NETL-ORD
Office of Research and Development

NEWS

*Shared Intellect • Shared Laboratories • Shared Resources*

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# Two Years in a Row: Another NETL-ORD Affiliated Researcher Wins Prestigious Presidential Award

**Brian Anderson's** productive research into natural gas hydrates, geothermal systems, and sustainable energy earned him the 2012 Presidential Early Career Award for Scientists and Engineers (PECASE). He received the award at a ceremony on April 14, 2014, in Washington, DC. It is the second year in a row that a National Energy Technology Laboratory-Office of Research and Development (NETL-ORD) affiliated researcher has won the award. The PECASE is the most prestigious award that the federal government gives to scientists or engineers who are early in their independent research careers. The Department of Energy nominated Anderson for the award in recognition of a combination of projects, the centerpiece of which was the reservoir simulations that he helped to develop of the Iġnik Sikumi reservoir. The project brought together researchers from NETL, ConocoPhillips, and the Japan Oil, Gas and Metals National Corporation to investigate how gas hydrate reservoirs on the Alaska North Slope respond to carbon dioxide ($CO_2$) injection. Anderson calls his NETL research partners "right at the cutting edge of scientific understanding of gas hydrates," his main area of research. "It's really been unbelievably fruitful to have a collaboration with [them]." Anderson has worked on several projects with various NETL-ORD scientists and researchers since 2006. His most recent NETL-ORD projects include plume modeling for the High-Pressure Water Tunnel Facility and reservoir simulations as part of the NETL-ORD hydrates research team.

*Dr. Brian Anderson, WVU, 2012 PECASE recipient*

Anderson is the GE Plastics Materials Engineering Professor of Chemical Engineering at West Virginia University (WVU). The PECASE is not the first recognition Anderson's work has garnered. The help he provided in responding to the Deepwater Horizon oil spill prompted Secretary of Energy Steven Chu to honor him with an award in 2011 as part of the NETL-led Nodal Analysis Team. In 2010, Anderson was selected to participate in the National Academy of Engineering's second Frontiers of Engineering program, an event that brought together some of the nation's "most innovative young engineering educators."[1] His efforts in the classroom have earned him praise as well. He was the 2010 Teacher of the Year in WVU's Benjamin M. Statler College of Engineering and Mineral Resources.

Anderson feels honored to have earned the award. He finds it "very humbling to look through the list of other awardees and the tremendous work they are doing across the country."

[1] National Academies, *Innovative Early-Career Engineering Faculty Selected to Participate in NAE's Second Frontiers of Engineering Education Symposium*, October 18, 2010, http://www8.nationalacademies.org/onpinews/newsitem.aspx?RecordID=10182010b, accessed March 18, 2014.

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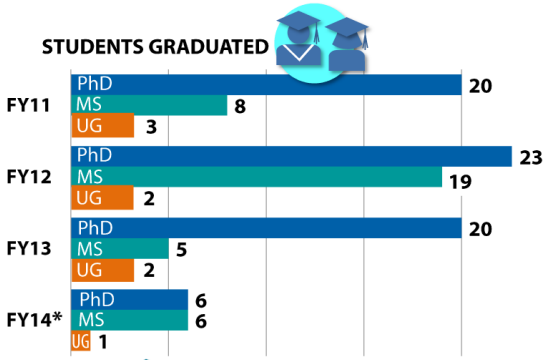
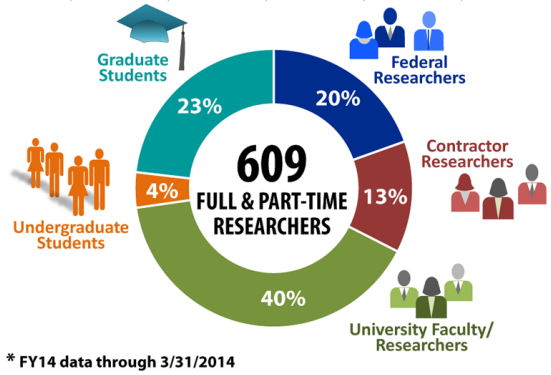
**PRODUCTS**

| | FY11 | FY12 | FY13 | FY14* |
|---|---|---|---|---|
| Publications | 194 | 195 | 163 | 64 |
| Patents Issued | 11 | 12 | 7 | 4 |
| Licenses | 9 | 4 | 0 | 1 |




* FY14 data through 3/31/2014

# Building Attractive Membranes with Poly Ionic Salts

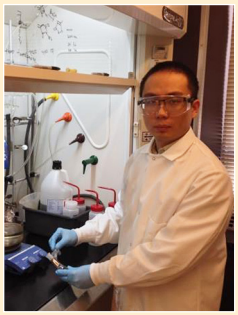
A key strategy for NETL-ORD is strength through collaboration. That principle is illustrated perfectly by the advances being made by the NETL-ORD's Carbon Capture research team, coordinated by NETL scientist **Dave Luebke** and comprising researchers from industry, academia, and national laboratories. Their successes are abundant and include recent work developing a new class of materials that shows promise in the area of carbon capture.

Membranes are an often-investigated tool for selectively separating $CO_2$ from gas mixtures. Ionic liquids (ILs) are salt-like materials that are liquid below 100 degrees Celsius (°C). These materials have good solubility and selectivity for $CO_2$ but, as liquids, cannot be easily formed into membranes. The goal was to incorporate IL gas separation and polymer processability into one material.

The collaborative research team, which included Professors **Krzysztof Matyjaszewski**, **Hunaid Nulwala** (also a research scientist at NETL), and **Meagan Mauter** of Carnegie Mellon University (CMU), pictured below, approached the problem by synthesizing and characterizing a new class of materials consisting of blocks of different polymerized monomers with distinct poly (IL) and structural domains.[2] These materials are new and required new characterization methodologies. The research team collaborated to solve the characterization challenges by developing a new gel permeation chromatography technique.[3] The resulting polymerized block copolymers (PIL-BCPs) can be cast into thin films, creating membranes with improved separation results for carbon and nitrogen. **Hongkun He**, a CMU graduate student involved in the work, explained that PIL-BCP properties can change depending on which anions, cations, and substituents are selected.[4]

Their approach to PIL-BCP synthesis involved conjugating cations to polymers using thiol-Michael (click chemistry), which allowed them to quickly develop a large library of materials including phase separated thin films, ion-gels, and liquid PIL-BCPS.

In addition to the researchers mentioned above, key team members also included **Erik Albenze** (URS), **Brian Adzima** (NETL/former Oak Ridge Institute for Science and Education (ORISE) graduate student), **Surendar R. Venna** (WVU), and **Mingjiang Zhong** (CMU).



*Left to right: Krzysztof (Kris) Matyjaszewski, Professor of Chemistry, CMU; Hunaid Nulwala, Task Technical Coordinator for Transformational Technologies at NETL and Assistant Research Professor of Chemistry, CMU; Meagan Mauter, Assistant Professor of Chemical Engineering, CMU; and Hongkun He, graduate student, CMU.*

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[2] Adzima, B. J., Taylor, S. C., He, H., Luebke, D. R., Matyjaszewski, K., & Nulwala, H. B. (2014). Vinyl-triazolium monomers: Versatile and new class of radically polymerizable ionic monomers. *Journal of Polymer Science Part A: Polymer Chemistry*, 52(3), 417–423. doi:10.1002/pola.27016.

[3] He, H., Zhong, M., Adzima, B., Luebke, D., Nulwala, H., & Matyjaszewski, K. (2013). A Simple and Universal Gel Permeation Chromatography Technique for Precise Molecular Weight Characterization of Well-Defined Poly(ionic liquid)s. *Journal of the American Chemical Society*, 135(11), 4227–4230. doi:10.1021/ja4012645.

[4] Adzima, B., Venna, S., Klara, S., He, H., Zhong, M., Mauter, M. S., Luebke, D., Matyjaszewski, K. & Nulwala, H. (2014). Modular Polymerized Ionic Liquid Block Copolymer Membranes for $CO_2/N_2$ Separation. *Journal of Materials Chemistry A*. doi:10.1039/c4ta00661e.

## *Technology Spotlight*

# Illuminating the Black Art of Surface Chemistry

"Catalysis is kind of a black art," says **Evan Granite**, a chemical engineer and member of the NETL-ORD Advanced Gasification research group. "People try different things without knowing what's going on at the surface."

We're talking about surface chemistry—the chemical reactions that take place on catalytic surfaces—and Granite's enthusiasm about it is infectious. Granite brings up an example that is relatable—our cars. Through surface chemistry, the three-way emissions catalyst in our cars removes unburned hydrocarbons, carbon monoxide (CO), and nitrogen oxides. The performance of the three-way catalyst is enhanced by an electrochemical oxygen sensor that keeps the air to fuel ratio in a range so that the catalyst can effectively do its job.

*Top view of electrochemical cell used to measure surface hydrogen on palladium.*

The team, which includes **James Miller**, a chemical engineering professor at CMU, **Karen Uffalussy**, an ORISE post-doctoral researcher, and **Bret Howard**, an NETL research chemist and team leader, is doing its part to create a renaissance for catalysis and make it less of a "dark art." The team studied the surface chemistry of palladium (Pd) sorbents. They employed an electrochemical cell reminiscent of the ones used in our cars. Palladium is commonly used as a sorbent, catalyst, and membrane for processing coal-derived syngas. Understanding the chemistry on the surface of this catalytic metal will allow researchers to optimize the use of Pd in gasification and other systems.

They first examined the surface of a Pd electrode in an electrochemical cell at temperatures between 100 and 300 °C. They discovered the partial pressure of hydrogen in the cell's gas is equal to the measured thermodynamic activity of hydrogen at the electrode surface. Under non-reaction conditions, the hydrogen in the gas comes to equilibrium with hydrogen on the Pd surface. They realized the cell functions as a hydrogen sensor, since the thermodynamic activity of hydrogen on the electrode is directly related to the concentration of hydrogen on the surface of Pd.

The team is currently repeating the lab-scale hydrogen surface measurements in the presence of syngas constituents such as CO, moisture, and $CO_2$. Other experiments involve Pd-alumina sorbents and their interactions with arsenic, phosphorus, and cadmium. Arsenic, phosphorus, and cadmium are well-known catalyst poisons, and are also effectively captured from syngas by Pd sorbents. Large-scale experiments at Southern Company's National Carbon Capture Facility, involving slipstreams of syngas and a 10 pound bed of Pd sorbent for capture of mercury, arsenic, and selenium, are also being conducted to validate the results at larger scale. Eventually, they expect to understand the mechanisms of molecular interactions at the surface of other materials, ultimately driving the development of better membranes, better sorbents, better catalysts, and a cleaner future.

For more information about NETL's Office of Research and Development and its programs, see http://www.netl.doe.gov/research/on-site-research.

## CMU Doctoral Candidate Brings Optimization Skills to Industry

**Alison Cozad's** oven runs five degrees too hot. She knows this because she "made a linear fit of what the oven says the temperature is versus what the thermometer says the temperature is," she says. Cozad began calibrating her ovens as an undergrad. Since then, whenever she moves out of an apartment, she leaves the information for future tenants—in the form of a graph and equation. It's no surprise that a scientist so committed to precision and practical knowledge has excelled at optimizing industry processes.

*"NETL has presented me with a lot of opportunities to present my work in front of an audience," says Cozad. The feedback she's received on her presentations has been especially valuable. "Each time you give a presentation, you're just honing it, again and again."*

To do so, Cozad has developed algebraic models of computer simulations based on optimization principles, machine learning, and statistical techniques. Her work as part of the Carbon Capture Simulation Initiative (CCSI) optimization group is one example. "Traditional optimization is done using a kind of handwritten algebraic or first-principles models," she says. Those models often lack the context that would make them meaningful. As part of her support for CCSI (a task funded by the Office of Fossil Energy [FE]), Cozad developed models to provide that missing context—or, in Cozad's words, to "bridge the gap between high-fidelity simulators and . . . advanced optimization solvers."

Cozad participated on the CCSI team while she pursued her Ph.D. in Chemical Engineering at CMU. During that time, she also worked with CMU chemical engineering professor **Nick Sahinidis** to develop ALAMO (Automatic Learning of Algebraic Models for Optimization), software that generates models noteworthy for their accuracy, simplicity, and minimal data requirements. What's more, she completed a summer internship with ExxonMobil, and after graduating in April, she will begin a full-time chemical engineering position at ExxonMobil's Fairfax, Virginia, office. One of the computational technologies Cozad developed for CCSI is of interest to ExxonMobil, reports **Madhava Syamlal**, director of CCSI. ExxonMobil is "looking at bringing in these ideas or maybe some of the software for some of their processes," Cozad explains, "depending on how this moves forward." But no matter how it moves forward, one thing seems certain: Cozad will optimize ExxonMobil's processes as aptly as she's optimized CCSI—and her own apartment.

# *Featured Facilities*

## Stay Put: Engineered Natural Systems Lab Supports NETL-ORD Research into Carbon Storage

Putting $CO_2$ underground isn't such a complicated task. The tricky part is getting it to stay there. NETL's Engineered Natural Systems Laboratory in Morgantown, WV, removes some of the mystery that surrounds the process. The lab's pressure vessels, CT scanners, and other equipment reveal how $CO_2$-storage scenarios play out. As **Grant Bromhal**, the Fluid-Rock Geophysics Team lead in ORD's Predictive Geosciences Division and the National Risk Assessment Partnership (NRAP) team technical leader, explains, "Most of what we do [in the lab] is try to re-create subsurface conditions to see what's going on inside the core, how the rock and the fluids interact, how easy it is to get $CO_2$ into the rock, how quickly it dissolves or mineralizes, and how good of a barrier certain rocks would be to [$CO_2$] flow."

Because the lab isn't restricted to NETL scientists, researchers from across academia and industry can use it. In fact, according to Bromhal, day-to-day operations in the lab are mostly run by URS, and universities contribute to a lot of the simulation work there.

The lab helps further the mission of NRAP, an FE-funded initiative that aims to help scientists predict, quantify, and respond to the risks associated with $CO_2$ storage projects. The initiative is led by NETL and includes partners Los Alamos, Lawrence Berkeley, Lawrence Livermore, and Pacific Northwest National Labs. "We're [also] focused on being able to most efficiently design a monitoring network for a site based on its risks," says Bromhal. Doing so requires meticulously constructing computer models on different scales. Some deal with just wellbores or the $CO_2$ reservoir itself; others deal with the whole engineered–natural system into which $CO_2$ is injected. In any case, those models have to be verified. Because of the Engineered Natural Systems Lab, researchers don't always have to venture into the field to confirm that their models reflect reality. Instead, they can use the lab's equipment to effectively peer inside the earth and devise ways to make $CO_2$ storage a less risky proposition.

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