

# **Chemical Engineering**

#### **UNIVERSITY** OF **WYOMING**

### www.uwyo.edu/ceas

**Chemical Engineering Newsletter** 

# **Message from the Head:**

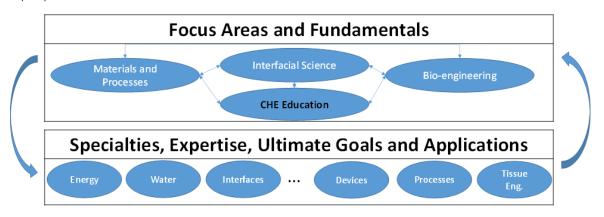
This is my first year as Head of the Department of Chemical Engineering (CHE) at the University of Wyoming. This is a privilege that I do not take lightly. CHE has a long history, but functioned as the Department of Chemical and Petroleum Engineering for 22 years. Since 2015, the two programs operate independently. Coincidentally, I also celebrated my 10<sup>th</sup> year on campus in September. We count with an enthusiastic group of colleagues and staff who embrace change as a way to substantiate healthy growth. Student enrollment comprises 208 undergrads, 10 Masters and 22 PhD students mentored by 9 faculty. The department teaches all the core courses, including traditional Engineering and Science content such as Fluid Dynamics. This is a departure from the College ES program. The un-



October 2016

ronmental Engineering and Graduate School Preparation. Undergrads can pursue a pre-med option as well as minors. Our curriculum is being remapped to enhance hands-on experience starting in the sophomore year (active-classroom model). We launched initiatives to highlight an underlying culture of excellence in teaching, research and service. As a group, we developed departmental research focus areas (see below).

We are actively recruiting undergraduate students. Our first Webinar will be held on October 7, 2016 from 8:30-9:30 am (MST); Link: <u>https://wyocast.uwyo.edu/WyoCast/Play/dee4fecbdbcc411a8fc5f2584f6487f71d</u>. We are also fundraising to enhance our Process Fundamentals and Process Control capabilities. Our Unit Operations Labs are housed in our recently renovated Process Fundamentals Laboratory. This lab will house many of our active classroom activities. Contact us if you have an interest in partnering with our department. We are also fundraising for professorships in connection with our focus areas. Contact us at HWarren@uwyo.edu (Heather Warren) or valvarad@uwyo.edu (Vladimir Alvarado). Our main office phone # is (307) 766-2500.



**In This Issue:** Message from the Head; AIChE Chapter Information; SWE Chapter Information; Biological & Environmental Engineering; The Wawrousek Lab; Ongoing Projects, and Faculty 2016 Publications.

### **AIChE Student Chapter**

American Institute of Chemical Engineers (AIChE) is a recognized Registered Student Organization (RSO) that helps students build professional relationships and learn more about Chemical Engineering. Nationally, AIChE offers resources to students on careers and job searching, graduate school programs and current research in the field. Locally, our chapter provides students with the opportunity to attend national and regional conferences to network with companies and graduate programs across the nation. Many members of our student chapter achieve success in the classroom and in industry after school. For example, Ben Pelton and Aaron Cheese, two active AIChE members in college, were the top students of their graduating cohort.

Last year, AIChE members held many events and attended multiple conferences. The chapter organized a Dinner with Industry event during the Job Fair week. This event invites companies to attend a dinner where students from the department can visit and network with companies that attend the Job Fair. Many students have been successful in attaining internships or jobs with companies that they interacted with at the event. In addition, AIChE helped with the campus wide event Safe Treat, which allows kids to trick-or-treat in a safe environment. In the spring, AIChE also organizes a brewery tour event with New Belgium Brewery in Fort Collins, CO. The head chemist at New Belgium leads a tour geared toward a more scientific crowd. The tour gives students the opportunity to see the wide variety of career choices that a Chemical Engineering degree offers as well as a technical explanation of the science and equipment found at a brewery.

Every year, representatives from our student chapter travel to the national and regional conferences. At the conferences, we attend meetings for AIChE chapter development, informational talks, research presentations, and network with other schools in our area. In addition, we watch the ChemE Car competition where schools design a car that runs off of a chemical reaction. There are many emissions guidelines for the car, making combustion engines illegal to compete. Therefore, teams pursue clean energy, such as electrochemical reactions. A \$500 incentive to build a car that runs on biofuels exists. Our student chapter also competes in ChemE Jeopardy, where questions derived from the core classes are used to test team's knowledge. For both competitions, you must win at the regional conference to go to the national competition. Last year, our school proudly placed second in ChemE Jeopardy at the regional conference and we hope to contend for national qualification again this year. The national conference also includes a Grad Fair that allows students to meet and network with different universities offering Chemical Engineering or related Graduate Programs . AIChE industry members often overlap with students at meetings, offering networking opportunities.

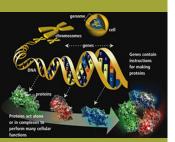
The AIChE student chapter is extremely fortunate to have the support of the Chemical Engineering Department as well as the UWEFE Board. Every year both entities provide AIChE with funding to attend the national and regional conferences, allowing students the opportunity to participate in career and academic activities. These conferences are invaluable as they provide our chapter with new ideas for academic and social programming, further introduce us to up and coming topics in the field, and allow for networking and collaboration locally and nationally. The conferences push current students to dive further into their education by promoting research, analytical thinking, understanding of fundamental principles, and fun applications of chemical engineering though year-long team efforts such as ChemE Car and ChemE Jeopardy. Without their help, AIChE would not be able to participate in the conferences and utilize the provided resources.

This year, the officers for AIChE are William (Sandy) Duncan (President), Katie Nelson (Vice President), Emily Lynch (Treasurer), Sarah Kamphaus (Secretary), Bridger Martin (ChemE Car Leader), Katie Hopfensperger (JEC Rep), Holly Ramseier (JEC Rep) and Christian McWorkman (UWEFE Rep). AIChE is excited for many events this year. We are currently organizing Industry Dinner and hope that companies will attend, even in trying times. AIChE plans to attend both conferences again this year. We will also participate in Safe Treat in the fall and tour New Belgium in the spring. This year we are going to participate in the campus wide Big Event, which involves community service events around Laramie to show support of the University of Wyoming. We will also organize fundraisers to help offset conference costs. Next year, we plan to continue participating and organizing the same events as this year. The University of Wyoming's AIChE student chapter also plans to host the regional conference in the future.

If students want join AIChE, they can reach Sandy Duncan at wduncan2@uwyo.edu and also search for us on Collegiate Link. AIChE is open to collaborating with other RSO's or groups to fundraise or plan events. Meeting details are sent out over email from Heather Warren the day before the meeting and the day of the meeting. We look forward to this year and hope to grow as an RSO.



University of Wyoming AIChE Student Chapter Presidency Back: Katie Nelson, Christian McWorkman, Sarah Kamphaus, William Duncan Front: Seth Bassham, Emily Lynch, Kathe Hopfensperger



In general, biological engineering addresses two groups of technical challenges. First, biological engineering applies physical, chemical and mathematical principles to solve biological challenges. For example, human health presents many opportunities for biological engineering applications. These include developing drug delivery systems that may use nanoparticles to target individual disease agents,



constructing artificial organs that will function effectively and not cause immune system responses, and increasing capabilities in vision, hearing, and mobility for people who do not have those capabilities. Biological engineers working on these problems work closely with health care professionals, including medical doctors, and also with chemical, mechanical and electrical engineers.

Second, biological engineering applies biological principles, in addition to physical, chemical and mathematical principles to design biological systems that produce high value products. For example, many foods require additional biological processes to be used after the crops are harvested. Several tasty examples are cheese, yogurt and beer which are produced from milk (for both cheese and yogurt) and grain (for beer). Three different biological fermentation processes are required for these three products even though two of them start with the same raw material. Additionally, biological processes are used to produce fine chemicals including many pharmaceuticals. Another application that may also provide human health benefits is the development of genetic technologies for enhancing organism performance using selected DNA.

Environmental engineering overlaps extensively with the second group of technical challenges addressed by biological engineering. Specifically, an important component of environmental engineering is the use of biological systems to convert waste materials into high value products. One common application is the use of microbiological systems to degrade contaminants in wastewater. These processes are used at many municipal water reclamation facilities to produce water that is safe for discharge to natural water bodies as well as potential reuse, especially for irrigation. Another application of biological engineering in environmental engineering is the use of different microbiological systems to convert organic contaminants into biofuels, especially methane, the same molecule found in natural gas. These systems are used with a variety of raw materials, including wastewaters, municipal solid waste and animal manures.

At the University of Wyoming, Professor David M. Bagley in the Department of Chemical Engineering is working with his doctoral student, Mr. Judd Larson, to develop biological processes for rapidly converting the organic fraction of municipal solid waste into methane (biofuel). Other researchers have identified that the conversion rate is limited by how fast solid materials, such as waste food, can be solubilized, because the methane-producing microorganisms can only use soluble materials. Mr. Larson is examining how to stimulate the growth of microorganisms on the surfaces of solid, degradable materials by examining the biological process of quorum sensing. Dr. Bagley's and Mr. Larson's goal is to identify appropriate quorum sensing triggers that will dramatically increase colonization and activity of the necessary microorganisms. This work will lead to the design of smaller, more efficient, and more cost-effective reaction systems that convert potential environmental contaminants into high value products.



S W E



ASPIRE • ADVANCE • ACHIEVE





SCIENCE, TECHNOLOGY, ENGINEERING & MATHEMATICS

Dr. Dongmei Li and MS student, Audra DeStefano

The motto of Society of Women Engineers is Aspire, Advance, Achieve. Our goals are largely centered around stimulating and encouraging women in engineering and leadership positions to achieve their full potentials. This also entails acting as a positive force in the engineering profession by demonstrating the value of diversity and improving the quality of life. For our University of Wyoming Chapter, our specific goals are focused on increasing and retaining the underrepresented women in engineering. We are constantly working towards our mission, as it is one that can never be too successful, by advertising within the college, offering opportunities for networking, and improving cohesion within the College of Engineering and Applied Science via male and female member involvement.

Our chapter participates in one large event each semester. In the Fall Semester, at least eight of our members go to the SWE National Convention with all travel expenses paid. At this convention, members participate in professional and collegiate workshops that range from lowering stress levels to managing finances to learning about current developments in the engineering industry. In addition to the workshops, the convention hosts the largest women engineering career fair in the world, giving our members opportunities to both network with large companies from around the world and to explore graduate school programs. In the past, we have had several members interview for internships and full-time positions at this career fair. When the convention is over, the attending members present their educational findings and experiences from the convention to the members that were unable to attend.

In the Spring, our chapter hosts its annual Student-Faculty Banquet for the College of Engineering and Applied Science. This dinner is all-expenses paid for attendees. At the Spring 2016 Banquet, we had 72 students, faculty, and local engineers attend, offering a great opportunity to network and develop connections with one another outside of the typical classroom setting.

Our chapter also largely partakes in outreach events. Our members have spoken in engineering panels for visiting middle schools, presented engineering activities to local elementary schools, and volunteered our time as judges for high school activities. We are large proponents for Engineering Girls Day (part of Engineering Week in February). On Engineering Girls Day we offered coffee and cookies to engineering students to have a presence on campus and we had members speaking in elementary school classrooms about the importance of pursuing academic goals.

**Katie Hopfensperger,** President, Society of Women Engineers said, "As a Chemical Engineering senior, I am proud to say that chemical engineering majors are usually the most represented major within our society. Currently our Secretary, Marketing Chair, and myself (President) are all studying chemical engineering."

Our society also pairs up with the American Institute of Chemical Engineers to volunteer for the SafeTreat event on Halloween. This event entails offering candy and games on campus in order to ensure that families can safely celebrate Halloween.

Last fall, members from the SWE presidency presented to the Advisory Board and they would like to thank them for their contributions to our National Convention funds. They are always grateful for the amount of support that they receive from the College of Engineering and Applied Science and the Chemical Engineering Department.

### The Wawrousek Lab

The Wawrousek lab concentrates on using a biological approach to solve engineering problems. Biological approaches can be advantageous when using heterogeneous feedstocks or a traditional catalyst that is expensive or particularly sensitive to fouling. Microorganisms are well-suited to consume a wide variety of carbon sources, both and inorganic, for bioconversion to value-added products. The Wawrousek lab is currently working on several projects using microorganisms for bioconversion, with each microbe chosen to suit a particular process.

One of the Wawrousek lab's interests is the conversion of carbon monoxide to valueadded chemicals, with potential sources of CO being waste streams from steel manufacture and from synthesis gas. Industrial bioproduction of salable chemicals and chemical building blocks from carbon monoxide has recently emerged as a viable process, with both pilot and demonstration scale operations in place. These first bioproduction processes have all relied on a traditional fermentation of CO by microorganisms in the dark. Looking ahead, the Wawrousek lab is engineering a photosynthetic microorganism that ferments CO. This microorganism, Rubrivivax gelatinosus CBS, is a photosynthetic bacterium that grows on CO in the light or dark, and light is used to alieve energy limitations encountered during CO growth in the dark. Using synthetic biology, this bacterium has

been engineered to produce isoprene, the monomer used for synthetic rubber production. Current efforts involve using additional synthetic biology approaches to optimize isoprene production in this strain.

Interest in bioremediation of produced waters from the oil and gas industry drives the Wawrousek lab's work with microorganisms that consume a milieu

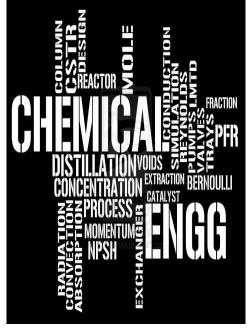
of hydrocarbons. A remediation process with bioremediation steps is currently in place in Pinedale, WY. Using synthetic biology, the Wawrousek lab is investigating microbes that could be engineered to produce a salable product when using hydrocarbons present in produced waters as a feedstock. Knowing that the composition of produced waters is quite variable and can depend on factors such as location in a formation and stage of drilling, bacteria were selected that could consume BTEX and other hydrocarbons, survive during starvation conditions when hydrocarbons are not plentiful, and could tolerate both salts and metals. Bacteria were grown on individual constituents of BTEX to identify the most promising strains for further development, and the Wawrousek lab has identified a strain that grows well on both ethylbenzene and xylene (Figure 1). This strain has grown on the hydrocarbons present in a sample of produced water, and the lab is current-



ly focused on engineering this bacterium to produce ethylene from hydrocarbons in produced water as a proof-of-concept. This bacterial conversion step will not fully remediate produced waters and additional steps for remediation are necessary, as this proposed step would only remove a fraction of the hydrocarbons. However, production of a salable product could improve current economics of produced water treatment.



Dr. Karen Wawrousek Assistant Professor Chemical Engineering





UW-CHE research focuses on added-value propositions and fundamental research in Materials and Processes, Bioengineering and Interfacial Science. Dollar amounts reflect overall funding level. Co-PIs are not listed, unless from CHE.

#### Carbon Initiative (WY – School of Energy Resources)

<u>Goal</u>. To develop, manufacture and engineer advanced processes to convert coal and coal byproducts into molecular intermediates or valuable (non-fuel) carbon materials that may be considered long term carbon sinks and/or co-processed with other hydrocarbon feedstock sources.

#### Ongoing CHE Projects

Project Title	Lead	Funding Level
Coal Conversion Process Characterization	Dr. David Bell	\$200,000.00
New Materials From Coal via Liquid Extraction	Dr. Dongmei (Katie) Li	\$104,078.00
Diamandoid and hard-carbon products from coal	Dr. John Ackerman & Dr. Patrick Johnson	\$240,000.00
Multi-functional Ceria-supported Metal Catalysts for Dry Reforming of Methane	Dr. Joseph Holles	\$200,000.00
An Experimental Investigation of Flow Instabilities and Time-Dependence of the Constitutive Relation- ships of Multiphase Flow in Porous Media.	Dr. Saman Aryana	\$110,000

<u>State</u>

Project Title	Lead	Program	Funding Level
Produced Water Treatment with Smart Materials for Reuse in Energy Exploration	Dr. Dongmei Li	WY Water Pro- gram	\$306,812.00
Produced Water Management and Resource Recov- ery: Initiative Cluster Technology Development and Value Extraction	Dr. Dongmei Li	Tier 1 Engineer- ing Initiative	\$400,000.00

#### Federal

Project Title	Lead	Agency	Funding Level
Integrated characterization of CO2 storage reser- voirs on the Rock Springs Uplift combining geome- chanics, geochemistry, and flow modeling	Dr. Vladimir Alvarado	DOE	\$1,400,255.00
Circulating Tumor Cell Capture and Re- lease from Degradable Hydrogel Surfaces	Dr. John Oakey	WY-INBRE NIH	\$225,000.00
Integration of Xenopus Extract and Micro- fluidics to Study Organelle Size Scaling	Dr. John Oakey	NIH	\$1,729,120.00
Spindle Assembly and Scaling via Microflu- idic Encapsulation of Xenopus Nuclei	Dr. John Oakey	NIH	\$312,919.00
Microfluidic Cell Encapsulation for High Throughput Screening and Rationally De- signed Biomaterials	Dr. John Oakey	NSF CAREER	\$400,071.00
Targeted Encapsulation and Inertial Focus- ing for Circulating Tumor Cell Isolation	Dr. John Oakey	DoD - CDMRP	\$523,209.00
Development of Molecular Separation Methods for Ionic Liquids Recycling from Carbon Feedstock/IL Mixtures Processing Using Ionic Liquids	Dr. Dongmei Li	Battelle Energy Alliance INL	\$150,000.00
Microfluidic Production of Multimodal Therapeutic PEG Hydrogel Nanoparticles	Dr. Dongmei Li	WY-INBRE NIH	\$79,706.00

#### Private Sector

Project Title	Lead	Company	Funding Level
Coal drying and mercury removal using steam from a NuScale reactor	Dr. David Bell	NuScale Power	\$254,000.00
Surfactant-enhanced waterflooding	Dr. Vladimir Alvarado	Baker Hughes	\$50,000.00

esearch Direction of Chemica

## **CHE Faculty 2016 Publications:**

- K. Mouzakis, A.K. Navarre-Sitchler<sup>\*</sup>, G. Rother, J.L. Banuelos, X. Wang, J. Kaszuba, Q.R.S. Miller, V. Alvarado, J. McCray, J. Heath, (2016), "An experimental study of porosity changes in caprocks exposed to supercritical CO2. I. Evolution of mineralogy, pore connectivity, pore size distribution, and surface area", accepted, Environmental Engineering Science. DOI: 10.1089/ees.2015.0588
- Q.R.S. Miller, X. Wang, J. Kaszuba\*, K. Mouzakis, A.K. Navarre-Sitchler, V. Alvarado, J. McCray, G. Rother, J.L. Banuelos, J. Heath, (2016), "An experimental study of porosity changes in shale caprocks exposed to CO2-saturated brine II. Insights from aqueous geochemistry", accepted, Environmental Engineering Science. DOI: 10.1089/ees.2015.0592
- G. Garcia-Olvera, T. M. Reilly, T. E. Lehmann and V. Alvarado\*, (2016), "Effect of Asphaltenes and Organic Acids on Crude Oil-Brine Interfacial Visco-Elasticity and Oil Recovery in Low-Salinity Waterflooding", Vol. 185, pp. 151-163, Fuel. DOI: 10.1016/j.fuel.2016.07.104
- 4. E. A. Taborda, C. A. Franco, S. A. Lopera, V. Alvarado and F. B. Cortés\*, (2016), "Effect of Nanoparticles/Nanofluids on the Rheology of Heavy Crude Oil and Its Mobility on Porous Media at Reservoir Condition", Vol. 184, pp. 222-232, Fuel. DOI: 10.1016/j.fuel.2016.07.013
- X. Wang, L. Fu, and V. Alvarado\*, (2016), "Analysis of Capillary Pressure and Relative Permeability Hysteresis under Low-Salinity Waterflooding Conditions", Vol. 180, pp. 228-243, Fuel. DOI: 10.1016/j.fuel.2016.04.039
- 6. P. Hoyer, M.S. Carvalho\* and V. Alvarado\*, (2016), "Snap-off in Constricted Capillary with Elastic Interface", Vol. 28, pp. 012104, Physics of Fluids. DOI: 10.1063/1.4939150
- G. Garcia-Olvera, T. Reilly, T. E. Lehmann, L. Wang and V. Alvarado\*, (2016), "Surfactant Behavior Analysis in EOR blends Using 1-D 1H NMR", Vol. 30 (1), pp. 63-71, Energy & Fuels. DOI: 10.1021/acs.energyfuels.5b01840
- 8. C. Zhang, , Q. Lai, and J.H. Holles, Ir@Pt Bimetallic Overlayer Catalysts for Aqueous Phase Glycerol Hydrodeoxygenation, Applied Catalysis A, 526 (2016) 113.
- C. Zhang, Q. Lai, and J.H. Holles, Influence of Adsorption Strength in Aqueous Phase Glycerol Hydrodeoxygenation over Ni@Pt and Co@Pt Overlayer Catalysts, Catalysis Science and Technology 6 (2016) 4632.
- Qinghua Lai, Michael D. Skoglund, Chen Zhang, Allen R. Morris, and Joseph H. Holles, "Use of Hydrogen Chemisorption and Ethylene Hydrogenation as Predictors for Aqueous Phase Reforming of Lactose over Ni@Pt and Co@Pt Bimetallic Overlayer Catalysts", Energy and Fuels, in press.
- 11. Qinghua Lai, Chen Zhang, Joseph H. Holles, "Hydrodeoxygenation of guaiacol over Ni@Pd and Ni@Pt bimetallic overlayer Catalysts", Applied Catalysis A 528 (2016) 1-13.
- Shuai Tan, Steve Paglieri and Dongmei Li, Nano-scale Sulfur-Tolerant Lanthanide Oxysulfide/Oxysulfate Catalysts for Water-Gas-Shi= Reac?on in a Novel Reactor Configuration, Catalysis Communica:ons, 73, p. 16–21, 2016.
- 13. Shibely Saha, Bridger Martin, Brian Leonard and **Dongmei Li**, Probing Synergetic Effects Between Platinum Nanoparticles Deposited via Atomic Layer Deposition and Molybdenum Carbide Nanotube Support through Surface Characterization and Device Performance, Journal of Materials Chemistry A, 4, 9253 9265, 2016.
- Dongmei Li and Shibely Saha, Durable and Active Catalyst PlaNorm Consisting of Phase-pure Transition Metal Carbide Support and Metal Nanoparticle Deposited via Atomic Layer Deposition (ALD), US Provisional Patent, filed March 12, 2016, serial number: 62/307,450.
- 15. Dongmei Li, Shuai Tan and Shibely Saha, Achieving Ultra-low Pt Loading with Enhanced Ac:vity and Durability, US Provisional Patent, filed June 10, 2016, serial number: 62/348,158.
- 16. F. Guo and S.A. Aryana, An experimental investigation of nanoparticle-stabilized CO2 foam used in enhanced oil recovery. Fuel, 186 (2016), 430-442.
- 17. P.K. Torsu and S.A. Aryana, On Nonequilibrium models of spontaneous countercurrent imbibition. Computational Geosciences, 20, 1 (2016), 161–170.
- G.C. Woods, A.H.M.A. Sadmani, S.A. Andrews, D.M. Bagley and R.C. Andrews. 2016. Rejection of Pharmaceutically-Based N-Nitrosodimethylamine Precursors Using Nanofiltration, Water Research, 93:179-186.
- 19. S.Z. Wu, C.J. Bascom, K. Nelson, K., J. Oakey, M. Bezanilla, Long-term growth of an early diverging land plant in microfluidic devices enables subcellular studies in development, Plant Physiology, 172, 28-37, 2016.
- B. Xia, K. Krutkramelis, J. Oakey, Oxygen-purged microfluidic device to enhance cell viability in photopolymerized PEG hydrogel microparticles, Biomacromolecules, 2016.
- B. Morin, Y. Liu, V. Alvarado, J. Oakey, A Microfluidic Flow Focusing Platform to Screen the Evolution of Crude Oil-Brine Interfacial Elasticity, Lab on a Chip, 2016. Long-Range Forces Affecting Equilibrium Inertial Focusing Behavior in Straight High Aspect Ratio Microfluidic Channels, Reece, A.E., Oakey, J., Physics of Fluid, 28, 043303, 2016.
- 22. S. Masoudi, C.H.G. Wright, J.C. Gatlin, J.S. Oakey, Microtubule Motility Analysis Based on Time-Lapse Fluorescence Microscopy, ISA Biomed. Sci. Instrum, 50, 126-133, 2016.
- K. Krutkramelis, B. Xia, and J. Oakey, Monodisperse Polyethylene Glycol Diacrylate Hydrogel Microsphere Formation by Oxygen-Controlled Photo-Polymerization in a Microfluidic Device, Lab on a Chip, 16, 1457-1465, 2016.
- 24. B. Xia, Z. Liang, B. Noren, A. Reece, R. McBride, J. Oakey, Microfluidic Single Cell Analysis, Current Opinion in Biotechnology, 2016.
- J.T. McConnell, J. Oakey, Observed and Predicted Particle Dynamics Driven By Inertial Flows Within High Aspect Ratio Microfluidic Channels, Microfluidics and Nanofluidics, 20, 22, 2016.
- 26. A. E. Reece, A.E., J. Oakey, Long-Range Forces Affecting Equilibrium Inertial Focusing Behavior in Straight High Aspect Ratio Microfluidic Channels, Physics of Fluid, 28, 043303, 2016.
- 27. Y. Wang and D. A. Bell, Competition between H<sub>2</sub>O and CO<sub>2</sub> during the gasification of Powder River basin coal, Fuel, 187 (2017) 94-102.