

Interdisciplinary Research (IDR) Origination Awards

Project Title

Combining the Forces of Experiment, Simulation, and Data Science to Develop New Catalysis Technology for Natural Gas Conversion

Principal Investigator(s) (full-time faculty)

Name (PI listed first)	Department	College
Morris Argyle	Chemical Engineering	Engineering
Kara Stowers	Chemistry and Biochemistry	Physical and Mathematical Sciences
David Wingate	Computer Science	Physical and Mathematical Sciences
Dan Ess	Chemistry and Biochemistry	Physical and Mathematical Sciences
Dennis Della Corte	Physics and Astronomy	Physical and Mathematical Sciences

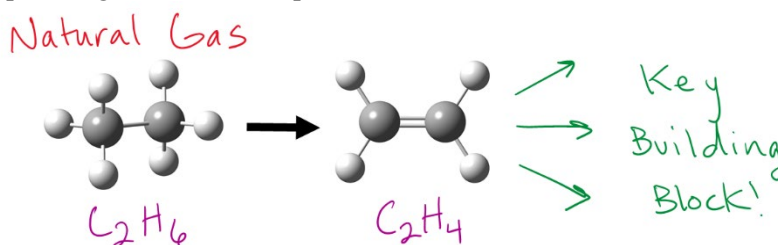
Track: Track one

Abstract

The US has massive amounts of oil and natural gas. Unfortunately, this excess results in significant waste and underutilization. For example, refineries in North Salt Lake routinely wastefully flare natural gas (as shown). As a major effort to dampen the impact of natural gas loss and more efficiently use hydrocarbons, our big-picture goal is to develop



new catalyst technology to convert ethane (C_2H_6) to ethylene (C_2H_4), which is the most critical chemical building block in the world (>150 million metric tons/year produced). Current technology to catalyze the seemingly simple removal of two hydrogen atoms



from ethane to make ethylene is very inefficient and unselective (i.e., it generates a mixture of wanted and unwanted products). The development of new, lower temperature, more selective catalysts for ethane to ethylene conversion is a “holy grail” chemistry problem and progress has been slow over several decades. Therefore, we have assembled a team that has unique synergy to develop new catalyst technology. We will leverage experiment (Argyle and Stowers), computer simulations (Della Corte and Ess), and data science (AI/machine learning: Wingate) to develop new catalysts based on a relatively new and emerging solid-state material technology called metal organic frameworks (MOFs), which combine transition metal centers with organic linking molecules to make 3D porous materials. Simultaneous use of experiment, simulation, and data science to solve this holy grail problem is necessary and novel because there are 10,000’s of potential MOFs and an experimental only trial and error-based approach is not tractable.

Summary of Plans for External Funding

The National Science Foundation (NSF) Division of Chemical, Bioengineering, Environmental and Transport (CBET) Systems Catalysis program maintains an open call for proposals that we will target in late 2021, after collecting preliminary data within this IDR project (~\$500,000 funding opportunity).

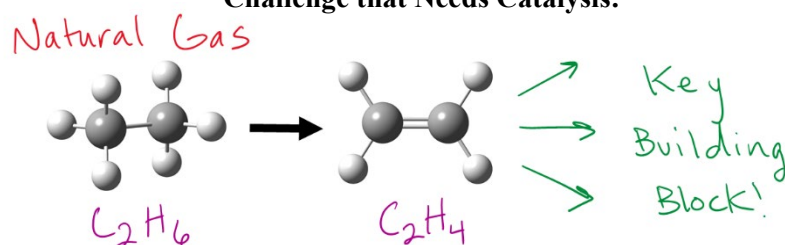
NSF Designing Materials to Revolutionize and Engineer our Future (DMREF). This is a biennial request for proposals that is next open in early 2023 and is ideally suited to our team because it requires materials discovery through both experiment and simulation. Importantly, to secure this type of high-level funding, a full two years of preliminary data from our team and coauthor publications is required. Therefore, 2021 is the correct time to target the 2023 submission. IDR funding would allow our team to collect the needed preliminary results and proof of concept to secure this ~\$1.8 million funding opportunity.

Combining the Forces of Experiment, Simulation, and Data Science to Develop New Catalysis Technology for Natural Gas Conversion

Introduction

The US and the rest of the world underutilizes a significant portion of our hydrocarbon natural gas resources. The example in the abstract showed that a large quantity of natural gas is burned, which is called flaring, because there is no economical way to convert the gas to useful chemical building blocks and it is not cost effective to compress or to liquify it. Our long-term goal is to develop new catalyst technology to convert ethane (C_2H_6), which is a major component of natural gas [1], to ethylene (C_2H_4), which is perhaps the very most critical chemical building block in the world (typically >150 million metric tons produced per year). The conversion of ethane to ethylene is called an oxidation reaction and therefore requires a catalyst capable of selective oxidation with oxygen (O_2) at a rapid rate. This ethane to ethylene reaction with oxygen is known as oxidative dehydrogenation (ODH) [2]. As the reviewer may know, catalysts are critical because they significantly reduce the energy needed for a chemical transformation, thereby speeding up the reaction rate and often increasing selectivity or efficiency (i.e., generate exclusively the desired product).

Challenge that Needs Catalysis:



Catalysts are critical for ODH because current technology without catalysts requires very high temperatures that demand significant energy input. Additionally, non-catalytic processes are not very selective due to a breakdown of the reagents into deposits of unusable soot-like carbon [3]. A particular category of catalysts that are well-suited for ODH are called metal oxides (see Figure 1). These solid-state materials are a combination of metal atoms with embedded oxygen atoms, which naturally can supply the needed oxygen atoms for oxidation as well as facilitate the reorganization of the chemical bonding of ethane to form ethylene. Moreover, metal oxides are generally stable and can be chemically modified, for example, by including small amounts of other atoms called dopants.

While metal oxide catalysts have several major advantages, no current metal oxide catalyst (e.g.

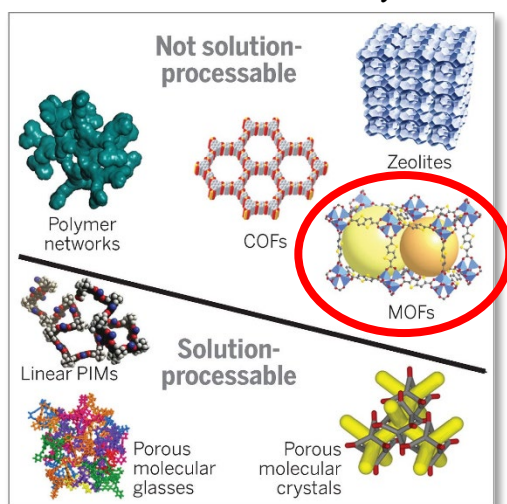


Figure 1: Metal oxides

established zeolite technology) is good enough to displace the existing inefficient, noncatalytic ODH process. We believe that a superior, game-changing metal oxide catalyst has not been discovered because these metal oxide catalysts are made with traditional methods that do not allow for new catalyst structures as well as consistent size, shape, and location of highly active metal sites that react with the incoming ethane.

Because development of a catalyst for ODH is a “holy grail” type chemistry and engineering problem, our plan is to make a paradigm change in how the metal oxide catalysts are designed and created, which will allow new, more reactive, and selective catalysts to be made. Specifically, we plan to use the emerging technology of metal organic frameworks (MOFs, see left-hand figure for comparison to traditional materials). MOFs are organized,

porous materials (pore is shown with the yellow balls) with a metal node (like nickel or molybdenum) connected by organic linkers. Importantly, the Stowers group is a world's leading expert in converting MOFs to metal oxide catalysts. The best way to think about this is that the MOF serves as a template device. Importantly, the Stowers group and other groups already have preliminary evidence that metal oxides generated through MOF templating generates more reactive metal oxide catalysts than traditional zeolite materials [4-8].

While MOFs are a highly promising material, there are 10,000's of potential MOFs that could be made, and it remains unclear which would give a highly active and highly selective catalyst after removal of the organic linkers. Therefore, we have a 3-pillar approach to the design, synthesis, and experimental testing of new metal oxides made from MOFs. The 3 pillars are: 1) experiment, 2) computer modeling, and 3) data science. Our team's strength dovetails with these pillars. The Stowers (Chemistry) and Argyle (Chemical Engineering) labs have closely collaborated on the ODH reaction employing traditionally made metal oxide catalysts. The unique combination of chemistry and engineering is critical to develop an industrial-type process as well as make fundamental advances. The Ess lab (Chemistry) is expert in atomistic molecular simulations, which can provide key details of structures and transformations of MOFs and resulting metal oxides. The Della Corte (Physics) and Wingate (Computer Science) labs have an established close collaboration that combines atomistic modelling and deep learning. This expertise is key because data science will be used to screen and predict MOF structures, properties, resulting metal oxide catalyst structure, reactivity, and selectivity. A data science approach is necessary because of the massive number of possible MOFs to create and the impossibility of simulating each with molecular modeling.

Research Plan

We propose to develop tools for modeling MOF decomposition that will allow for rational design and prediction of metal oxide catalysts and materials. The decomposed MOFs generally retain a degree of their previous patterned structure, producing materials with higher surface areas and a higher concentration of controlled active sites than obtained in metal oxide catalysts produced through traditional synthetic methods. Further, we will use computationally intensive tools, such as density functional theory (DFT), to train faster models that retain the predictive power of the more complex models at lower computational costs to identify key characteristics of hundreds of models (e.g., atomic charges, band energies, highest occupied molecular orbital (HOMO)/lowest unoccupied molecular orbital (LUMO) gaps that are key characteristics of semiconducting and catalytic materials, and structural features such as surface area, porosity, pore diameter, pore size distribution, etc.). Our approach will be to combine a synergistic effort of experiment, simulation, and data science to: *i*) experimentally synthesize MOFs, induce thermal decomposition for catalyst formation, and test the performance of metal oxide catalysts for alkane dehydrogenation; *ii*) use calculations and simulation to model MOF conversion to metal oxides as well as generate data for machine learning (ML) based analysis of MOFs and metal oxides; and *iii*) develop tools to analyze MOF databases and make predictions for metal oxide properties produced via MOF decomposition. More details regarding these aims are in the following sections.

Expected Outcomes

We expect that this project will have broad benefits beyond the field of catalysis, as these metal oxide materials have far ranging applications including semiconductors, photocatalysts, sensors and gas/energy storage [9, 10]. This research will provide avenues for harnessing the vast library of MOF materials for each application in an efficient and artificially intelligent method. We also expect that our research into metal oxides for ODH reactions will provide a low-cost highly efficient catalyst for ethane to ethylene conversion. Because the ethane to ethylene conversion is the most difficult of the alkane conversions, we also expect that these principles can be applied to other oil refining partial oxidations, such as methane, propane, and other light hydrocarbon conversions to more useful materials.

Project Methodology

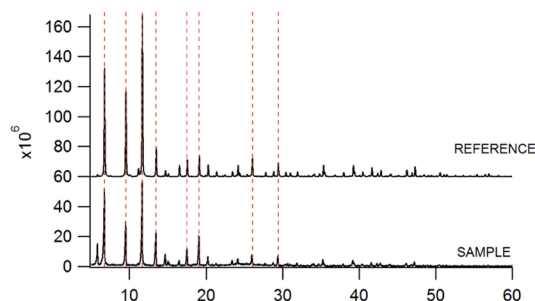


Figure 1: X-ray diffraction patterns. Top: HKUST-1 sample, Bottom: Synthesized HKUST-1 on carbon supports.

at crystal orientations which are consistent with the Cu-analogue of the Ni-MOF. These data demonstrate that we can make and characterize these materials. We will characterize the new materials we make and benchmark them against the published materials prior to decomposition. In addition to single metal oxides, we will study synergistic effects between metals that can increase activity. It is difficult to achieve patterned structured bimetallic metal oxides through traditional methods, but using MOFs allows us to get specifics in properties of the metal oxides. We will build relationships between MOF topologies/properties (e.g. linker composition, linker length, bonding, metal oxidation state, etc.) and the resulting metal oxide structure (surface area, metal geometry and coordination number, oxidation state and composition) through identifying a subset of targeted metal oxides that are catalytically excellent for partial oxidation reactions. These metal oxides will be kinetically evaluated for catalysis of partial oxidation reactions. Through review of the CoRE 2019 MOF database [11], we can target a variety of structures through an analysis of the nodes and linkers and determine which ten structures to target based on their substructures. We will then synthesize the different MOFs and compare the physical and chemical properties with those in the database.

With the MOF-powders synthesized, they will then be decomposed under inert and oxidizing environments comparable to what has been done in other studies. The Cu-based MOF structure (shown in Figure 1) decomposes through release of carbon dioxide and polymerizes the rest of the aromatic carbons. Figure 2 shows the differences in nanoparticle formation for Cu-based MOF upon decompositions under

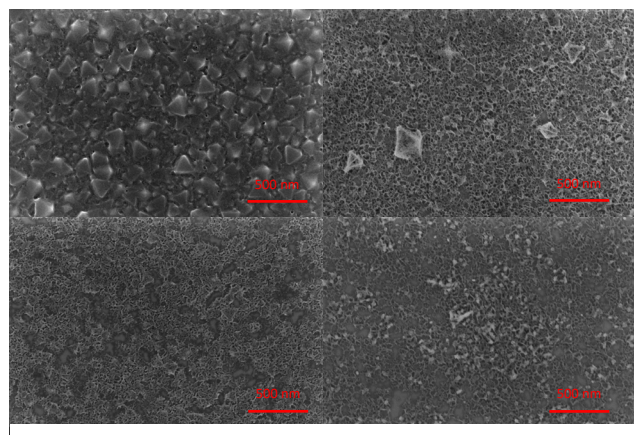


Figure 2: Top left: Undecomposed HKUST-1, Decomposed at 400 °C in, Top right: 70% N₂ 30% O₂, Bottom Left: 80% N₂ 20% O₂, Bottom Right: 90% N₂ 10% O₂.

Aim 1: Parameter collection for catalyst optimization

We will start by synthesizing known MOFs with nickel (Ni), vanadium (V), and molybdenum (Mo) to transform to oxides for partial oxidation reactions as these are the most efficient for conversion of ethane to ethylene. In the database, there are 100's of Ni- and V-based MOFs, but only a handful of Mo-based MOFs. We will use an organic linker similar to all three MOFs, the carboxylate-based aromatic ligand. We have been successful at making the nickel (Ni)- and copper (Cu)-based carboxylate-based organic linker MOFs for different reactions in our lab. Figure 1 shows the X-ray diffraction pattern for a Cu-based MOF showing shifts

different oxygen concentrations. As shown, particle size increases as temperature decreases and surface area stays nearly consistent. These data demonstrate that we have already been able to start work regarding decomposition conditions and characterization. We will decompose the Ni-, V-, Mo-, and other transition metal MOF materials to form metal oxides. Our research will overcome challenges regarding how properties are related to catalyst preparation by categorizing decomposition methods in terms of temperature, atmosphere, and time in order to understand how these variables affect chemical and physical properties of the catalysts.

We will then characterize the physical and chemical properties of the decomposed materials. This information will be used to inform the

computational models and studies regarding decomposition to be done by the computational and modeling part of the team. We will characterize and parameterize known design features that allow prediction of the resulting metal oxide structures from starting MOF topologies. We will also map out the detailed chemical process of MOF conversion to metal oxide catalyst structure. Our use of calculations and simulation to model MOF conversion to metal oxides will generate data for machine learning (ML) based analysis of MOFs and metal oxides. These will result in tools to analyze MOF databases and make predictions for metal oxides. These experiments will provide foundational data for simulation and data science efforts that will provide rational design of new highly active catalysts and other advanced metal oxide materials.

The catalytic testing of materials derived from MOFs will then be completed to determine how the metal sites and surface area properties affect the outcomes of the reaction for partial oxidations. We will also look at oxygen vacancies and Fermi levels and put them in the context of semiconductors in order to categorize these materials to benefit machine learning of future materials. With the catalytic activity of the metal oxides obtained for ODH, we will use the data to identify the most important features needed for designing highly-active catalysts. Machine learning will be used to identify the next 10 targets from the database of >1000 metal-based structures.

We will decompose these MOF structures in two ways: 1) decomposition at the lowest temperature and shortest times to obtain the full metal oxide in an oxidizing environment and 2) decomposition first under an inert nitrogen atmosphere to decompose the carbon ligand structure followed by quick oxidation in an oxidizing atmosphere to obtain the full metal oxide (carbon removal). These derived catalysts will then be characterized for full physical and chemical properties. Following the characterization, catalytic dehydrogenation experiments will be conducted to characterize kinetic analysis of activity. In tandem with catalytic evaluation, all of the before and after characterization will be used to effectively model decomposition of the materials.

Aim 2: Atomistic simulation and property analysis of MOFs and metal oxides

Currently, it is unknown how (i.e., the mechanism) MOFs undergo thermal loss of organic linkers to generate metal oxides. It is very likely that the resulting metal oxide materials formed in this fashion are in a “kinetic trap”, meaning that the metal oxides are not the most stable form. This is important because kinetically formed metal oxides can be highly reactive compared with more thermodynamically stable forms. Therefore, to understand this process and to enable prediction of materials, Ess will use atomistic modeling to examine the exact reaction steps and intermediates that occur during organic linker decomposition. These atomistic simulations will be directly tied to experimental characterization of properties and reactivity by the Stowers and Argyle groups. Importantly, the use of so-called first principles density functional theory (DFT) modeling needs to be benchmarked and compared to reality.

After an initial round of high-level DFT modeling has been completed, and simulations validated, the Ess group will then develop a suite of methods that allow massively faster analysis of reaction mechanisms and prediction of resulting metal oxide structures from starting MOFs. However, even using extremely fast modeling techniques, such as a reactive force field, the Ess group will only be able to simulate and predict the structure and properties of hundreds of materials. Therefore, this initial data generated during year one will provide the basis for developing a robust deep learning model by Della Corte and Wingate. It is likely with complete simulation of several hundred MOF to metal oxide reactions and harvesting of MOF and metal oxide properties for features that a highly accurate and robust machine learning model can be developed.

Aim 3: Machine learning analysis and predictions for rational catalyst design

We aim to explore using ML tools (especially recurrent, deep graph neural networks) to combine the salient features from our simulated data sets with the features of known good catalysts to predict which other MOF structures within the database will also be successful catalysts. After these predictions have been tested, we will use ML for rationally designing a new MOF material that would result in an optimized catalyst. As an important, synergistic research thrust on the ML side, we propose to explore how first-

principles information (including basic knowledge of chemical and quantum processes) can be directly incorporated into ML models to reduce the amount of required data and improve results.

Machine learning is notoriously data hungry; while we can generate large amounts of data from molecular dynamics and DFT simulations, it may still not be enough. As a synergistic research thrust, we will investigate the incorporation of first-principles knowledge into our models, including knowledge of chemical processes, material properties, quantum processes, and material interactions. This knowledge will be incorporated through initialization, objective functions, and architecture design, and could result in a radical reduction in sample complexity. If successful, such a mix of deep learning with domain expertise could have significant impact in other chemistry contexts, as well as other domains such as life sciences or physics.

Schedule

In the first six months of the project, we will make, characterize, and decompose a series of up to 10 representative MOFs. Over the next two months, those MOFs will be decomposed and the decomposition process will be optimized. Over the next four months, these materials will be tested as ODH catalysts. Simultaneously during the first year of the project, the modeling and machine learning tools will be developed to be applied and validated as experimental data are obtained. During the last year of the project, several candidate MOFs identified by machine learning will be made, characterized, decomposed, and tested as ODH catalysts to verify and tune the computational models.

Milestones

- 1: create up to 10 MOFs (expected to be done by six months).
- 2: decompose the MOFs into metal oxides for use as catalysts (expected completion by eight months)
- 3: submission of initial proposal to NSF CBET Catalysis Program (planned in late 2021).
- 4: complete ODH testing (expected completion by twelve months).
- 5: complete simulation of the MOF decomposition process (expected completion by 15 months).
- 6: complete machine learning process to back-predict MOF candidates (expected completion by 18 mo.).
- 7: submission of NSF DMREF proposal in January 2023.
- 8: complete MOF synthesis, decomposition, characterization, ODH testing of several candidate materials identified by machine learning (expected completion by 24 months)

Team Description

Professor Stowers has experience making MOFs, while she and Professor Argyle have closely collaborated on ODH catalysts. Collectively, they have the needed experimental experience to make, characterize, and test both the MOFs and the derived catalysts. Professor Argyle brings needed reactor design and modeling experience. Professor Ess has the required experience with both model catalysts and predictive power for previously unused MOF materials. Professors Della Corte and Wingate have the required experience with atomistic modelling and deep machine learning needed to train a deep learning model for MOFs and their decomposed structures. All five PI's are needed to perform this project that tackles the grand challenge of efficient catalytic ethylene production with broader metal oxide applications to vital areas such as energy production and storage using solid oxide fuel cells or supercapacitors and solar hydrogen production through water splitting on tuned band gap semiconductors [10, 11].

Expected Research Outcomes

The combination of experiment, simulation, and machine learning will provide a general understanding of metal oxide catalyst structure resulting from thermal decomposition of MOF templates. The correlation of derived metal oxides to kinetic catalytic properties will also provide pathways for rational design of high-performance catalysts predicted from available MOF materials. Ultimately, these benchmarking studies will be coupled with ML to perform faster, more efficient, neuralnetwork based searches of MOF databases and eventually predict new MOF structures that are not in current databases.

Budget and Budget Narrative

	Year 1	Year 2	Total
Supplies	\$6,849	\$10,296	\$17,145
Salaries			
Graduate	\$54,000	\$27,810	\$81,810
Post-doctoral researcher	\$6,000	\$12,000	\$18,000
Travel	\$1,500	\$1,545	\$3,045
Totals	\$68,349	\$51,651	\$120,000

Supplies include MOF precursor chemicals in year 1 (e.g., 500 g vanadium oxychloride, 99.9% purity; 250 g titanium tetrachloride, 99.9%; 10 g molybdenum chloride, 99.99%; and 100 g 2,6-naphthalenedicarboxylic acid, 95%; all prices from Sigma Aldrich), reactant and gas chromatograph gases (2 cylinders ethane, 99.99%; 2 cylinders C₂H₆, 2 cylinders O₂, 6 cylinders UHP He, 6 cylinders in Year 1 and double that amount in Year 2; all prices from AirGas), and miscellaneous glassware and laboratory consumables (e.g., flasks, filter paper, stoppers, rubber gloves, estimated at \$1200/year) in both years. All values carried over to Year 2 have been escalated at a 3% inflation rate.

Two graduate students (at \$27,000/year) will be funded by the project, one for one year in the Wingate and Della Corte labs and one for both years in the Stowers and Argyle labs. A portion of a post-doctoral researcher will be funded in the Ess lab.

Travel is to allow one Principal Investigator or student travel to a national conference, such as the American Chemical Society or the American Institute of Chemical Engineers annual meeting, to present results each year.

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Plans for external funding

The National Science Foundation (NSF) Division of Chemical, Bioengineering, Environmental and Transport (CBET) Systems Catalysis Program maintains an open call for proposals that we will target in late 2021. As is typical for the NSF, proposals are generally only successful with sufficient preliminary data. Therefore, the IDR funding is crucial for our efforts to develop this needed preliminary data. The available funding is typically ~\$500,000 for a period of performance of three years. Writing this proposal will serve as a foundation for a larger funding opportunity, discussed next.

The NSF also has a multi-disciplinary program called Designing Materials to Revolutionize and Engineer our Future (DMREF). This program has a biennial request for proposals that is next open in early 2023. It is ideally suited to our team because it requires materials discovery through both experiment and simulation. IDR funding would allow our team to collect the needed preliminary results and proof of concept to secure this ~\$1.8 million funding opportunity with a four year period of performance. Importantly, to secure this type of high-level funding, a full two years of preliminary data from our team and coauthor publications is required. Therefore, IDR funding in 2021 is the correct time to target the 2023 DMREF submission.

Proposal Timeline:

Proposal	1Q21	2Q21	3Q21	4Q21	1Q22	2Q22	3Q22	4Q22	1Q23
NSF CBET Catalysis Program									
NSF CBET Catalysis Program (resubmission, if required)									
NSF DMREF									

Biographical Sketches

Curriculum Vitae: **Morris D. Argyle**
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Education and Training

University of California at Berkeley, Chemical Engineering, Ph.D.,	2003
Brigham Young University, Chemical Engineering, B.S.	1990

Research and Professional Experience

Associate Professor, Chemical Engineering Department, Brigham Young University	8/2009-present
Department Head, University of Wyoming, Dept. of Chemical and Petroleum Eng.	7/2008-6/2009
Associate Professor, University of Wyoming, Dept. of Chemical and Petroleum Eng.	7/2008-6/2009
Assistant Professor, University of Wyoming, Dept. of Chemical and Petroleum Eng.	9/2003-6/2008
Technical & Process Supervisor; Operations Support & Design Engineer, Exxon Co. USA	1990-1998
Professional Engineer , Texas License Number 82571	1996—present

Publications (11 shown of 56 peer reviewed, archival journal publications; 1 book chapter, 2 edited books)

- M. D. Argyle, K. D. Chen, A. T. Bell, E. Iglesia, "Effect of Catalyst Structure on Oxidative Dehydrogenation of Ethane and Propane on Alumina-Supported Vanadia." *Journal of Catalysis*, 208, 139-149, 2002. <http://dx.doi.org/10.1006/jcat.2002.3570>
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- M. D. Argyle, C. Krebs, C. Resini, K. D. Chen, A. T. Bell, E. Iglesia, "Quantification of Reduced Centers in Metal Oxide Catalysts during Propane Oxidative Dehydrogenation Using UV-visible Spectroscopy." *Chemical Communications*, 2082-2083, 2003. <http://dx.doi.org/10.1039/B305264H>
- T. Waku, M. D. Argyle, A. T. Bell, E. Iglesia, "Effects of O₂ Concentration on the Rate and Selectivity in Oxidative Dehydrogenation of Ethane Catalyzed by Vanadium Oxide: Implications for O₂ Staging and Membrane Reactors." *Industrial & Engineering Chemistry Research*, 42, 5462-5466, 2003. <http://dx.doi.org/10.1021/ie0304661>
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- J. L. Park, K. A. Canizales, M. D. Argyle, B. F. Woodfield, K. J. Stowers. “The effects of doping alumina with silica in alumina-supported NiO catalysts for oxidative dehydrogenation of ethane.” *Microporous and Mesoporous Materials*, 293, 109799, 2020. <https://doi.org/10.1016/j.micromeso.2019.109799>
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- M. D. Argyle, C. H. Bartholomew, “Heterogeneous Catalyst Deactivation and Regeneration: A Review.” *Catalysts*, 5, 145-269, 2015. <http://dx.doi.org/10.3390/catal5010145>
- B. B. Hallac, K. Keyvanloo, K., J. D. Hedengren, W. C. Hecker, M. D. Argyle, “An optimized simulation model for iron-based Fischer-Tropsch catalyst design: Transfer limitations as functions of operating and design conditions.” *Chem. Eng. J.* 263, 268-279, 2015. <http://dx.doi.org/10.1016/j.cej.2014.10.108>
- M. Rahmati, M.-Saeed Safdari, T. H. Fletcher, M. D. Argyle, C. H. Bartholomew. “Chemical and Thermal Sintering of Supported Metals with Emphasis on Cobalt Catalysts During Fischer–Tropsch Synthesis.” *Chemical Reviews*, 120, 4455-4533, 2020. <https://dx.doi.org/10.1021/acs.chemrev.9b00417>
- M. Rahmati, B. Huang, M. K. Mortensen, Jr., T. H. Fletcher, B. F. Woodfield, W. C. Hecker, M. D. Argyle, “Effect of Different Alumina Supports on Performance of Cobalt Fischer-Tropsch Catalysts.” *Journal of Catalysis*, 359, 92-100, 2018. <https://doi.org/10.1016/j.jcat.2017.12.022>.

Patents

Co-inventor on 6 US and 1 European Patents

Research Supervision and Mentoring

Currently supervising 5 undergraduate researchers

Previously supervised 5 PhD, 6 MS, and 35 undergraduate researchers

Previous Research Funding

Principal Investigator or Co-Principal Investigator on 12 externally funded grants totaling ~\$3.2 million and 3 internally funded grants totaling \$55,000.

Synergistic Activities

Leader of the BYU Fischer-Tropsch Consortium.

Technical consultant for Cosmas Inc., a company involved in nanoparticle and catalyst manufacture.

Rocky Mountain Catalysis Society Director, 2018-present. President, 2012-2018. Secretary/Treasurer, 2009-2012.

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Research and Professional Experience

Assistant Professor of Chemistry <i>Brigham Young University, Provo, UT</i>	2014-present
Postdoctoral Fellow <i>Harvard University, Cambridge, MA</i>	2012-2014

Education and Training

Doctor of Philosophy in Chemistry, Organic Chemistry	2008-2012
Master of Science in Chemistry <i>University of Michigan-Ann Arbor Ann Arbor, MI</i>	2006-2008
Bachelor of Science in Chemical Engineering	2002-2006
Bachelor of Science in Chemistry <i>University of Utah, Salt Lake City, UT</i>	2002-2006

Publications (12 most relevant shown of 21 peer reviewed, archival journal publications)

- Nguyen-Sorenson, A. H. T.; Wu, Y.; Orcutt, E. K.; Kent, R. V.; Anderson, H. C.; Matzger, A. J.; Stowers, K. J.* Energetic decomposition yields efficient bimetallic Cu MOF-derived catalysts. *J. Mater. Chem. A*, 2020, 8, 15066-15073
- Park, J. L.; Canizales, K. A.; Argyle, M. A.; Woodfield, B. F.; Stowers, K. J.* "The effects of doping alumina with silica in alumina-supported NiO catalysts for oxidative dehydrogenation of ethane." *Micro. Meso. Mater.* **2019**, 293, 109799.
- Zhou, Z.; Orcutt, E. K.; Anderson, H. A.; Stowers, K. J.* "H₂ surface modification of a carbon nanotube catalyst for the improvement of ethane oxidative dehydrogenation" *Carbon* **2019**, 152, 924-931.
- Nguyen-Sorenson, A. H. T.; Anderson, C. M.; Balijepalli, S. K.; McDonald, K. A.; Matzger, A. J.; Stowers, K. J.* "Highly active copper catalyst obtained through rapid MOF decomposition" *Inorg. Chem. Front.* **2019**, 6, 521-526.
- Zhou, Z.; Balijepalli, S. K.; Nguyen-Sorenson, A.; Anderson, C. M.; Park, J. L.; Stowers, K. J.* "Steam stable covalently-bonded polyethyleneimine modified multiwall carbon nanotubes for carbon dioxide capture" *Energy Fuels* **2018**, 32, 11701-11709.
- Park, J. L.; Balijepalli, S. K.; Argyle, M. A.; Stowers, K. J.* Low Temperature Oxidative Dehydrogenation of Ethane by Ce-Modified NiNb Catalysts *Ind. Eng. Chem. Res.*, **2018**, 57, 5234-5240 (*Invited article*)

- Zhou, Z.; Anderson, C. M.; Butler, S. K.; Thompson, S. K.; Whitty, K. J.; Shen, T.-C.; Stowers, K. J.* Stability and efficiency of CO₂ capture using linear amine polymer modified carbon nanotubes. *J. Mater. Chem. A*, **2017**, 5, 10486-10494
- Zugic, B.; Karakalos, S.; Stowers, K. J.; Biener, M.M.; Biener J.; Friend, C. M.; Madix, R. J. Continuous Catalytic Production of Methyl Acrylates from Unsaturated Alcohols by Gold: The Strong Effect of C=C Unsaturation on Reaction Selectivity. *ACS Catalysis*, **2016**, 6, 1833-1839.
- Karakalos, S.; Zugic, B.; Stowers, K. J.; Biener, M.M.; Biener J.; Friend, C. M.; Madix, R. J. Catalytic production of methyl acrylates by gold-mediated cross coupling of unsaturated aldehydes with methanol. *Surf. Sci.*, **2016**, 652, 58-66.
- Stowers, K. J.; Biener, M.M.; Biener J.; Friend, C. M.; Madix, R. J. Facile Ester Synthesis on Ag-Modified Nanoporous Au: Oxidative Coupling of Ethanol and 1-Butanol under UHV Conditions. *Cat. Lett.*, **2015**, 6, 1217-1223.
- Wang, L.C.; Stowers, K. J.; Zugic, B.; Personick, M. J.; Biener, M.M.; Biener J.; Friend, C. M.; Madix, R. J. Exploiting basic principles to control the selectivity of the vapor phase catalytic oxidative cross-coupling of primary alcohols over nanoporous gold catalysts. *J. Catal.*, **2015**, 329, 78-86.
- Wang, L.C.; Stowers, K. J.; Zugic, B.; Baumer, M.; Biener, M.M.; Biener J.; Friend, C. M.; Madix, R. J. Methyl ester synthesis catalyzed by nanoporous gold: from 10⁻⁹ Torr to 1 atm. *Cat. Sci. Tech.*, **2015**, 5, 1299-1306.

Previous Research Funding

Principal investigator of Co-Principal Investigator on 4 externally funded grants totaling ~\$900,000 and 1 internally funded grant totaling \$19,000

Research Supervision and Mentoring

Currently supervising 2 graduate students and 5 undergraduate researchers
Previously supervised 3 PhD, 1 MS, and 21 undergraduate researchers

Synergistic Activities

Grant Reviewer, National Science Foundation, ACS Petroleum Research Fund 2016-present

Journal Article Reviewer 2011-Present

Journal of the American Chemical Society, Organic Letters, Surface Science, Catalysis Science and Technology, Journal of Materials Chemistry A, Applied Catalysis A: Gen, Applied Catalysis B: Env, ACS Catalysis, Journal of Materials Science, Industrial and Chemical Engineering Research, Carbon, Surface Science Reports, ChemCatChem

Chem Camp Co-Director 2015-2019

NSF Biochemistry and Chemistry BYU REU Site Director 2017-present

DANIEL H. ESS

Professor

Department of Chemistry and Biochemistry

Brigham Young University

<https://esslab.byu.edu/>

E-mail: dhe@chem.byu.edu

EDUCATION

Ph.D. Comp. Chemistry

University of California, Los Angeles (9/03-10/07)

Advisor: K. N. Houk

B.S. Biochemistry

Brigham Young University, Provo, Utah (2000)

PROFESSIONAL POSITIONS

Professor

Brigham Young University, Provo Utah (9/20-present)

Associate Professor

Brigham Young University, Provo Utah (9/16-9/20)

Assistant Professor

Brigham Young University, Provo Utah (7/10-8/16)

Postdoctoral Scholar

University of North Carolina at Chapel Hill (10/09-6/10)

Comp. Inorganic

Advisors: Cynthia K. Schauer and Thomas J. Meyer

Postdoctoral Scholar

The Scripps Research Institute, Florida (10/07-10/09)

Comp. & Experimental Catalysis

Advisor: Roy A. Periana

California Institute of Technology (10/07-10/09)

Advisor: William A. Goddard, III

CURRENT AWARDS (Total for all awards = \$3,100,876)

- *National Science Foundation*, “Dynamical Organometallic Mechanisms” CHE-1952420 (PI, 2020-2023) \$265,338
- *Chevron Phillips Chemical Co.*, “Design of Homogeneous Alpha Olefin Catalysts” (PI, 2014-2021) \$710,000
- *Phillips 66*, “Computational Optimization of Solid Acid Metal-Organic Frameworks” (PI, 2019-2021) \$217,519
- *National Science Foundation*, “Theory and Design of Transition-Metal Heterodinuclear and Homodinuclear Catalytic Reactions” CHE-1764194 (PI, 2018-2021) \$234,205
- *National Science Foundation*, “Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career” CHE-1757627 (PI, 2018-2021) \$331,950; renewal (PI, 2021-2024) CHE-2050872 \$371,250
- *U.S. Department of Energy, Office of Basic Energy Sciences, Catalysis Sciences*, “Theory of Main-Group, p-Block Hydrocarbon Functionalization Reactions” (PI, 2017-2020) and renewal “Modeling and Design of Main-Group Metal Catalyzed Alkane C-H Functionalization Reactions” (PI, 2020-2023) DE-SC0018329 \$343,312
- *National Institutes of Health, NIGMS*, “Asymmetric N-H/N-alkyl olefin aziridinations and ring-opening transformations” 1R35GM136373- 01 (subcontract, 2020-2025) \$160,720

SOFTWARE DEVELOPMENT

<https://esslab.byu.edu/software>

- Milo: a quasiclassical direct dynamics program (Python). C++ version also available.
- MECPro: Efficient Python program to locate minimum energy crossing points for organometallic reactions.

EXTERNAL SERVICE HIGHLIGHTS

- Guest editor for *Chemical Reviews* Volume 119, Issue 11 on “Computational Design of Catalysts from Molecules to Materials”. Authored editorial: <https://doi.org/10.1021/acs.chemrev.9b00296>.
- Reviewer of >300 journal articles. Example of journals are: *Science*, *Nature*, *Nature Chemistry*, *Nature Catalysis*, *Journal of the American Chemical Society*, *Chemical Science*, *ACS Catalysis*, *Inorganic Chemistry*, *Journal of Physical Chemistry*, and *Organometallics*.

BYU AWARDS

- Karl G. Maeser Research and Creative Arts Award (2019)
- Richard Roskelly Teaching and Learning Fellowship (2017-2018)
- BYU Young Scholar Award (2015)
- BYU College of Physical and Mathematical Sciences Young Scholar Award (2014)

BYU PUBLICATION STATISTICS & HIGHLIGHTS

- h-index = 40; i10-index = 86 (Google Scholar for all publications on 11/08/2020)
- Total publications = 134
- BYU publications = 103
- Total senior author/corresponding author publications = 76
- *Science* publications = 3
- Publications with impact factor >8 = 35
- Publications with graduate students = 38
- Publications with undergraduate coauthors = 33

EXAMPLE ISSUED PATENT (Total 4)

Bischof, S. M.; Kilgore, U. J.; Sydora, O. L.; Ess, D. H.; Fuller, III, J. T.; Kwon, D.-H. “Fluorinated N2-Phosphinyl Amidine Compounds, Chromium Salt Complexes, Catalyst Systems, and Their Use to Oligomerize Ethylene” (with Chevron Phillips Chem. Co. LP) US 10,493,442 B2. Issued 12/03/2019.

Ess, D. H.; Falck, J. R. Jat, J. L. Kürti, L. “Direct Stereospecific Synthesis of Unprotected Aziridines from Olefins” US 9,988,349 B2. Issued 06/05/2018.

EXAMPLE BYU PUBLICATIONS

132. Smith, J. A.; Schouten, A.; Wilde, J. H.; Westendorff, K. S.; Dickie, D. A.; Ess, D. H.*; Harmen, W. D. “Experiments and Direct Dynamics Simulations Reveal a Network of Reaction Pathways for Tungsten η^2 -Arene - Aryl Hydride Equilibria” *J. Am. Chem. Soc.* **2020**, *142*, 16437-16454. <https://doi.org/10.1021/jacs.0c08032>

129. Maley, S. M.; Kwon, D.-H.; Rollins, N.^A; Stanley, J. C.; Sydora, O. L.; Bischof, S. M.; Ess, D. H.* “Quantum-Mechanical Transition-State Model Combined with Machine Learning Provides Catalyst Design Features for Selective Cr Olefin Oligomerization” *Chem. Sci.* **2020**, 9665-9674. <https://doi.org/10.1039/D0SC03552A>

126. Rollins, N.; Pugh, S. L.; Maley, S. M.; Grant, B. O.; Hamilton, S. R.; Teynor, M. S.; Carlsen, R.; Jenkins, J. R., Ess, D. H.* “Machine Learning Analysis of Direct Dynamics Trajectory Outcomes for Thermal Deazetization of 2,3-Diazabicyclo[2.2.1]hept-2-ene” *J. Phys. Chem. A* **2020**, *124*, 4813-4826. <https://doi.org/10.1021/acs.jpca.9b10410>

3332 TMCB
Department of Computer Science
Brigham Young University
Provo, UT 84602

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Cell: (508) 808-0619
Office: (801) 422-6350
Homepage: <http://pcc.cs.byu.edu/>

Education

Ph.D. Computer Science, University of Michigan. April, 2008.
M.S. Computer Science, Brigham Young University. April, 2004.
B.S. Computer Science, Brigham Young University. December, 2002.

Research Experience

Assistant Professor, BYU
Director, Lyric Labs, ADI
Research Scientist, Lyric Labs, ADI
Research Scientist, MIT
Postdoctoral Research Associate, MIT
Research Fellow, University of Michigan

August 2015 - Present
July 2014 - August 2015
May 2012 - July 2014
June 2010 - May 2012
Jan. 2008 - June 2010
Aug. 2004 - Dec. 2007

Most Relevant Publications

- [1] Z. Brown, N. Tibbetts, D. Wingate and N. Fulda. Towards Neural Programming Interfaces. NeurIPS, 2020.
- [2] A. Carr and D. Wingate. Wasserstein Neural Processes. NeurIPS Workshop on Optimal Transport, 2019.
- [3] Iris Seaman, Jan-Willem van de Meent, David Wingate. Modeling Theory of Mind for Autonomous Agents with Probabilistic Programs. ICML Workshop on Imitation, Intent, and Interaction (oral), 2019.
- [4] Iris Seaman, Jan-Willem van de Meent, David Wingate. Modeling Theory of Mind for Autonomous Agents with Probabilistic Programs. ICML Workshop on Generative Modeling and Model-Based Reasoning for Robotics and AI, 2019.
- [5] Chandramouli Nyshadham, Matthias Rupp, Brayden Bekker, Alexander V Shapeev, Tim Mueller, Conrad W Rosenbrock, Gabor Csanyi, David Wingate, Gus LW Hart. Machine-learned multi-system surrogate models for materials prediction. npj Computational Materials, 5:1, pg 1-6, 2019.
- [6] P Hyatt, D Wingate, MD Killpack. Model-based Control of Soft Actuators Using Learned Nonlinear Discrete-time Models. Frontiers in Robotics and AI 6, 22, 2019.
- [7] Chandramouli Nyshadham, Matthias Rupp, Brayden Bekker, Alexander Shapeev, Tim Mueller, Conrad Rosenbrock, Gabor Csanyi, David Wingate, Gus Hart. General machine learning models for materials prediction. Bulletin of the American Physical Society, 63, 2018.
- [8] N. Fulda, T. Etchart, W. Myers, D. Ricks, Z. Brown, J. Szendre, B. Murdoch, A. Carr and D. Wingate. BYU-EVE: Mixed-Initiative Dialog via Structured Knowledge Graph Traversal and Conversational Scaffolding. Alexa Prize Proceedings, 2018.

Patents

2020 Focused capacitive sensing. D Wingate. US Patent 10,684,728
2020 Portless and membrane-free microphone. D Wingate, IC Novet. US Patent 10,547,953
2019 Audio processing using an intelligent microphone. D Wingate. US Patent 10,269,343
2016 Signal source separation. D Wingate, N Stein. US Patent 9,460,732
2016 Time-frequency directional processing of audio signals. N Stein, J Traa, D Wingate. US Patent 9,420,368
2016 Microphone calibration. J Ranieri, D Wingate, ND Stein. US Patent 9,232,332
2016 Apparatus, systems, and methods for calibration of microphones. J Ranieri, D Wingate, ND Stein. US Patent 9,232,333

Professional Activities

- Workshops co-chair and senior program committee, AAAI 2017, AAAI 2018
- Associate Editor, IROS 2017
- NSF Robust Intelligence panel reviewer, 2017, 2018, 2020
- Area Chair, ICML 2009, ICML 2014, ICML 2015
- Co-organizer, 2012 AAAI Spring Symposium: “Designing Intelligent Robots: Reintegrating AI” (with George Konidaris, Sarah Osentoski, Todd Hester, Stephen Hart and Byron Boots)
- Co-organizer, 2011 ICML Workshop on Planning and Acting with Uncertain Models (with Finale Doshi-Velez)
- General chair, 2009 Reinforcement Learning Competition
- Co-organizer, NIPS 2006 Workshop on Grounding Perception, Knowledge and Cognition in Sensori-Motor Experience (with Brian Tanner and Michael James).
- Conference and journal reviewing / program committee member
JMLR{05,06,07,08,09,10,11,14}, ML{08,10,10}, AAAI{05,07,08,10,16,17,20}, ICRA16, PEERJ15, ICML{07,08,09,11,12,13,14,16,17,18,20}, NECO, NWO, IJCAI07, ECML09, RSS10, AISTATS{11,12,17}, UAI11, NeurIPS{05,07,08,09,10,11,12,13,14,15,16,17,18,19,20}, ICLR17,20, CORL17.

Honors and Grants

2020 Class of 1949 BYU Young Scholar of the Year
NSF EFRI, 2019; \$2M grant (\$1M to BYU; \$500k to my lab)
Alexa Prize 2018 semi-finalist; \$250k grant
DARPA PPAML, 2017 - \$500k; sole PI
NSF CUAS, 2016-2017 - \$90k
Internal funding - \$30k
External gifts - \$515k
Best poster award, *International Joint Conference on Artificial Intelligence (IJCAI)*, 2011
Best paper award, *International Conference on Autonomic Computing and Communications (ICAC)*, 2010
NSF Graduate Research Fellow, 2004-2007
Best paper award, *International Conference on Machine Learning and Applications (ICMLA)*, 2003

Biographical Sketch

Dr. Dennis Della Corte
Brigham Young University, Department of Physics and Astrophysics,
N361 ESC, Provo UT 84602, Phone (801) 494-6827, E-mail dennis.dellacorte@byu.edu

Professional Preparation

TU Dortmund/University of Utah	Physics	B.S. (2008-2011)
Heinrich Heine Universität Düsseldorf	Medical Physics	MS (2011-2012)
FH Aachen	Biomedical Engineering	MS (2014-2017)
Forschungszentrum Jülich / Stanford University	Biophysics	Dr.rer.nat (2012-2015)
Bayer Business Services GmbH	Senior Project Manager	2016-2018

Academic Appointments

Assistant Professor of Chemistry (Brigham Young University, 2018-today)

Publications Most Closely Related to the Proposed Project

1. Della Corte D, van Beek HL, Syberg F, et al. Engineering and application of a biosensor with focused ligand specificity. *Nature communications*. 2020;11(1):1-11.
2. Billings WM, Hedelius B, Millicam T, Wingate D, Della Corte D. ProSPR: Democratized Implementation of AlphaFold Protein Distance Prediction Network. *BioRxiv*. 2019:830273.
3. Coates T, Young N, Jarrett A, Morris JC, Moody J, Della Corte D. Current Computational Methods for Enzyme Design. *Modern Physics Letters B* (accepted). 2020.
4. Morris JC, Della Corte D. Using molecular docking and molecular dynamics to investigate protein-ligand interactions. *Modern Physics Letters B* (accepted). 2020.
5. Stern KL, Smith MS, Billings WM, et al. Context-dependent stabilizing interactions among solvent-exposed residues along the surface of a trimeric helix bundle. *Biochemistry*. 2020;59(17):1672-1679.
6. Billings W, Morris C, Della Corte D. The Whole is Greater than its Parts--Ensembling Improves Protein Contact Prediction. *Authorea Preprints*. 2020. (under review)
7. Coupling an Ensemble of Homologues Improves Refinement of Protein Homology Models André Wildberg, Dennis Della Corte, and Gunnar F. Schröder *J. Chem. Theory Comput.* 11 (12), 5578-5582 (2015).
8. Protein structure refinement with adaptively restrained homologous replicas, Dennis Della Corte, André Wildberg, and Gunnar F. Schröder, Eleventh Meeting on the Critical Assessment of Techniques for Protein Structure Prediction (September 2016). *Proteins: Struct., Funct., Bioinf.* 84 (S1), (2015).
9. Integrated NMR, Fluorescence and MD Benchmark Study of Protein Mechanics and Hydrodynamics, Christina Möckel, Jakub Kubiak, Oliver Schillinger, Ralf Kuehnemuth, Dennis Della Corte, Gunnar F. Schröder, ... (4 other authors). *J. Phys. Chem. B*, (2018).

Current and pending support

Investigator: Morris D. Argyle			
Support:	<input type="checkbox"/> Current	<input checked="" type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: Tritium Combustion Kinetics [Professor Larry Baxter in BYU Chemical Engineering is PI, Argyle is co-			
Overlap Statement: There is no overlap with the current proposal.			
Source of Support: Savannah River National Laboratory			
Total Award Amount: \$250,000		Total Award Period Covered: July 2021-June 2023	
Location of Project: Provo, UT			
Person-Months Per Year Committed to the Project.		Cal:	Acad: Sumr: 0.5
Support:	<input checked="" type="checkbox"/> Current	<input type="checkbox"/> Pending	<input type="checkbox"/> Submission Planned in Near Future
Project/Proposal Title: DOE SRNL 0000395264 [Professor Larry Baxter in BYU Chemical Engineering is PI, Argyle is co-PI]			
Overlap Statement: There is no overlap with the current proposal.			
Source of Support: Savannah River National Laboratory			
Total Award Amount: \$135,537		Total Award Period Covered: Sept. 2018-August 2021	
Location of Project: Provo, UT			
Person-Months Per Year Committed to the Project.		0	Cal: Acad: Sumr: 1

Investigator:

Kara Stowers—no current or pending support

Daniel H. Ess

Active

Project Title: Design of Homogeneous Alpha Olefin Catalysts

Source of Support: Chevron Phillips Chemical Co. LP

Role: PI

Total Costs: \$710,000

Starting Date: 01/01/2014

Ending Date: 12/31/2021

Person-months Per Year Committed to the Project: 1.0 for all years

Project goals: The goal of this work is to use computational methods to design new transition metal catalysts for ethylene oligomerization.

Project Title: Theory of Main-Group, p-Block Hydrocarbon Functionalization Reactions and Modeling and Design of Main-Group Metal Catalyzed Alkane C-H Functionalization Reactions

Source of Support: Basic Energy Sciences, Department of Energy (DOE) Office of Science.

Role: PI

Total Costs: \$343,312

Starting Date: 09/15/2017

Ending Date: 09/14/2023

Person-months Per Year Committed to the Project: 1.0 for years 2 and 3

Project goals: The goal of this work is to use computational methods to examine the mechanisms and reactivity of main-group p-block metals to promote conversion of C-H bonds to C-O bonds.

Project Title: Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career

Source of Support: National Science Foundation

Role: PI

Total Costs: \$331,950

Starting Date: 03/2018

Ending Date: 02/2021

Person-months Per Year Committed to the Project: 0.0

Project goals: The goal of this work is to host visiting summer undergraduate students for a research experience.

Project Title: Theory of Transition-Metal Dinuclear Catalyzed Reactions

Source of Support: National Science Foundation

Role: PI

Total Costs: \$234,205

Starting Date: 09/01/2018

Ending Date: 08/31/2021

Person-months Per Year Committed to the Project: 1.0 for years 2 and 3

Project goals: The goal of this work is to use DFT methods to examine the mechanisms and reactivity of dinuclear catalyzed organic transformations and compare them to monometallic catalyzed reactions.

Project Title: Computational Optimization of Acids

Annual Direct Costs: Phillips 66

Role: PI

Total Award Amount: \$217,519

Starting Date: 06/01/2019

Ending Date: 12/31/2021
Person-months Per Year Committed to the Project: 0.0
Project goals: The goal of this work is to use computational methods to examine acids for petrochemical organic transformations.

Project Title: Dynamical Organometallic Mechanisms
Source of Support: National Science Foundation
Role: PI
Total Costs: \$265,338
Proposed Starting Date: 09/01/2020
Proposed Ending Date: 08/31/2023
Person-months Per Year Committed to the Project: 1.0 for years 2 and 3
Project goals: The goal of this work is to develop and apply computational methods to the direct dynamics trajectories of organometallic reactions.

Project Title: R35GM136373 (subcontract)
Source of Support: NIH (subcontract through Rice University; Kurti is PI)
Role: Subcontractor
Total Costs: \$160,720
Proposed Starting Date: 01/01/2020
Proposed Ending Date: 12/31/2025
Person-months Per Year Committed to the Project: 1.0 for all years

Pending Support

Project Title: Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career
Source of Support: National Science Foundation
Role: PI
Annual Direct Costs: \$371,250
Starting Date: 09/2021
Ending Date: 08/2024
Person-months Per Year Committed to the Project: 0.0
Project goals: The goal of this work is to host visiting summer undergraduate students for a research experience.

Project Title: R15 GM143721-01 (subcontract)
Source of Support: NIH (subcontract through Utah State University; Liu is PI)
Role: Subcontractor
Total Costs: \$133,499
Proposed Starting Date: 04/01/2021
Proposed Ending Date: 3/31/2024
Person-months Per Year Committed to the Project: 0.25 for all years
Project goals: The goal of this work is use quantum mechanical calculations to investigate reaction mechanisms and predict new reagents and reactions for electrocatalytic cross-coupling reactions.

Projects/Proposals

1.*Project/Proposal Title :

*Status of Support : Current Pending Submission Planned Transfer of Support

Proposal/Award Number (if available):

*Source of Support:

*Primary Place of Performance :

Project/Proposal Start Date (MM/YYYY) (if available) :

Project/Proposal End Date (MM/YYYY) (if available) :

*Total Award Amount (including Indirect Costs): \$

*Person-Month(s) (or Partial Person-Months) Per Year Committed to the Project

*Year (YYYY)	*Person Months (##.##)	Year (YYYY)	Person Months (##.##)
1.		4.	
2.		5.	
3.			

2.* Project/Proposal Title :

*Status of Support : Current Pending Submission Planned Transfer of Support

Proposal/Award Number (if available):

*Source of Support:

*Primary Place of Performance :

Project/Proposal Start Date (MM/YYYY) (if available) :

Project/Proposal End Date (MM/YYYY) (if available) :

*Total Award Amount (including Indirect Costs): \$

*Person-Month(s) (or Partial Person-Months) Per Year Committed to the Project

*Year (YYYY)	*Person Months (##.##)	Year (YYYY)	Person Months (##.##)
1.		4.	
2.		5.	
3.			

Projects/Proposals

3.*Project/Proposal Title :

*Status of Support : Current Pending Submission Planned Transfer of Support

Proposal/Award Number (if available):

*Source of Support:

*Primary Place of Performance :

Project/Proposal Start Date (MM/YYYY) (if available) :

Project/Proposal End Date (MM/YYYY) (if available) :

*Total Award Amount (including Indirect Costs): \$

*Person-Month(s) (or Partial Person-Months) Per Year Committed to the Project

*Year (YYYY)	*Person Months (##.##)	Year (YYYY)	Person Months (##.##)
1.		4.	
2.		5.	
3.			

4.* Project/Proposal Title :

*Status of Support : Current Pending Submission Planned Transfer of Support

Proposal/Award Number (if available):

*Source of Support:

*Primary Place of Performance :

Project/Proposal Start Date (MM/YYYY) (if available) :

Project/Proposal End Date (MM/YYYY) (if available) :

*Total Award Amount (including Indirect Costs): \$

*Person-Month(s) (or Partial Person-Months) Per Year Committed to the Project

*Year (YYYY)	*Person Months (##.##)	Year (YYYY)	Person Months (##.##)
1.		4.	
2.		5.	
3.			

Current and Pending Support for Dr. Dennis Della Corte, BYU

Support: Current

Project/Proposal Title: Predictive Structure-based Guidelines for Identifying Optimal PEGylation Sites within Proteins and Understanding the Context-Dependence of Non-covalent Interaction Strength

Source of Support: NIH

Total Award Amount: \$435,751

Total Award Period Covered: 4/1/2020-3/31/2023

Person-Months Per Year Committed to the Project:

Cal: 0.0 Acad: 0.0 Sumr: 1.0

Support: Pending

Project/Proposal Title: DMREF: GOALI: Platform to Discover and Tune Enzymatic Degradation of Conventional Polymers

Source of Support: NSF

Total Award Amount: \$1,800,000

Total Award Period Covered: 9/1/2021-8/31/2025

Person-Months Per Year Committed to the Project:

Cal: 0.0 Acad: 0.0 Sumr: 1.0