructed other research assistants in proper collection and maintenance of samples and machines
- Reduced back log of sample analysis by 8 months in a 3-month span
- Programmed hybrid aerosol model optimization in MATLAB

SAMPLE OF PUBLICATIONS (31 total)

1. **Russell, C. K.**, Saxena, A., Miller, J. T. (2022). Impact of PtZn nanoparticles on propylene aromatization on H-ZSM-5. (*Submitted May 2022*)
2. Qi, L., Zhang, Y., Conrad, M. A., **Russell, C. K.**, Miller, J., & Bell, A. T. (2020). Ethanol Conversion to Butadiene over Isolated Zinc and Yttrium Sites Grafted onto Dealuminated Beta Zeolite. *Journal of the American Chemical Society*, *142*(34), 14674–14687. https://doi.org/10.1021/jacs.0c06906
3. Lardinois, T. M., Bates, J. S., Lippie, H. H., **Russell, C. K.**, Miller, J. T., Meyer, H. M., Unocic, K. A., Prikhodko, V., Wei, X., Lambert, C. K., Getsoian, A. B., & Gounder, R. (2021). Structural Interconversion between Agglomerated Palladium Domains and Mononuclear Pd(II) Cations in Chabazite Zeolites. *Chemistry of Materials*, *33*(5), 1698–1713. https://doi.org/10.1021/acs.chemmater.0c04465
4. Toan, S., O'Dell, W., **Russell, C. K.**, Zhao, S., Lai, Q., Song, H., Zhao, Y., & Fan, M. (2019). Thermodynamics of $NaHCO_3$ decomposition during Na_2CO_3-based CO_2 capture. *Journal of Environmental Sciences (China)*, *78*, 74–80. https://doi.org/10.1016/j.jes.2018.07.005
5. Sun, Z., Liu, H., Bai, H., Yu, S., **Russell, C. K.**, Zeng, L., & Sun, Z. (2022). The crucial role of deoxygenation in syngas refinement and carbon dioxide utilization during chemical looping-based biomass gasification. *Chemical Engineering Journal*, *428*. https://doi.org/10.1016/j.cej.2021.132068
6. Gao, Y., He, X., Mao, K., **Russell, C. K.**, Toan, S., Wang, A., Chien, T., Cheng, F., Russell, A. G., Zeng, X. C., Fan, M. (2022). Ultrasonically Activated Dually Functionalized Carbon Nanotubes for Catalyzing Monoethanolamine-based CO_2 Capture. (*Submitted to Advanced Energy Materials*).
7. Yuda, A., Kumar, A., Reesh, I. A., **Russell, C. K.**, Miller, J. T., Saad, M. A. S., Al-Marri, M. J. (2022). Electro-oxidation of methanol on At, AgNi, and AgCo catalysts prepared by combustion synthesis technique. (Submitted to International Journal of Energy Research).

AWARDS AND HONORS

Zell Miller Scholar	2011 – 2015
Delta Chi Officer of the Year (Risk Manager)	2013 – 2014
Georgia Tech record for most intramural sports teams (99)	2015
Georgia Tech ChBE External Advisory Board Student Representative	2012, 2014
Georgia Tech Delta Chi Executive Board Member	2012 – 2015

COMMUNITY OUTREACH AND INVOLVEMENT

Purdue ChE GSO Social Chair and Outreach Chair	2019 – 2021, 2022-2023
Purdue Men's Club Volleyball Team (Tournament Director)	2018 – present, 2022-2023
Murdock Elementary School Afterschool Volunteer, Science Day	2019-present
Blood Donor (5 gallons)	2009-present

Kaustabh Sarkar

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EDUCATION

Purdue University, West Lafayette, IN **July 2022**
Ph.D. in Chemical Engineering
Advisor: You-Yeon Won
Research Topic: Radioluminescent nanoparticles for multimodal cancer treatment
Activities and Societies: Leslie Bottorff Fellow, Graduate Student Organization, Post Graduate Student Government, Chemical Engineering Safety Committee

Institute of Chemical Technology, Mumbai, India **May 2022**
Bachelors in Chemical Engineering
Activities and Societies: TEDxICTMumbai, Literary Club,

CAREER OBJECTIVE

Ph.D. candidate graduating from Purdue University with 5 years of research laboratory experience in preclinical *in vitro* and *in vivo* testing of nanoparticle drug delivery systems with prior/current research in process scale-up and optimization in developing safer alternatives for small molecule chemotherapeutic drug delivery.

SKILLS

Solid-state characterization
- X-ray diffractometry (XRD)
- Thermal analysis (DSC, TGA)
- Spectroscopy (FT-IR, RS, 1D NMR, 2D NMR)
- Particle size (DLS)
- Microscopy (TEM, FDM)
- UV-visible spectrophotometry
- HPLC/SEC
- Circular Dichroism spectroscopy (CD)
- Atomic Absorption Spectroscopy (AAS)
- MestreNova

***In vitro* testing**
- Controlled release
- Cell culture
- Cytotoxicity assays
- Clonogenic assays

***In vivo* testing**
- Efficacy studies
- Biodistribution studies
- Pharmacokinetic studies
- MATLAB PK modelling
- MicroCT imaging and analysis
- Kaplan Meier analysis
- GraphPad Prism
- Histological analysis

Manufacturing
- Hydrothermal synthesis
- Solvent exchange synthesis
- Emulsion evaporation
- Lyophilization
- Process scale-up and optimization

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **August 2017-Present**

- Synthesized a novel radioluminescent nanoparticle formulation for radiation-controlled paclitaxel drug release for intratumoral chemoradiotherapy
- Established *in vitro* efficacy and safety via clonogenic and MTT assays
- Examined therapeutic efficacy in immune-deficient and immune-competent murine models
- Investigated the effects of stereochemistry of paclitaxel on the *in vitro* and *in vivo* efficacy
- Designed strategies to expand the scope of the platform to other anti-cancer drugs

- Participated in professional development courses like Applied Management Principles for Ph.D. students

Undergraduate Research Assistant, Reliance Industries **May- June 2016**

- Established PI relations for an algal species to develop a hydrothermal synthesis procedure
- Optimized growth conditions to increase productivity of raceway pond reactors
- Developed model to obtain process optimization parameters for a continuous raceway pond reactor using obtained PI relations with real time insolation prediction and evaporative losses

Undergraduate Research Assistant, Bhabha Atomic Research Centre **May-June 2014**

- Synthesized $Y_2Sn_2O_7$ nanoparticles and studied their luminescence properties
- Examined the effects of Er and Sm doping on luminescence of $Y_2Sn_2O_7$ nanoparticles
- Increased the luminescence by 20% with Sm doping

LEADERSHIP AND PROFESSIONAL SERVICES

Laboratory Safety Officer, Won Research Group **May 2019- June 2021**

- Ensure safe laboratory practices, conduct laboratory training for new graduate students, organize and participate in laboratory cleanup activities, report near misses and safety incidents, nominated for the departmental "Excellence in Safety" award

Graduate Teaching Assistant, Purdue University **Aug- Dec 2018, Jan-March 2020**

- Teaching assistant for CHE205 (Chemical Engineering Calculations) and CHE435 (Chemical Engineering Laboratory)

Graduate Student Organization (GSO) Officer, Purdue University **May 2018- May 2020**

- Served as the senator representing the department in the Graduate Student Government

PUBLICATIONS, PATENTS AND PRESENTATIONS

1. **Sarkar K.**, Torregrossa-Allen S.E., Elzey B.D., Narayanan S., Langer M.P., Durm G.A., Won Y-Y. Effect of Paclitaxel Stereochemistry on X-Ray-Triggered Release of Paclitaxel from $CaWO_4$ /Paclitaxel-Coloaded PEG-PLA Nanoparticles, *Molecular Pharmaceutics*, 2022
2. Misra R., **Sarkar K.**, Lee J., Pizzuti V., Lee D.S., Currie M., Torregrossa-Allen S., Long D., Durm G.A., Langer M.P., Elzey B.D., Won Y-Y. Radioluminescent nanoparticles for radiation-controlled release of drugs, *Journal of Controlled Release*, 2019
3. Patel A.P., Schorr C.R., Viswanath D., **Sarkar K.,** Streb N.J., Pizzuti V., Misra R., Lee J., Won Y-Y. Pilot-Scale Optimization of the Solvent Exchange Production and Lyophilization Processing of PEG–PLA Block Copolymer-Encapsulated $CaWO_4$ Radioluminescent Nanoparticles for Theranostic Applications, *Industrial and Engineering Chemistry Research*, 2021
4. Won Y-Y., Misra R., Lee J., **Sarkar K.,** Pizzuti V.J. *Radioluminescent Nanoparticles for Radiation-Triggered Controlled Release Drugs*, pending PCT/US Provisional Patent, Application No.18/49823, PRF Reference No. 68028-02, filed on September 7, 2018
5. **Sarkar K.** et al. Effect of drug hydrophobicity on X-ray-triggered drug release from PEG-PLA/CaWO4 nanoparticles. *AIChE Annual Meeting*, Boston, MA, November 2021
6. **Sarkar K.** et al. Radioluminescent nanoparticles for combination chemoradiotherapy of locally advanced head and neck cancers. *Indiana Clinical and Translational Sciences Institute (CTSI) Annual Meeting*, Virtual, September 2020.

AWARDS AND HONORS

- Leslie Bottoroff Fellowship **August 2019- August 2022**
- Chemical Engineering Departmental Travel Grant Award **2020**
- Best Poster, Health and Disease Research Symposium **2020**

Kaustubh Sawant

480 W Stadium Avenue, West Lafayette, IN, 47907
(765)-775-8858
sawantk@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **Expected Spring 2023**
PhD in Chemical Engineering | GPA: 3.82/4.00
Advisor: Jeffrey Greeley
Research Topic: Elucidating Structure-Property Relationships at Metal-Metal Oxide Interfaces for Heterogeneous Catalysis.
Activities and Societies: Purdue Catalysis Center, Graduate Soccer Team

Institute of Chemical Technology, Mumbai, India **2014-2018**
B.E in Chemical Engineering | GPA: 9.36/10.00
GRE: 329/340 | TOEFL: 113/120
Activities and Societies: Vortex Organizing Head (2016), Tennis Club, Soccer Club

CAREER OBJECTIVE

Chemical Engineering PhD candidate with proven experience in software engineering, materials modeling, machine learning, and data analytics. Seeking positions to work in highly collaborative teams and provide solutions for a better future.

SKILLS

Programming Languages: Shell/Bash, Python, HTML/CSS, Excel/VBA, MATLAB
Modeling/Data Science Tools:

- Density Functional Theory Simulations - VASP, GPAW, QBOX
- Molecular Dynamics Simulations - VASP, LAMMPS, ASE
- Process Simulations - Aspen plus, Pyomo
- AI/ML - TensorFlow, PyTorch, Scikit-learn, Pandas, Networkx

Technologies: High Performance Computing (CPU/GPU), Git, Povray
Languages: English (fluent), Marathi (native), Hindi (native)

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **2018-Present**
Thermodynamic Formulism for Surface Science Experiments

- Developed a novel framework to make *ab initio* thermodynamic hull diagrams for ultra-high vacuum (UHV) surface science experiments including atomic layer deposition experiments.
- Proposed a thermodynamic scheme to bridge the gap between UHV experiments and industrially relevant reaction conditions.

Universal Properties of Metal Supported Oxide Films

- Developed models to accurately predict the formation of metal supported metal oxide films.
- Proposed a new bonding model to explain deviations from bond order conservation principles.
- Worked in close collaboration with experimental groups at Purdue University to develop prediction tools for overlayer formation in strong metal support interaction.
- Proposed a theory to explain the change in the chemical properties of key intermediates due to the presence of the thin film oxides using charge transfer.

Kaustubh Sawant

Discovery of New Materials for Oxygen Reduction Reaction

- Predicted the existence of stable single atom and 2d metal oxide dopants that can enhance the activity and stability of Pt group catalysts for oxygen reduction reaction.
- Developed a local strain based model to explain the enhancement in activity.

Method Development [github.itap.purdue.edu/sawantk]

- Developed lattice matching algorithm to enumerate non pseudomorphic film structures.
- Developed an active deep learning method for simulating metal-water interfaces.
- Developed non mean field cluster expansion and microkinetic model calculator.

Summer Design Intern, Jacobs Engineering **Summer 2017**

- Reduced ~2hrs of manual work by developing an automated system (Excel/VBA) to optimize three phase chemical separators and storage tanks.
- Performed systematic check of process and instrumentation diagrams to ensure consistency.

Summer Intern, Vanguard Industrial Hygiene Laboratory **Summer 2016**

- Collaborated with Certified Industrial Hygienist Subhash Nikam to mitigate volatile solvent at Lupin Research Park, Pune. Prepared report identifying causes for solvent leaks and provided strategies for safe handling of volatile solvents.

PUBLICATIONS

- Gao, J*.; **Sawant, K. J*.;** Miller, J. T.; Zeng, Z.; Zemlyanov, D.; Greeley, J. P.; Structural and Chemical Transformations of Zinc Oxide Ultrathin Films on Pd(111) Surfaces. ACS Appl. Mater. Interfaces 2021, *13* (29), 35113–35123. *(* Co first author*)
- **Sawant, K. J**.; Zeng, Z.; Greeley, J. P.; Universal properties of metal-supported oxide films from linear scaling relationships: Elucidation of Strong Metal Support Interactions. (*In peer review*)

In preparation: (*Drafts available on request*)

- **Sawant, K. J*.;** Gao, J*.; Miller, J. T.; Zeng, Z.; Zemlyanov, D.; Greeley, J. P.; Tuning adsorption properties of metals through metal-hydroxide interaction. *(* Co first author*)
- Smith, J.; **Sawant, K. J**.; Zeng, Z.; Greeley, J. P.; Gao, W.; Chemistry under atomic resolution microscopy – visualizing chemical reactions by tracking the behaviors of atoms.
- **Sawant, K. J**.; Zeng, Z.; Greeley, J. P.; Stability of metal oxides on metal nanoparticles and its impact on oxygen reduction reaction.

EXTRACURRICULAR EXPERIENCE

Organizing Coordinator and Webmaster, Purdue Catalysis Center **2021-Present**

- Organized weekly scientific talks and presentations to nurture collaborative work.
- Improved and maintained the Purdue Catalysis Center website to promote graduate research.

Overall Head and Secretary, Vortex ICT, Mumbai **2016-2017**

- Led a team of 100+, planned and organized Vortex, ICT's technical festival.
- Member of the ICT students' council and ensuring collaboration between industry and students.

TEACHING

DFT Coding Assistant, Advanced Modeling for Catalysis (ChE 697) **Spring 2022**
Teaching Assistant, Design and Analysis of Processing Systems (ChE 450) **Spring 2021**
Teaching Assistant, Chemical Engineering Thermodynamics (ChE 211) **Fall 2020**

AWARDS

K.C. Chao and Jiun Chao Graduate Education Endowment **2020**

Natasha Singh

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EDUCATION

Purdue University, West Lafayette, IN **Expected: March. 2022**
PhD in Chemical Engineering | GPA: 3.7/4.0
Advisor: Vivek Narsimhan
Research Topic: Impact of surface viscosity on droplet dynamics (Fluid Mechanics)

Indian Institute of Technology Kanpur **May. 2018**
B.Tech in Chemical Engineering | GPA: 8.6/10.0

CAREER OBJECTIVE

I am a senior PhD student working on understanding the impact of interfacial rheology on single droplet dynamics (i.e., droplet deformation, breakup, sedimentation, and coalescence) using perturbation theories and boundary-integral simulations. Because of my exposure to computational fluids research, parallel programming and computational geometry courses, and recent internship at the AMD HPC team, I have developed an interest in high-performance computing in scientific applications. After graduation, I would like to work in the industry research and software development division, where I can apply my domain knowledge and technical skillset.

TECHNICAL SKILLS

- `C, C++, Python, Bash, MATLAB, OpenMP, MPI, HIP, CUDA, Git, LAPACK, PETSc, Docker, LATEX`

RESEARCH AND WORK EXPERIENCE

PhD Thesis: Impact of Interfacial Rheology on Droplet Dynamics **Fall 2018 – Present**
Graduate Research Assistant, Purdue University

- Theoretically investigated the impact of interfacial viscosity on the stability of a single droplet subjected to weak shear and extensional flows under stokes flow regime using turning point bifurcation analysis
- Developed an axisymmetric boundary element simulation model from scratch in `C++` to numerically examine the role of surface viscosity on the stability of droplet shapes during sedimentation under gravity
- Extended the codebase to analyze the influence of surface viscosity on single droplet deformation and breakup under external flow by combining boundary-integral and finite element analysis. Achieved good qualitative agreement between theories and simulations
- Using `MPI` and `PETSc`, designed a highly parallel axisymmetric boundary element simulation model in `C++` to capture the effect of surface rheology on the coalescence of two droplets approaching each other under external flow

Performance Analysis of HPCG Benchmark **Summer 2022**
Summer Intern in Data Center GPU Customer Engineering Team, AMD

- Familiarized with fundamentals of `AMD GPU` architecture, `ROCm` software platform, and `HIP` programming language
- Built, profiled and did root cause analysis of the performance of application benchmark on `GPU` accelerated platforms

- Explored the benefits of different code optimization techniques and runtime environments in terms of performance

Computational Fluid Dynamics of 2D Phenomena **Fall 2020**
Course Project in Computing for Science and Engineering, Purdue University

- Developed an interactive CFD tool for inviscid flow simulations that took predefined shapes or hand-drawn prototypes as input and provided aerodynamic parameters back to the user as output

Droplet Depinning on Inclined Surfaces at High Reynolds Numbers **Summer 2017**
Visiting Research Scholar under Prof. Edward White and Prof. Sungyon Lee, Texas A&M

- Performed experiments for a single droplet adhering to a solid surface exposed to wind and gravity modalities and examined critical conditions for droplet depinning

PUBLICATIONS

1. **Natasha Singh** and Vivek Narsimhan, "Impact of surface viscosity on droplet breakup and relaxation", *Journal of Fluid Mechanics*, Accepted, (2022).
   ***Conference talks*:** 74th Annual Meeting of the APS Division of Fluid Dynamics 2021
2. **Natasha Singh** and Vivek Narsimhan, "Impact of surface viscosity on the stability of a droplet translating through a stagnant fluid", *Journal of Fluid Mechanics*, 927, pp A44, (2021).
   ***Conference talks**:* APS March Meeting 2021 and 95th Colloid and Surface Science Symposium 2021
3. **Natasha Singh** and Vivek Narsimhan, "Deformation and burst of a liquid droplet with viscous surface moduli in a linear flow field", *Physical Review Fluids*, 5(6), 063601, (2020).
   ***Conference talks**:* 73rd Annual Meeting of the APS Division of Fluid Dynamics 2020 and 2020 Virtual AIChE Annual Meeting

AWARDS AND HONORS

1. TAMU-IITK summer undergraduate research scholarship
   (Awarded to two junior undergraduates per department) 2017
2. Academic Excellence Award, IIT Kanpur
   (Awarded to top 7% students in the institute) 2016, 2017

RELEVANT COURSEWORK

Departmental Core Courses:
Finite Element Analysis, Stability Instability and Singularities in Transport Phenomena, Advanced transport Phenomena, Advanced Thermodynamics, Linear Operators, Rheology of Complex Fluids

Programming & Computer Science Courses:
Computational Geometry, Parallel Computing, Computing for Science and Engineering, Data Science, Data Structures and Algorithms, Programming in C, Interactive Computer Graphics, Artificial Intelligence, Fundamentals of Deep Learning (NVIDIA workshop)

Hosup Song

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EDUCATION

Purdue University — West Lafayette, IN
Ph.D. in Chemical Engineering — Expected Dec 2022

University of Minnesota — Twin Cities, MN
Bachelor of Chemical Engineering — May 2018

RESEARCH EXPERIENCE

Caruthers Research Group — **Aug 2018 - Present**
Graduate Assistant
Thermomechanical behaviors of glass forming polymers and its implications on constitutive modeling

- Characterization of various amorphous glass forming polymers using Dynamic Mechanical Analysis techniques on a rheometer
- Systematic study of the effects of temperature on the relaxation spectra of an amorphous polymer through utilization of Dynamic Mechanical Analysis and Stress Relaxation
- Perform thermal analysis of materials in various states of matter by using a Differential Scanning Calorimeter to calculate the glass transition temperatures and heat capacities
- Explore the effects of complex deformation histories on the mechanical performance of amorphous polymers through mechanical tensile testing
- Develop a MATLAB scrip to calculate the stress and strain values from a time-lapse video using image analysis tools
- Prediction of transition state molecular geometry as a precursor to calculations of transition state activation energy using Machine Learning algorithms

Neurock Research Group — **May 2017 - May 2018**
Undergraduate Researcher
Catalytic dehydrogenation of n-propanol to propyl aldehyde

- Researched under the advisor on catalytic dehydrogenation of n-propanol to propyl aldehyde, using computer simulations of molecular energy levels
- Used DFT calculations in VASP on SSH to calculate the absolute energies of surface-molecule systems and the corresponding reaction energies

Jong Seok Jeong Research Group — **April 2016 - May 2018**
Undergraduate Researcher
Analysis of electron beam propagation through crystalline Strontium Titanate ($SrTiO_3$) with respect to the sub-lattice position of the beam

- Researched the oscillation of electron beams in CTEM and STEM images of thin, non-amorphous specimen of Strontium Titanate
- Simulate CTEM/STEM and develop high resolution images of electron beam locations oscillating through crystalline Strontium Titanate
- Developed a MATLAB code to process raw TIFF images of wave functions to a Jet image series

Analysis of electron beam broadening patterns in both crystalline and amorphous materials

- Researched on observed electron beam broadening patterns when electron beams are shot through amorphous elements with thickness of 100 nm or larger
- Used Wolfram Mathematica to process computer simulation results by normalizing and radially integrating the electron beam intensity values obtained in array form

Hosup Song

TEACHING EXPERIENCE

TA for Chemical Engineering Calculations — Spring 2021
TA for Senior Chemical Engineering Lab — Spring 2020
Tutor for Organic Chemistry at Chemistry department of UMN — January 2017 – May 2018
Tutor for Math, Chemistry, and Physics at Taylor tutor center for College of Engineering and Science — January 2016 – May 2018

PUBLICATIONS

1. **Song, H.**, Medvedev, G. A. & Caruthers, J. M. (*in progress)*
2. **Song, H.**, Medvedev, G. A. & Caruthers, J. M. Structural relaxation of an epoxy resin at temperatures well below Tg. *Polym. Eng. Sci.* **62**, 537–552 (2022).
3. Ni, Y., **Song, H.**, Wilcox, D. A., Medvedev, G. A., Boudouris, B. W. & Caruthers, J. M. Rethinking the Analysis of the Linear Viscoelastic Behavior of an Epoxy Polymer near and above the Glass Transition. *Macromolecules* **53**, 1867–1880 (2020).
4. Jeong, J. S., **Song, H.**, Held, J. T. & Mkhoyan, A. K. Subatomic Channeling and Helicon-Type Beams in $SrTiO_3$. *Phys. Rev. Lett.* **122**, 75501 (2019).

PRESENTATIONS

Effect of Large Deformation on the Linear Viscoelastic Response of a Glassy Polymer
2022 APS, Oral

Structural Relaxation of an Epoxy Resin at Temperatures well below Tg
2021 Purdue ChE GSO Symposium, Poster

Structural relaxation in a polymeric glass well below Tg
2021 APS, Oral

Structural Relaxation of an Epoxy Resin at Temperatures well below Tg
2019 Purdue ChE GSO Symposium, Poster

Thermo-mechanical Behaviors of Glassy Polymers
2019 Purdue ChE GSO Colloqium, Poster

RELEVANT COURSEWORK

- Engineering of High Polymers
- Polymer Reaction Engineering
- Theory of Elasticity
- Structure and Properties of Polymeric Materials

TECHNICAL SKILLS

- MATLAB
- ARES-G2 (Rheometer)
- Java
- Mechanical testing via Extensometer
- DSC
- Python
- Solidity

Ying Tan

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EDUCATION

Purdue University, West Lafayette, IN **Expected May 2023**
PhD in Chemical Engineering | GPA: 3.58/4.0
Advisors: Professor Brett Savoie and Professor Bryan Boudouris
Research Topic: Design Features for Charge Transport in Radical Polymers

Zhejiang University **September 2014 – June 2018**
Bachelor of Engineering in Macromolecular Materials and Engineering | GPA: 3.83/4.0 | 11/92

CAREER OBJECTIVE

My ultimate career goal is to independently head a research laboratory focused on, but not limited to, the fields of polymer and soft matter materials, I plan on completing my graduate study in May 2023, and I will be trying to extend my skillset by acquiring a postdoctoral researcher position in the broad area of polymer physics, materials, and engineering. Also, given the minority of women in engineering, especially in academia, I would love to stand out and be a voice for women researchers.

SKILLS

Programming Languages- Python, C, MATLAB.
Synthetic Techniques- Organic synthesis and purification, Polymerization, Crystallization.
Chromatography- Gel Permeation (GPC), Thin Layer/Column.
Spectroscopy- Nuclear Magnetic Resonance (NMR), Ultraviolet-visible (UV-Vis), Electron Paramagnetic Resonance (EPR), Mass Spectroscopy (MS)
Other skills
Visualization Tools: Blender, VMD, Photoshop Statistics Software: JMP
Academic Software: Origin, ChemDraw, Mendeley Languages: Chinese, English

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **November. 2018 – Present**
Worked in a Simulation Research Group led by Prof. Brett Savoie

- Density functional theory of the charge transfer characteristics of a broad range of open-shell chemistries relevant to radical polymer conductors.
- Molecular dynamics simulations of different generations of radical dendritic macromolecules.
- Semi-empirical quantum chemistry calculations for the molecular design strategy of radical polymers with a combination of radicals, spacers, and polymer backbones.

Graduate Research Assistant, Purdue University **November. 2018 – Present**
Worked in a Polymer Research Group led by Prof. Bryan Boudouris

- Synthesis and characterizations of a series of radical oligomers as analogues of a radical polymer conductor champion to elucidate the molecular evidence of charge transfer.
- Single molecule open-shell electronics formed by the radical oligomers via a junction set-up. Performed transmission function calculations for single molecular open-shell electronics.

Ying Tan

RESEARCH AND WORK EXPERIENCE

Undergraduate Research Assistant, Zhejiang University **March. 2017 – May. 2018**

Worked at an Organic Semiconductor Lab led by Prof. Hanying Li

- Established the morphological revolution of calcite single crystals induced by the additive, citrate, and the agarose gel network matrix, uncovering the mechanism of hierarchical biominerals construction.

PUBLICATIONS AND PRESENTATIONS

1. "Electronic and Spintronic Open-Shell Macromolecules, Quo Vadis?," **Tan, Y**.; Hsu, S. N.; Tahir, H.; Dou, L.; Savoie, B. M.; Boudouris, B. W. *J. Am. Chem. Soc.* **2022**, *144*, 626–647.
2. Oral Presentation, "Molecular Design Features for Charge Transport in Radical Polymers." **Tan, Y**.; Savoie, B. M.; Boudouris, B. W. ACS Spring 2022 Meeting, San Diego, CA, March 20, 2022.
3. Oral Presentation, "Predicting Molecular Charge Transport in Radical Polymers." **Tan, Y**.; Savoie, B. M.; Boudouris, B. W. APS March 2022 Meeting, Chicago, IL, March 16, 2022.
4. "Molecular Design Features for Charge Transport in Non-Conjugated Radical Polymers," **Tan, Y**.; Casetti, N. C.; Boudouris, B. W.; Savoie, B. M. *J. Am. Chem. Soc.* **2021**, *143*, 11994-12002. (Selected as Supplementary cover art).
5. "Electronic and Magnetic Properties of a 3-Arm Nonconjugated Open-Shell Polymer," Yeo, H.; Akkiraju, S.; **Tan, Y**.; Tahir, H.; Dilley, N. R.; Savoie, B. M.; Boudouris, B. W. *ACS Polym. Au.* **2022**, *2*, 59–68.
6. "Design of an n-Type Low Glass Transition Temperature Radical Polymer," Chi, T.; Akkiraju, S.; Liang, Z.; **Tan, Y**.; Kim, H. J.; Zhao, X.; Savoie, B. M.; Boudouris, B. W. *Polym. Chem.* **2021**, *12*, 1448-1457. (Selected as Back cover art).
7. "Assessing the Synergy Effect of Additive and Matrix on Single-crystal Growth: Morphological Revolution Resulted from Gel-mediated Enhancement on CIT-Calcite Interaction," Liu, Y.; **Tan, Y**.; Ren, J.; Chen, H.; Li, H. *Chin. Chem. Lett.* **2018**, *29*, 1296-1300.

AWARDS AND HONORS

Ziek Travel Grant, Davidson School of Chemical Engineering, Purdue University	2022
College of Engineering Conference Travel Grants, Purdue University	2022
Poster award (2nd Prize) in Division of Polymer Physics, 2021 APS March Meeting, USA	2021
Scholarship for Outstanding Students, Zhejiang University, China	2015-2017
Outstanding Student Leader Award, Zhejiang University, China	2016

TEACHING EXPERIENCE

Graduate Research Assistant, Purdue University

- Teaching Assistant for Chemical Engineering Calculations, Fall 2019
- Teaching Assistant for Statistical Modeling and Quality Enhancement, Spring 2021

Jessica Elvira Torres

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jetorres425@gmail.com

EDUCATION

Purdue University, West Lafayette, IN **Expected Spring 2023**
PhD Candidate in Chemical Engineering
Advisor: Dr. Julie Liu
Research Topic: Protein-Based Biomaterials for Biomedical Applications

Massachusetts Institute of Technology, Cambridge, MA **2016**
BS in Chemical Biological Engineering

RESEARCH EXPERIENCE

Graduate Research Assistant, Purdue University, West Lafayette, IN **2017 – Present**

- Designed elastin-like polypeptide formulations modified with adhesive L-3,4-dihydroxyphenylalanine residues combined with crosslinkers to function as a surgical sealant
- Created an *in vitro* tissue model with collagen and hyaluronic acid to mimic large molecule drug diffusion and recovery
- Developed a polymer-based outreach activity that increased interest and career alignment in chemical engineering

Post-Bachelor Researcher, U.S. Department of Energy, **2016 – 2017**
Oak Ridge National Laboratory, Oak Ridge, TN

- Built biomass fast pyrolysis reactor simulations for optimization of bio-oil production
- Modeled residence time distributions and pressure drop of polydisperse materials in fast pyrolysis reactors using computational fluid dynamics discrete element model

Research Intern, Massachusetts Institute of Technology Langer Laboratory **2015**

- Developed nanoparticles to target inflammation in the gastrointestinal tract for drug delivery
- Optimized conditions for nanoparticle production using BSA to attain quality nanoparticles via dialysis, weight measurements, and spectrophotometry

SELECTED PUBLICATIONS

1. **J. E. Torres**, S. Hollingshead, D. Boucher, J. C. Liu "Biomimetic Adhesives for Clinical Applications" in Biomimetic Protein Based Elastomers, RSC Biomaterials Science, (2022).
2. S. Hollingshead, **J. E. Torres**, J. C. Liu "Effect of cross-linkers on mussel- and elastin-inspired adhesives on physiological substrates" ACS Applied Biomaterials 5 (2022).
3. Q. Xu, **J. Torres**, M. Hakim, P. M. Babiak, P. Pal, C. M. Battistoni, M. Nguyen, A. Panitch, L. Solorio, J. Liu "Collagen- and hyaluronic acid-based hydrogels and their biomedical applications" Materials Science and Engineering: R 146 (2021).
4. **J. E. Torres**, F. Meng, S. Bhattacharya, K. Buno, A. Ahmadzadedgan, S. Madduri, P. Babiak, P. Vlachos, L. Solorio, Y. Yeo, J. C. Liu "In Vitro Tissue Modeling of Collagen and Aldehyde/Hydrazide-Modified Hyaluronic Acid Hydrogels" (In Preparation).
5. **J. E. Torres** and J. C. Liu "Effect of coacervation and cross-linkers on mussel- and elastin-inspired surgical sealing" (In Preparation).
6. **J. E. Torres** and J. C. Liu "Enhancing chemical engineering identity in young women with a biomedical polymer outreach activity" (In Preparation).

Jessica Elvira Torres

SELECTED CONFERENCE PRESENTATIONS

1. **J. E. Torres**, F. Meng, S. Madduri, K. Buno, L. Solorio, Y. Yeo, J. C. Liu "In Vitro Tissue Model with Collagen and Aldehyde/Hydrazide-Modified Hyaluronic Acid Hydrogels." Society for Biomaterials Annual Meeting, April 2022, Baltimore, MD.
2. **J. E. Torres**, J. C. Liu "Bioinspired Elastin-Based DOPA-Modified Protein Lung Sealants." Society for Biomaterials Annual Meeting, April 2021, Chicago, IL.
3. **J. E. Torres**, F. Meng, K. Buno, Y. Yeo, L. Solorio, J. C. Liu "Collagen I and Modified Hyaluronic Acid Hydrogels for Tissue Engineering." Society for Biomaterials Annual Meeting, April 2021, Chicago, IL.
4. **J. E. Torres**, J. C. Liu "Formulation Design of a Recombinant Protein-Based Lung Sealant." International Conference on Biological and Biomimetic Adhesives, February 2021, Aveiro, Portugal.

AWARDS AND HONORS

Outstanding Service Award **2022**
- Purdue College of Engineering award recognizing a student who contributed to the quality, reputation, and success of the graduate student community, school, college, and university

Marilyn Forney Trailblazer Award **2021**
- Purdue Chemical Engineering award recognizing a student who helped pave the way for women in the field of engineering

National Science Foundation Graduate Research Fellowship **2019**
- National Science Foundation 3-year fellowship

Leslie Bottorff Innovation for Clinical Translation Fellowship **2019**
- Purdue University College of Engineering and Indiana University School of Medicine
- 2-year fellowship targeting new innovations for near-term translation into hospital settings

Purdue Doctoral Fellowship **2017**
- Purdue University 4-year fellowship

Mickey Leland Energy Fellowship **2015**
- U.S. Department of Energy summer fellowship

SKILLS

Laboratory Skills:	Confocal microscopy, scanning electron cryomicroscopy, colorimetric assays, bacterial fermentation, recombinant protein production and purification, immunofluorescence, cell culture, cytocompatibility
Material Testing:	Compression testing, burst pressure testing, swelling, adhesive testing, rheology
Computational Modeling:	MATLAB, Python, C, C++, JMP, SAS

Suraj Ugrani

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EDUCATION

Purdue University, West Lafayette, IN **May 2023**
PhD in Chemical Engineering | GPA: 3.42/4.0
Advisor: Sangtae Kim
Research Topic: Computer-aided drug discovery

Indian Institute of Technology Bombay, Mumbai, India **July 2016**
M.Tech. in Chemical Engineering| GPA: 8.47/10.0

University of Mumbai, Mumbai, India **May 2013**
B.E. in Chemical Engineering| First Class with Distinction-73.87%

CAREER OBJECTIVE

I am a PhD candidate in Chemical Engineering with a passion for drug discovery and possess a diverse skill set which includes computational chemistry techniques, data science, and programming. I am seeking a stimulating work environment to apply my knowledge to solve challenging problems in drug discovery while simultaneously expanding my capabilities.

SKILLS

Structure-Based Computer-Aided Drug Discovery

- Proficient in related techniques including molecular docking, MD simulation, homology modeling, and application of machine learning

UCSF DOCK/AutoDock Vina	GROMACS
MODELLER (protein structure modeling)	Python
RDKit	MATLAB

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2018 – Present**
'Application of the "Hydrogen Bond-Wrapping" Concept for Computer-Aided Discovery of TMPRSS2 Inhibitors'

- Validating a novel descriptor based on extent of 'wrapping' around a protein's hydrogen bonds using machine learning models for application in drug discovery
- Designing inhibitors of human protein TMPRSS2, which are potential broad-spectrum antivirals, using information from the machine learning models

Research Fellow, Indian Institute of Technology Bombay **Apr. 2017 – Jul. 2018**
'Development of an Exclusive Flavor Encapsulation Technology based on Spray Drying, Melt Injection or Other Novel Processes'

- Optimized existing spray drying process conditions and slurry composition leading to improved particle morphology and retention of active ingredient
- Designed a lab-scale prototype for melt extrusion to synthesize cylindrical particles

'Preparation and Rheological Characterization of LiFePO4 based Cathode Slurry for Li-ion batteries' (Side project)

Suraj

Research Fellow, Institute of Chemical Technology, Mumbai **Jan. 2017 – Mar. 2017**
'Investigation of Properties of Molten Salts as a Heat Storage Medium'

M.Tech. Research Assistant, Indian Institute of Technology Bombay **Jan. 2015 – Jul. 2016**
'Experimental Determination of Solute Critical Supersaturation (CSS) for Aerosol Synthesis of Drug Nanoparticles'

- Performed nanoparticles synthesis by spray drying, size analysis with a scanning mobility particle sizer, and computer simulations to determine CSS of various lipids and cancer drugs
- Devised drug-lipid-solvent systems to ensure formation of a lipid shell encapsulating the drug

PUBLICATIONS AND PRESENTATIONS

1. Jain, M.; Vaze, R. G.; **Ugrani, S.**; Sharma, K. P. Mechanoresponsive and Recyclable Biocatalytic Sponges from Enzyme-Polymer Surfactant Conjugates and Nanoparticles. *RSC Adv*. **2018**, 8 (68), 39029–39038. https://doi.org/10.1039/C8RA08221A.
2. Sapra, M.; **Ugrani, S.**; Mayya, Y. S.; Venkataraman, C. Estimation of Critical Supersaturation Solubility Ratio for Predicting Diameters of Dry Particles Prepared by Air-Jet Atomization of Solutions. *J. Colloid Interface Sci.* **2017**, 500, 172–181. https://doi.org/10.1016/j.jcis.2017.04.008.

AWARDS AND HONORS

Winner of 'Best Overall Poster Pitch' at the 2021 Virtual Purdue Chemical Engineering Graduate Student Organization Symposium

HOBBIES AND INTERESTS

- Music (guitar) – improvisation, composition, experimentation
- Basketball – member of school teams from middle-school through undergraduate final year
- Moral philosophy – particularly ethics of consumption

Dhushyanth Viswanath

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dviswan@purdue.edu

EDUCATION

Purdue University, West Lafayette, IN **Expected Summer 2023**
PhD in Chemical Engineering | GPA: 3.81/4.0
Advisor: Dr. You-Yeon Won
Research Topic: Radioluminescent Nanoparticle Formulations for Multimodal Treatment of Cancer

University of Wisconsin-Madison, WI **May 2018**
Bachelor of Science in Chemical Engineering | GPA: 3.74/4.0
Academic Honors: Graduated with Distinction (Top 15%), Deans List (All Semesters)

SKILLS

Polymeric Nanoparticle Formulation Development

- Co-loading of inorganic nanoparticles and hydrophobic small molecule drugs in PEG-PLA micelles via emulsion/evaporation, solvent exchange, dialysis & microfluidic mixing methods

Block copolymer synthesis & characterization	Confocal microscopy
Inorganic nanoparticle synthesis & characterization	Flow cytometry
Mammalian cell culture	*In vivo* efficacy testing
Colorimetric & fluorescent assays	Biodistribution & pharmacokinetic modelling

RESEARCH EXPERIENCE

Graduate Research Assistant, Purdue University **Aug 2018 – Present**

- Designed block co-polymer-encapsulated radioluminescent nanoparticles as novel tools to achieve concomitant radio- and photodynamic- therapy of solid tumors
- Probing synergy between radiation-induced photodynamic therapy and blockage of key immune markers towards inciting systemic abscopal response for patients with metastatic disease
- Adept in various organic and inorganic synthesis, formulation, and characterization techniques
- Highly experienced in conducting pre-clinical safety and efficacy testing via cell culture and murine models and possess expertise in associated data analysis and statistical methods
- Frequently collaborate with veterinary and clinical oncologists at Purdue University and IU School of Medicine, respectively, to identify and address potential downstream obstacles hindering clinical translation

Undergraduate Researcher, Klingenberg Lab, UW-Madison **Jan 2017 – Jun 2017**

- Characterized changes in apparent viscosity of aqueous fiber suspensions with varying shear rate, fiber type, concentration, and morphology using a lignocellulosic biomass rheometer

Undergraduate Researcher, Yan Lab, National University of Singapore **Summer 2016**

- Designed experimental parameters for synthesis of glucosamine from chitin via acid-catalyzed hydrolysis and deacetylation

LEADERSHIP EXPERIENCE

Lab Safety Officer, Won Lab, Purdue University **Jun 2021 – Present**

- Established structured chemical waste disposal and lab safety practices for researchers in wet chemistry and biosafety level-2 labs in compliance with OSHA and university guidelines
- Mentored over 10 researchers from high school to graduate background on lab safety resulting in 0 safety incidents during tenure

Dhushyanth Viswanath

Chemical Engineering Department Safety Committee, Purdue University Jun 2021 – Present

- Conducted monthly inspections across 30 research groups to identify potential safety hazards
- Developed and documented lab safety and ergonomic protocols impacting daily activity of over 200 researchers in the department
- Innovated solutions to address unprecedented COVID-19-related workplace complications

Chemical Engineering Safety Seminar Committee, Purdue University Aug 2019 – Jun 2020

- Operated in a 4-member team to organize seminars regarding lab safety and ergonomics
- Implemented strategies to promote student interest and involvement thereby growing average seminar attendance from 10 to 40 people in one semester on a $500 budget

Teaching Assistant, Chemical Engineering Lab, Purdue University Fall 2019 & Spring 2021

- Mentored 60 undergraduate students on research methodology, i.e., developing hypotheses, acquiring data through experimentation, and communicating results effectively in presentations and reports
- Served as lab safety officer and as liaison between professor, lab technician, and students

AWARDS AND HONORS

- **Leslie Bottorff Fellowship,** Purdue University **2021 - Present**
- **1st Place in Poster Competition** **Sep 2020**
  2020 Annual Meeting of the Indiana Clinical and Translational Science Institute (CTSI)
- **1st Place in Poster Competition** **Aug 2020**
  29th Annual Purdue Chemical Engineering GSO Symposium
- **2nd Place in Poster Competition** **Feb 2020**
  Heath and Disease: Science, Technology, Culture, and Policy Research Symposium, Purdue University
- **Ellis C. Riplinger Scholarship**, UW – Madison **Aug 2017**
- **DCS Scholarship**, UW – Madison **May 2017**

PUBLICATIONS

1. **First Author: Viswanath, D.**; Won, Y.-Y., Combining Radiotherapy (RT) and Photodynamic Therapy (PDT): Clinical Studies on Conventional RT-PDT Approaches, and Novel Nanoparticle-Based RT-PDT Approaches Under Preclinical Evaluation. *ACS Biomaterials Science & Engineering* 2022 (Submitted)
2. **Co-First Author:** Pizzuti, V.; **Viswanath, D.**; Won, Y.-Y.; et al., Bilirubin-Coated Radio-Luminescent Particles for Radiation-Induced Photodynamic Therapy. *ACS Applied Bio Materials* 2020, 3, 8, 4858–4872
3. **Co-Author:** Yoo, J.; **Viswanath, D.**; Won, Y.-Y., Strategy for Synthesis of Statistically Sequence-Controlled Uniform PLGA and Effects of Sequence Distribution on Interaction and Drug Release Properties. *ACS Macro Letters* 2021, 1510-1516
4. **Co-Author:** Patel, A. P.; Schorr, C. R.; **Viswanath, D.**; et al., Pilot-Scale Optimization of the Solvent Exchange Production and Lyophilization Processing of PEG–PLA Block Copolymer-Encapsulated $CaWO_4$ Radioluminescent Nanoparticles for Theranostic Applications. *Industrial & Engineering Chemistry Research* 2021, 60 (19), 7081-7096

Zitang Wei

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EDUCATION

Purdue University, West Lafayette, IN **Expected May. 2023**
PhD in Chemical Engineering
Advisor: Letian Dou
Research Topic: Topochemical polymer single crystals with quantitative recyclability and tunable mechanical properties

University of California, Santa Barbara, Santa Barbara, CA **Sept 2014 – Apr. 2018**
Bachelor of Science, Chemistry, College of Creative Studies
Undergraduate Research Advisor: Fred Wudl
Research Topic: Synthesis of heterocycle-containing conjugated molecules for organic solar cells

CAREER OBJECTIVE

Design and synthesize cheap and easily accessible polymer materials for next-generation recyclable plastics.

SKILLS

Organic Molecule Design and Synthesis

- Air and moisture-free reaction design and synthesis, flash column chromatography, TLC, recrystallization, distillation.

Thin Film Fabrication
X-ray Diffraction
Operation of Diamond Anvil Cell
Single Crystal Preparation and Analysis
Nuclear Magnetic Resonance Spectroscopy
Operation of Ball Milling Machine

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2018 – Present**
Quantitative depolymerization of polyindenedione derivatives for next-generation recyclable plastics

- Designed and synthesized conjugated polyindenedione derivatives via topochemical polymerizations.
- Developed the solution-processed depolymerization method of polyindenedione derivatives.
- Characterized the polymer materials by NMR, single crystal XRD, DSC, and TGA.
- Processed one-dimensional polymer single crystals into two-dimensional thin films using ultrasonication and vacuum filtration.

Tuning Elastic Modulus of Topochemical Polymer Single Crystals by Side Chain Design

- Functionalized the side chains of polymer single crystals by introducing unsaturated groups, bulkiness, and heteroatoms. Prepared monomer single crystals with distinct side chains and tested the topochemical reactivity.
- Tested the elastic modulus of polymer single crystals using nano-indentation.

Novel selenophene-containing organic ligand for Sn-based 2D perovskite materials

- Designed and synthesized a novel selenophene-containing organic ligand and incorporated the ligand into 2D Sn-based perovskites.
- Utilized the 2D Sn-based perovskites into field-effect transistors and light-emitting diodes.

Zitang Wei

PUBLICATIONS AND PRESENTATIONS

Publications:

1. Luo, X.[+]; **Wei, Z.**[+]; Seo, B.[+]; Hu, Q.; Wang, X.; Romo, J.A.; Jain, M.; Cakamak, C.; Boudouris, B.W.; Zhao, K.; Mei, j.; Savoie, B.M.; Dou, L. Circularly Recyclable Polymers Featuring Topochemically Weakened Carbon-Carbon Bonds. *J. Am. Chem. Soc*. 2022. Accepted. [+]Equal contribution first author.
2. **Wei, Z.**; Wang, X.; Seo, B.; Luo, X.; Hu, Q.; Jones, J.; Zeller, M.; Savoie, B.M.; Zhao, K.; Dou, L. Side-Chain Control of Topochemical Polymer Single Crystals with Tunable Elastic Modulus. *Angew. Chemie Int. Ed*, 2022. Manuscript under review.
3. **Wei, Z.**; Wang, K.; Zhao, W.; Gao, Y.; Hu, Q.; Chen, K.; Dou, L. A selenophene-containing conjugated organic ligand for two-dimensional halide perovskites. *Chem. Commun*. 2021, 57, 11469-11472.
4. **Wei, Z.**; Li, X.; Wudl, F.; Zheng, Y. Facile synthesis of thiophene/selenophene-fused acene and their optoelectronic properties. *Tetrahedron*. 2017, 73, 7100-7104.
5. Gao, Y.; **Wei, Z.**; Yoo, P.; Shi, E.; Zeller, M.; Liao, P.; Dou, L. Highly stable lead-free perovskite field-effect transistors incorporating linear π-conjugated organic ligands. *J. Am. Chem. Soc.* 2019, 141, 15577-15585.
6. Gao, Y.; **Wei, Z.**; Hsu, S.N.; Boudouris, B.W.; Dou, L. Two-dimensional halide perovskites featuring semiconducting organic building blocks. *Mater. Chem. Front.* 2020, 4, 3400-3814.
7. Liang, A.; Gao, Y.; Asadpour, R.; **Wei, Z.**; Finkenauer, B. P.; Jin, L.; Yang, J.; Wang, K.; Chen, K.; Liao, P.; Zhu, C.; Huang, L.; Boudouris, B.W.; Alam, M.A., Dou, L. Ligand-driven grain engineering of high mobility two-dimensional perovskite thin-film transistors. *J. Am. Chem. Soc*. 2021, 37, 15215-15223.
8. Ma, K.; Hsu, S.N.; Gao, Y.; **Wei, Z.**; Jin, L.; Finkenauer, B.P.; Huang, L.; Boudouris, B.W.; Mei, J.; Dou, L. Organic Cation Engineering for Vertical Charge Transport in Lead-Free Perovskite Quantum Wells. *Small. Sci*. 2021, 1, 2000024.
9. Finkenauer, B.P.; Gao, Y.; Wang, X.; Tian, Y.; **Wei, Z.**; Zhu, C.; Rokke, D.J.; Jin, L.; Meng, L.; Yang, Y.; Huang, L.; Zhao, K.; Dou, L. Mechanically robust and self-healable perovskite solar cells. *Cell Rep. Phys. Sci*. 2021, 2, 100320.
10. Wang, K.; Jin, L.; Gao, Y.; Liang, A.; Finkenauer, B.P.; Zhao, W.; **Wei, Z.**; Zhu, C.; Guo, T.F.; Huang, L.; Dou, L. Lead-free organic–perovskite hybrid quantum wells for highly stable light-emitting diodes. *ACS Nano*. 2021, 15, 6316-6325.
11. Li, X.; Wang, H.; Schneider, J.A.; **Wei, Z.**; Lai, W.Y.; Huang, W.; Wudl, F.; Zheng, Y. Catalyst-free one-step synthesis of ortho-tetraaryl perylene diimides for efficient OPV non-fullerene acceptors. *J. Mater. Chem. C*. 2017, 5, 2781-2785.

Presentations:

1. **Wei, Z.** A Selenophene-Containing Conjugated Organic Ligand for Two-Dimensional Halide Perovskite. MRS Spring 2022, Honolulu, HI, May 2022.
2. **Wei, Z.** Two-Dimensional Organic-Inorganic Halide Perovskites Design and Synthesis. Purdue Process Safety & Assurance Center Fall 2019 Conference, West Lafayette, IN, Sept 2019.
3. **Wei, Z.** Perovskite Material Design for Thin Film Electronics. Mi-Bio Summit on Flexible and Stretchable Bioelectronics. West Lafayette, IN, Jul 2019.

TEACHING EXERIENCES

Graduate Teaching Assistant, Purdue University

- ChE 435: Chemical Engineering Laboratory — Fall 2019
- ChE 211: Introduction to Chemical Engineering Thermodynamics — Spring 2021

Junkai Xie

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EDUCATION

Purdue University, West Lafayette, IN **Expected 2023**
PhD in Chemical Engineering | GPA: 3.45/4.0
Bachelor's in Chemical Engineering | GPA: 3.82/4.0 **May 2018**

TECHNICAL SKILLS

I have proficient skills in maintaining and differentiating iPSC and regular cells lines as cell models. I can efficiently isolate genomic DNA, total RNA from TC culture and plasmid DNA from bacterial culture. In addition, I can construct cDNA by reverse transcription and quantify using q-PCR to determine the relative change in transcription. Related skills in molecular cloning such as primer design, PCR reaction, gel electrophoresis and cell transformation are my daily routines. From the protein engineering perspective, skills such as blotting, protein expression, purification and FPLC have been demonstrated in some of my research protect. Immunohistochemistry and immunofluorescence were routinely used on cells and animal tissues and further visualized via confocal microscopy and super resolution microscopy.

COMPUTATION

- Specialized Software: Ingenuity Pathway Analysis (IPA), OriginPro, MATLAB, Python, BLAST, KEGG
- Engineering Software: Aspen
- Statistical Software: Minitab, SAS
- General Software: Office, Endnote, Photoshop

WORK EXPERIENCE

Graduate Research Assistant, PURDUE CHE **2018 – Present**

- Reveal the contribution of environmental toxicant exposure to the risk of early on-set of neurodegenerative diseases.
- Understanding of the molecular mechanism connecting between traumatic injuries and late on-set neurodegenerative disease including Alzheimer's Disease and Parkinson's Disease.

Research Assistant, Novozymes **2017**

- Development and optimization of recombinant lactase used in lactose-free milk production.

Undergraduate Research Assistant, PURDUE Chemistry and CHE **2015 – 2018**

- Development of DNA aptamer-based small molecules detection platform.

Undergraduate Teaching Assistant, PURDUE Dept. of Engineering Education **2015 – 2017**

- Teaching assistant for ENGR13X courses focusing on engineering modeling and MATLAB programming.

PEER REVIEWED PUBLICATIONS

1. **J Xie,** Y Ho, H Zhao, H Szadowski, C Yuan and R Huang. "NatD modulated nucleosomal conformation and stability." Under Preparation.
2. **J Xie,** X Ping, X Jin and C Yuan. "Molecular mechanism of acupuncture mediated pain relief after tibial nerve injury" Under Preparation.
3. **J Xie**, S Herr, R Shi and C Yuan. "Transcriptomic analysis of motor cortex post spinal cord injury." Under Preparation.
4. S Wang, C Bryan, **J Xie**, H Zhao, L Lin, J Tai, K Horzmann, O Sanchez, M Zhang, J Freeman and C Yuan. "Atrazine Exposure in Zebrafish Induces Aberrant Genome-Wide Methylation." (2021) Submitted.
5. **J Xie**, S Herr, D Ma, H Zhao, S Sun, Z Ma, M Chan, K Li, Y Yang, F Huang, R Shi and C Yuan.

"Acute transcriptomic and epigenetic alterations at T12 after T10 spinal cord contusive injury." (2021) Submitted.

6. O Sanchez, L Lin, **J Xie**, J Freeman and C Yuan. "Lead Exposure Induces Dysregulation of Constitutive Heterochromatin Hallmarks in Live Cells." Current Research in Toxicology (2021) Accepted.
7. Z Que, MI Olivero-Acosta, J Zhang, M Eaton, A Tukker, X Chen, J Wu, **J Xie**, T Xiao, K Wettschurack, L Yunis, J Shafer, J Schaber, J Rochet, A Bowman, C Yuan, Z Huang, C Hu, D Trader, W Skarnes and Y Yang. "Hyperexcitability and pharmacological responsiveness of cortical neurons derived from human iPSCs carrying epilepsy-associated sodium channel Nav1.2-L1342P genetic variant." Journal of Neuroscience (2021)
8. H Zhao, D Ma, **J Xie**, OF Sanchez, F Huang and C Yuan. "Live cell probe for in-situ single cell monitoring of mitochondrial DNA methylation." ACS Sensor 6(10):3575-3586 (2021).
9. A Mendonca, OF Sanchez, **J Xie**, A Carneiro, L Lin and C Yuan. "Identifying distinct heterochromatin regions using combinatorial epigenetic probes in live cells." Biochimica et Biophysica Acta (BBA) – Gene Regulatory Mechanisms, 194725, (2021).
10. **J Xie**, L Lin, O Sanchez, C Bryan, JF Freeman and C Yuan. "Pre-differentiation exposure to low-dose of atrazine results in persistent phenotypic changes in human neuronal cell lines." Environmental Pollution, 116379, (2021).
11. LF Lin, **J Xie**, OF Sanchez, C Bryan, JL Freeman and C Yuan. "Low dose lead exposure induces alterations on the heterochromatin hallmarks persisting through SH-SY5Y cell differentiation." Chemosphere 264, 128486, (2021).
12. **J Xie**, K Wettschurack and C Yuan. Review: "*In vitro* Cell Platform for Understanding Developmental Toxicity" Frontiers in Genetics 11, (2020).
13. K Wettschurack*, **J Xie***, O Sanchez and C Yuan. Review: "Engineering in situ biosensors for tracking cellular events." Current Opinion in Chemical Engineering 30, 34-41, (2020). *: Equal contribution.
14. OF Sanchez, L Lin, C Bryan**, J Xie**, JL Freeman and C Yuan. "Profiling epigenetic changes in human cell line induced by atrazine exposure." Environmental Pollution 258, 113712, (2020).

CONFERENCES & POSTER PRESENTATIONS

- 2021 AIChE Annual Meeting Presentation: "*Transcriptome and Methylome Analysis of Distal Spinal Cord Location after Spinal Cord Injury*."
- 2021 AIChE Annual Meeting Presentation "*Development of Human iPSC-Derived Neuron Culture to Study the Contribution of Gene Environmental Interactions to the on-set of Alzheimer's Disease*."
- 2020 AIChE Annual Meeting (Virtual) Presentation: "Unveil Epigenetic Memory Conferring Parkinson's Disease Risks Arising from Exposure to Environmental Chemicals"
- 2020 AIChE Annual Meeting (Virtual) Poster Presentation "A Novel Platform of Monitoring DNA Hydroxymethylation (5-hmC) Change in Live Cells"

AWARDS & FELLOWSHIPS

Charles C. Chappelle Research Fellowship 2018 – 2019
Leslie Bottorff Innovation for Clinical Translation Fellowship 2021 – 2023

LANGUAGE SKILLS

English | Chinese | German

PROFESSIONAL MEMBERSHIP

American Institute of Chemical Engineers 2015 - present
American Chemical Society Member 2014 - 2015

Han Zhao

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EDUCATION

Purdue University, West Lafayette, IN **Expected Jun. 2023**
PhD in Chemical Engineering
Advisor: Chongli Yuan
Research Topic: Multi-organelle interactome and liquid-liquid phase separation of chromatin in Parkinson's disease

University of Science and Technology of China, Hefei, China **May. 2017**
BS in Physical Chemistry

CAREER OBJECTIVE

My future research interest is to systematically quantify organelle interaction of neurons during Parkinson's disease (PD) progression and build organelle interaction network that drives PD onset. PD is an intrinsically complicated disease affecting multiple organelles, including mitochondria, lysosome, endoplasmic reticulum, synapse, and epigenetic landscape in nucleus. Onset of PD triggers dysfunction of more than one organelle mentioned above. Different cellular compartments crosstalk through direct contact or exchanging of signaling molecules. The current approaches focus on individual organelles, while neglecting the crosstalk between organelles. There is limited knowledge regarding dynamics and causal relationship between various dysfunctional organelles during the onset of PD, thus leaving the molecular mechanism of PD poorly understood. To fill this knowledge gap, my future research will focus on 1) establish a humanized brain culture model consisting of different neuron types; 2) build a library of toolset to probe and perturb protein-protein interaction (PPI) across various organelles; and 3) explore the organelle interactome via advanced quantitative microscopy coupled with machine learning algorithm to predict causal relationship from timelapse dataset. The foundation of my proposed research is built upon my research expertise in cell biology, protein engineering and system biology. For example, I successfully derived dopaminergic (DA) neurons from human induced pluripotent stem cells (hiPSCs) with PD-like phenotype after atrazine exposure at developmental stage. Furthermore, we developed live-cell compatible probe targeting mitochondrial DNA methylation in my previous work. Additionally, I performed quantitative measurement of interaction of two heterochromatin markers, namely ^{me}CpG and H3K9me3, using fluorescent lifetime imaging microscope (FLIM), during neuron differentiation. In another project, I used regression-based model to predict dominant epigenetic features that can distinguish cells from different treatment group. Collectively, my training from PhD research will support my accomplishment of proposed research objectives.

SKILLS

Experimental Skills: Confocal microscopy, Quantitative microscopy (fluorescence lifetime microscopy and fluorescent correlation microscopy), Cell culture.
Programming Skills: R.

Han Zhao

RESEARCH AND WORK EXPERIENCE

Graduate Research Assistant, Purdue University **Aug. 2017 – Present**

- Designed and validated a novel live-cell compatible probe targeting mitochondrial DNA methylation and revealed spatial distribution of mitochondrial DNA methylation in mammalian cell line.
- Evaluated neurotoxicity of forever chemical PFOA and discovered altered DNA methylation level and mitochondria morphology in dopaminergic-like neurons after developmental exposure to PFOA.
- Examined changes in heterochromatin markers systematically during drug resistance development of breast cancer using single-cell imaging-based approach and identified DNA methylation as potential driving factor for drug resistance development.
- Derived dopaminergic neurons from hiPSCs, assessed the changes of heterochromatin markers and neuronal activity and observed Parkinson's disease phenotype after developmental exposure to atrazine.
- Tracked the dynamics of heterochromatin markers (5mC and H3K9me3) of single cell during neuron differentiation and performed biophysical measurements of selected markers, i.e. fluorescent lifetime and diffusivity to understand interaction between essential proteins for heterochromatin establishment.

PUBLICATIONS

1. **Zhao, H.**; Xie, J.; Wu, S.; Sánchez, O. F.; Zhang, X.; Freeman, J. L.; Yuan, C., Pre-differentiation exposure of PFOA induced persistent changes in DNA methylation and mitochondrial morphology in human dopaminergic-like neurons. *Environmental Pollution* (2022)
2. **Zhao, H**.; Lin, L. F.; Hahn, J.; Xie, J.; Holman, H. F.; Yuan, C., Single-Cell Image-Based Analysis Reveals Chromatin Changes during the Acquisition of Tamoxifen Drug Resistance. *Life* (2022)
3. **Zhao, H**.; Ma, D.; Xie, J.; Sanchez, O.; Huang, F.; Yuan, C., Live-Cell Probe for In Situ Single-Cell Monitoring of Mitochondrial DNA Methylation. *ACS Sensors* (2021)
4. Wang, S.; Bryan, C.; Xie, J.; **Zhao, H**.; Lin, L. F.; Tai, J. A. C.; Horzmann, K. A.; Sanchez, O. F.; Zhang, M.; Freeman, J. L.; Yuan, C., Atrazine exposure in zebrafish induces aberrant genome-wide methylation. *Neurotoxicology and Teratology* (2022)
5. Yuan, C.; Freeman, J. L.; Xie, J.; **Zhao, H**., The Role of Dynamic Epigenetic Changes in Modulating Homeostasis after Exposure to Low-dose Environmental Chemicals. *Genomic and Epigenomic Biomarkers of Toxicology and Disease* (2022)
6. Mendonca, A.; Sánchez, O.; **Zhao, H**.; Lin, L.; Min, A.; Yuan, C., Development and application of novel BiFC probes for cell sorting based on epigenetic modification. *Cytometry Part A* (2022)

AWARDS AND HONORS

2nd place in Sensor Competition Session of 2021 AIChE Annual Meeting 2021

Acknowledgements

The Graduate Student Organization would like to thank the following companies for their financial support and attendance at the 31st Annual Graduate Research Symposium. Without their support, this event would not have been possible:

Notes

Notes