netlognews

NETL's Quarterly R&D newsletter — April 2014, Issue 33

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U.S. DEPARTMENT OF ENERGY | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Cover image: *Clusters of pyrite crystals in the Marcellus shale before gas production. After injection, the shale will be analyzed to evaluate any changes in the minerals or microbes.*

netlognews

newlognews is a quarterly newsletter highlighting recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

NETL/Boston Scientific Corporation-Developed PtCr Alloy Used in New Family of Bare Metal Coronary Stents

—Boston Scientific has received CE Mark approval for the REBEL™ Platinum Chromium Coronary Stent System, the company's latest generation bare metal stent for the treatment of coronary artery disease (CAD). Bare metal stents play an important role in treating CAD and represent a significant share of the global stent market.

CE marking is a mandatory conformity marking for certain products sold within the European Economic Area (EEA) since 1985. This allows the marketing of these stents in most European countries along with areas of Africa and the Middle East.

Scientists from NETL and Boston Scientific collaborated to develop the platinum chromium stent alloy. This alloy was the recipient of an R&D 100 Award in 2011; in 2012, it was recognized both by the Federal Laboratory Consortium (FLC) with the Award for Excellence in Technology Transfer and by the Secretary's Award for Excellence. It has been nominated for the United States Patent Office's Presidential Medal for Innovation in 2013 and for the American Society for Materials' Engineering Materials Achievement Award in 2014.

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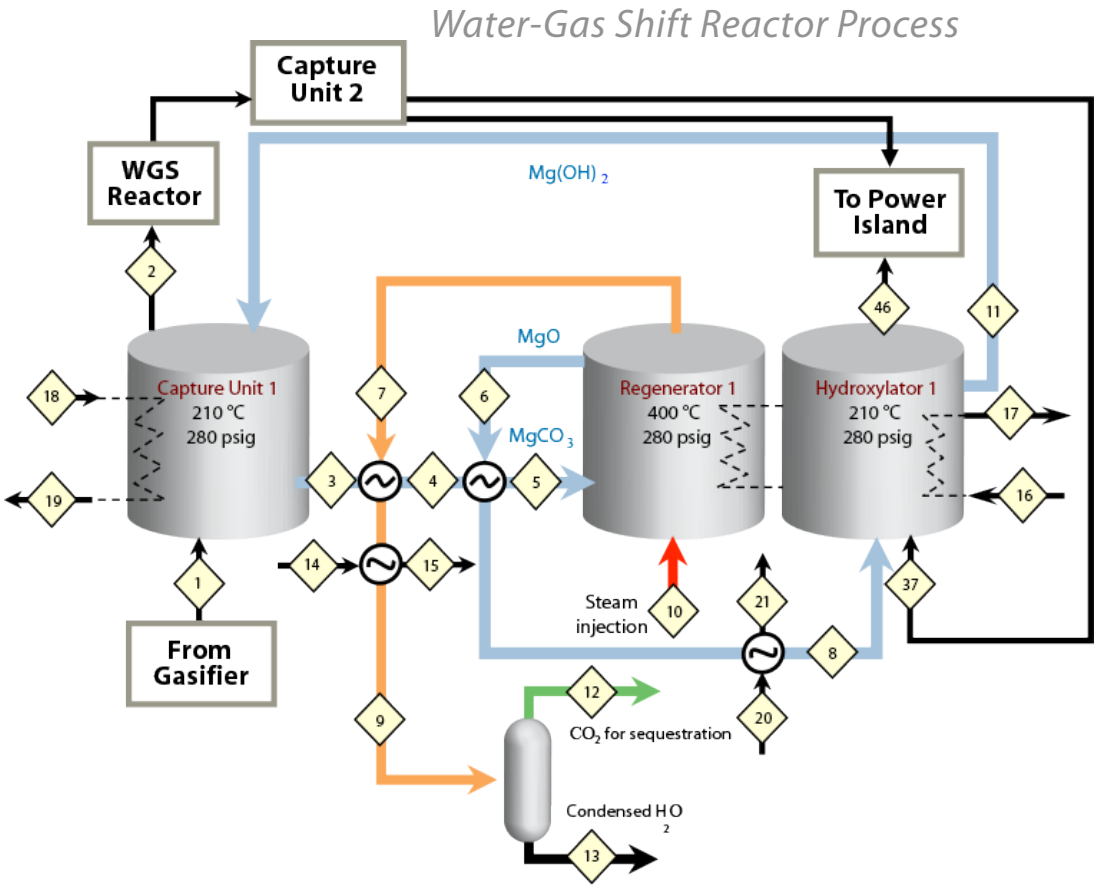

Novel CO_2 Capture Process Patented—U.S. Patent # 8,617,499 was issued to scientists at NETL for a CO_2 capture process that minimizes steam required for regeneration while enhancing the water-gas shift reaction to produce H_2 from synthesis gas from precombustion gas streams.

The water-gas shift (WGS) reaction is a chemical reaction in which carbon monoxide (CO) reacts with water vapor (H_2O) to form carbon dioxide (CO_2) and hydrogen (H_2). The water-gas shift reaction is a highly significant industrial reaction and is used in conjunction with reforming of methane and other hydrocarbons for the production of high purity hydrogen, among other applications.

"Minimization of steam requirements and enhancement of water-gas shift reaction with warm gas temperature CO_2 removal" describes a process for CO_2 separation at warm gas temperatures (150-250 °C) from high pressure (> 380 psi) gas streams such as coal gasification gas streams using magnesium hydroxide known as $Mg(OH)_2$. A $Mg(OH)_2$ sorbent is used prior to the water-gas shift reactor to remove carbon dioxide and provide steam generated during CO_2 removal for the water-gas shift reaction. The $Mg(OH)_2$ sorbent is also used after the water-gas shift reactor to remove the remaining CO_2 formed in the water-gas shift reactor to produce pure H_2. This novel process contributes to a significant increase in overall power plant efficiency due to enhancement of the water-gas shift reactor performance.

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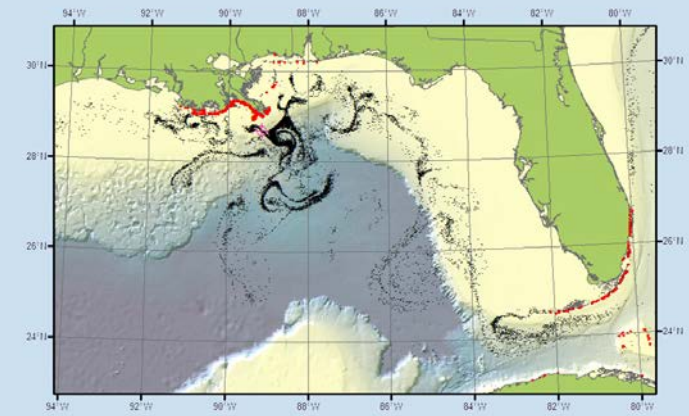

The image shows the predicted spill trajectory 40 days after a hypothetical blowout. It also shows the predicted location of beached oil as a result of this hypothetical spill.

Researchers Evaluate Capabilities of BLOSOM, NETL's Blowout Oil Spill Model

—Scientists at NETL set out to create a data and modeling system to support DOE's mission to produce science-based evaluations of engineered and natural systems, ensure sustainable, environmentally responsible access to U.S. resources, and help prevent future hydrocarbon spills and impacts. One result of this effort is NETL's Blowout and Spill Occurrence Model (BLOSOM), an integrated system designed to simulate offshore oil spills resulting from deepwater (greater than 500 feet) and ultra-deepwater (greater than 5,000 feet) well blowouts.

Recently, researchers used BLOSOM in an international oil spill model intercomparison study focused on improving understanding and predictions of plume dynamics and droplet-size distributions associated with subsea hydrocarbon spills or seeps. The American Petroleum Institute (API) led the effort that included modelers from Texas to Norway. The purpose of the study was to determine the relative strengths of each model and identify areas of large uncertainty with these predictive modeling tools. Another goal was to better understand the formation of subsurface plumes and the effect of dispersants on them—phenomena that are currently poorly understood and lack substantial real world data

In addition to the API-led study, the Ultra-Deepwater Risk Assessment team at NETL also recently received a request from the Bureau of Safety and Environmental Enforcement's (BSEE) Oil Spill Response Division for a review of BLOSOM. BSEE is seeking new computational modeling and assessment tools for its efforts.

These outside opportunities and interest in BLOSOM have offered NETL researchers the opportunity to evaluate the performance of BLOSOM. In addition, the team has gained key insights into the model's current capabilities and relevance to DOE's current hydrocarbon spill prevention goals for offshore systems, as well as potential future uses of this tool.

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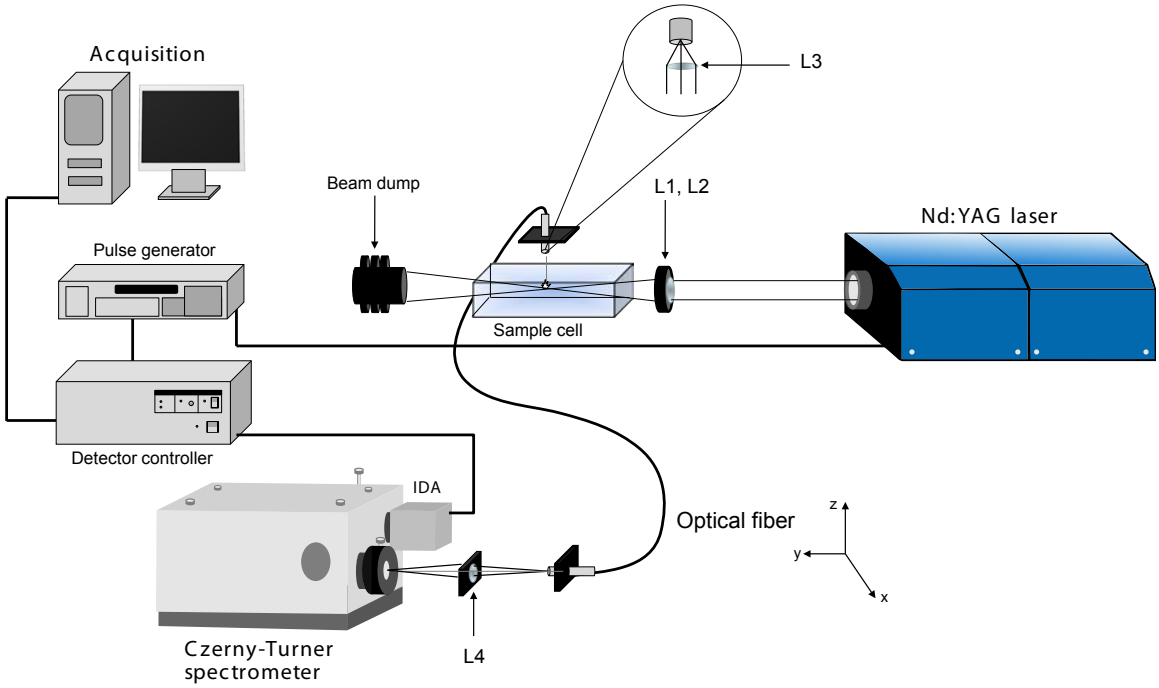
Diagram showing how the LIBS system works.



Analytical Technique Shows Promise for Sensing CO_2 Leakage in Deep Saline Formations

—Leakage of injected carbon dioxide (CO_2) or resident fluids, such as brine, is a major concern associated with the injection of large volumes of CO_2 into deep saline formations. Migration of brine could contaminate drinking water resources by increasing their salinity or endanger vegetation and animal life as well as human health. The main objective of this study was to investigate the effect of sodium chloride concentration on the detection of calcium and potassium in brine samples using laser-induced breakdown spectroscopy (LIBS).

There were two major goals for the LIBS down hole sensor project: 1) to determine the suitability of the LIBS technique for in situ measurements of metal ion concentrations in sodium-rich solution, and 2) to develop a chemical sensor to quickly detect brine intrusion into formations used for domestic or agricultural water production.

A peer-reviewed manuscript about the results of this study titled "Effect of Sodium Chloride Concentration on Elemental Analysis of Brines by Laser-Induced Breakdown Spectroscopy (LIBS)" was recently published in the *Journal of Applied Spectroscopy* , 02/2014, 68 (2), 213-221.

This study showed that LIBS is a promising analytical technique for monitoring calcium and potassium concentrations in a saline-rich solution.

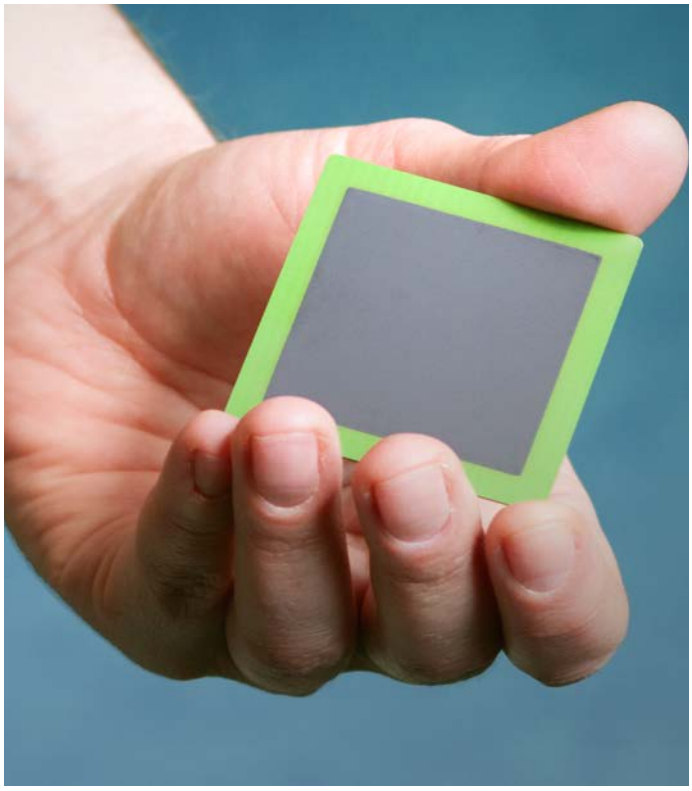
Contact: : Dustin McIntyre, 304-285-1374

NETL-RUA Study Provides Key Insight into SOFC Performance—Solid Oxide Fuel Cells (SOFCs) are electrochemical conversion devices, which transform chemical energy directly to electrical energy. SOFCs have been improved continuously over more than a decade of intense international research, and many current research efforts focus on reducing the operating temperature below 800 ºC. A significant technical challenge is improving the performance of the cathode, as activation of the oxygen reduction reaction (ORR) is a major source of performance loss in SOFCs at low temperatures.

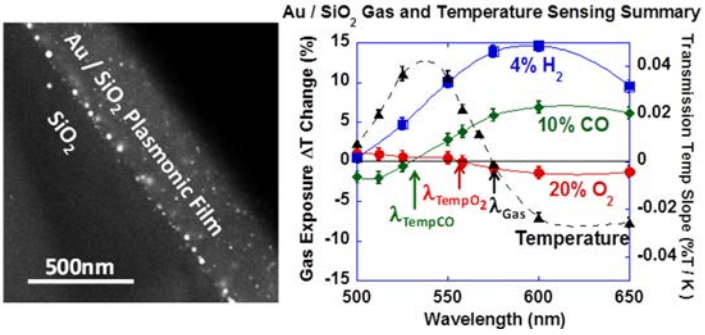
NETL Regional University Alliance researchers recently completed a detailed computational study of the oxidation reduction reaction, which improved model reliability. The ORR model retains treatment of cathode oxygen exchange as competitive between two reactive regions within the cathode, namely the 3-phase boundary (3PB) and the 2-phase boundary (2PB). Revisions to this model were completed to include the influence of surface adsorbed charge, which has a critical impact on the rate at which oxygen in the feed gas exchanges with the surface of the active electro-ceramic materials. The numerical investigation demonstrates that competition between 3PB and 2PB occurs at all operating conditions, but that at more aggressive operating conditions (higher current density), the 2PB reaction pathway becomes dominant. Furthermore, the refined models demonstrate that the character of the transition from 3PB to 2PB dominance (whether implicit or explicit) is strongly influenced by the nature of the materials composing the cathode, in qualitative agreement with independently reported experimental evidence.

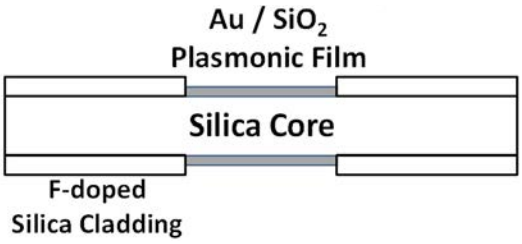
The study provides key insight to the ORR process, which ultimately would be used to create improved materials that are resistant to long-term degradation. This study called "Simulation of Surface-Potential Driven ORR Kinetics on SOFC Cathode with Parallel Reaction Pathways" was published in the *Journal of the Electrochemical Society* 161 (3) F344 (2014).

Contact: : Kirk Gerdes, 304-285-4342



A solid oxide fuel cell used in the NETL-RUA study.





NETL Researchers Demonstrate Extreme Temperature Sensing with Optical Fiber Sensors

—Embedded sensors capable of operation in extreme environments including high temperatures, high pressures, and highly reducing, oxidizing, and/or corrosive environments could make a significant impact on enhanced efficiencies and reduced greenhouse gas emissions of current and future fossil-based power generation systems. Relevant power generation technologies include solid oxide fuel cells, gas turbines, and advanced combustion systems.

Optical based sensors exhibit inherent advantages as compared to other sensing approaches due to (1) broadband wavelength and distributed interrogation compatibility, (2) immunity to electromagnetic interference, and (3) the elimination of electrical wires and contacts in the harsh environment which represents a common source of sensor device failure and a potential safety concern for application in explosive gas atmospheres.

NETL researchers have recently demonstrated a new optical fiber-based sensor technology that is potentially stable at temperatures approaching 900 ° to 1000 °C by monitoring the localized surface plasmon resonance absorption peak associated with Au nanoparticles embedded in a silica matrix. Characteristic shifts in the absorption peak arise due to changes in gas stream composition while a broadening and damping of the peak occurs with increasing temperatures. By using broadband wavelength interrogation techniques, these two effects can be potentially exploited to monitor both parameters with a single sensor element.

In addition to demonstrating useful responses in prototype sensors, the team has also theoretically modeled the sensing effect using waveguide-based models. Continued research by the team is focused on optimizing the sensing layers, developing harsh environment compatible packaging, and identifying higher temperature stable optical fiber core materials to enable the eventual realization of sensor devices based upon the demonstrated technology. Several provisional or non-provisional patent applications have been submitted on the technology that is described in more detail in a recent team publication: "Plasmonic Nanocomposite Thin Film Enabled Fiber Optic Sensors for Simultaneous Gas and Temperature Sensing at Extreme Temperatures," *Nanoscale*, Vol. 5 (19), 9030-9039, 2013.

Contact: Paul Ohodnicki, 412-386-7389

New Computational Tool Predicts Transport Properties in Advanced Alloys

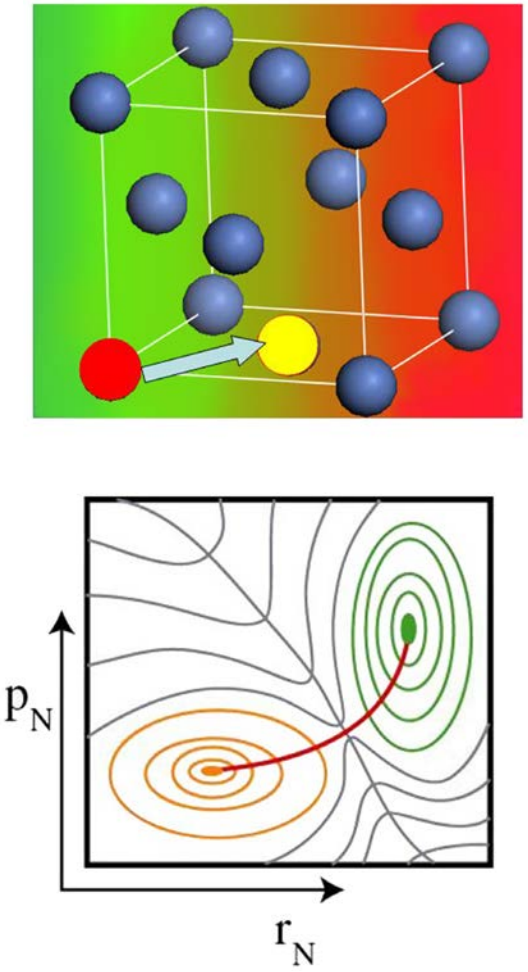
—The interaction between metal alloys and their environment is of critical importance to a variety of applications spanning energy, defense and healthcare. Although there are several fundamental properties dictating macroscopic success, the mobility of gases, defects and metal atoms within the metal alloy often dictates an alloy's overall chemical effectiveness (i.e., corrosion resistance).

NETL researchers Drs. Alfonso and Tafen have developed and are applying multi-scale computational approaches facilitating the rapid development of the next generation of advanced alloys that will enable future energy systems. Specifically, they have constructed a computational tool to examine transport properties in alumina forming nickel-based alloys. Their approach is based on the Kinetic Monte Carlo framework, which allows the prediction of atomic-scale mobility in alloys to macroscopic laboratory observations at relevant conditions.

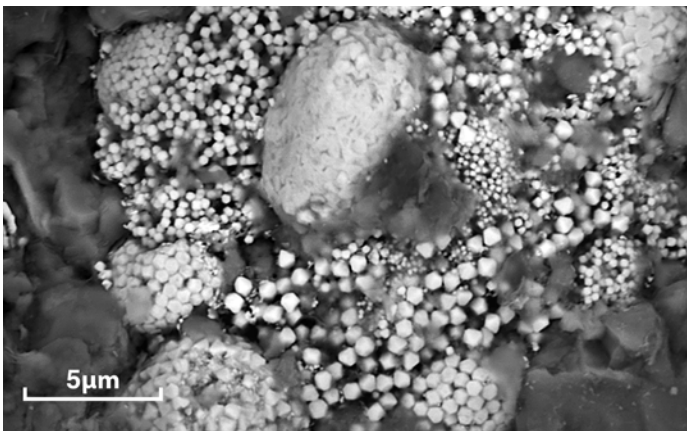
A computationally efficient analytical expression was used to capture the effect of the local environment. The ab initio "trained" model expression helps to determine hopping barriers under different local environments, which is otherwise impractical to calculate from ab initio methods even with the most efficient computer hardware. The entire computational machinery has been implemented in an in-house software code. The diffusion constants predicted from this tool are a key input into the Wagner model—a theoretical-based, well-defined strategy to design oxidation resistant alloys for advanced energy applications.

A distinct advantage of this tool is that the various effects of the diffusion properties can be disentangled at the atomic level. This tool contains generic building blocks for building probes specific to multiple research areas. A description of the earlier version of the code and its application to the investigation of mobility of oxygen in nickel was reported in the *Journal of Applied Physics*.

Contacts: Dominic Alfonso, 412-386-4113



On top– diffusion of atom (red sphere) in bulk nickel facilitated by a vacant site (yellow sphere). On the bottom– the so-called minimum energy pathway for diffusion.



Clusters of pyrite crystals in the Marcellus shale before gas production. After injection, the shale will be analyzed to evaluate any changes in the minerals or microbes.

NETL Researchers Investigate Underground Microbe Interaction—

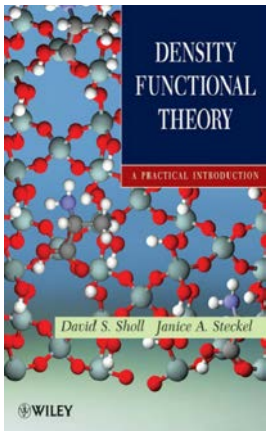
CO_2 storage and fossil fuel production have the potential to both affect and be affected by microbial populations. NETL is investigating the interactions of microbes with substances commonly injected into the subsurface – CO_2 used to enhance oil production, and fluids used for shale gas development. The goal is to learn more about how the subsurface changes when exposed to these substances, and how the microbes themselves participate in or are impacted by those changes.

Data from NETL's Carbon Capture, Utilization, and Storage (CCUS) database, NATCARB, was used to construct a map that lays the temperatures of active CCUS sites over a geothermal heat flow map of the United States. Temperatures and pressures found at active CCUS sites were used to determine which ones were likely hosts to microbes such as bacteria and archaea (single-celled organisms similar in size to bacteria but differing from them in molecular organization). Only three sites out of 94 had temperatures too high to be hospitable to microbes. The others could suit a variety of microbes, and those microbes could have distinct effects on CO_2 behavior.

"Microbes are an active part of the subsurface," says Kelley Rabjohns, a postgraduate Oak Ridge Institute of Science and Technology (ORISE) intern, "and should be considered when thinking about the effects of CO_2 sequestration."

More information about NETL's microbe study can be found in NETL's LabNotes.

Contact: : Circe Verba, 541-967-4437



Density Functional Theory Book is Translated to Turkish—

"Density Functional Theory, A Practical Introduction," coauthored by David Sholl of Georgia Tech and Jan Steckel, a computational chemist at NETL, originally published in English by Wiley in 2009, has been translated into the Turkish language and republished in January 2014. Other editions include a Google eBook and Kindle edition.

Density functional theory (DFT) is one of the most powerful and frequently used computational tools used to study and predict the properties of isolated molecules, bulk solids, and material interfaces, including surfaces. Although DFT theory is quite complicated, this book demonstrates that the basic concepts underlying the calculations are simple enough to be understood by anyone in a variety of scientific, mathematical, and engineering backgrounds. It also provides key information necessary to apply this powerful method to solve real-world problems.

Topics covered include molecules, solids, surfaces, vibrational frequencies, rates, phase diagrams, magnetic properties, and DFT-based molecular dynamics methods. The book discusses what DFT can do and how to do it, as well as what limitations and approximations users of the theory should be aware of. It has appeared on the syllabus for theoretical courses at various universities including the University of Pittsburgh, Carnegie Mellon, Georgia Tech, Uppsala Universitet, Universiteit Antwerpen, and Notre Dame. International interest in this book co authored at NETL helps to cement NETL's image as a strong player at the forefront of scientific research and education.

Contact: Jan Steckel, 412-386-4430

Recent NETL Publications

1.	Mahecha-Botero, Andres; Li, Tingwen; Haseidl, Franz, et al. March 17, 2014. Experimental and Computational Fluid Dynamic Study of the Change of Volumetric Flow in Fluidized-Bed Reactors, *Chemical Engineering Science*, 106, 231-241.
2.	Goueguel, Christian; Singh, Jagdisk P.; McIntyre, Dustin L., et al. February 2014. Effect of Sodium Chloride Concentration on Elemental Analysis of Brines by Laser-Induced Breakdown Spectroscopy (LIBS), *Applied Spectroscopy*, 68 (2) 213-221.
3.	Galvin, Janine E.; Benyahia, Sofiane. February 2014. The Effect of Cohesive Forces on the Fluidization of Aeratable Powders, *AIChE Journal*, 60 (2) 473-484.
4.	Adzima, Brian J.; Taylor, Steve C.; He, Hongkun; et al. February 1, 2014. Vinyl-Triazolium Monomers: Versatile and New Class of Radically Polymerizable Ionic Monomers, *J. Polymer Science Part A – Polymer Chemistry*, 52 (3) 417-423.
5.	Perry, Robert J.; Genovese, Sarah E.; Farnum, Rachel L.; et al. January 29, 2014. A Combined Experimental and Computational Study on Selected Physical Properties of Aminosilicones, *Industrial & Engineering Chemistry Research*, 53 (4) 1334-1341.
6.	Sorescu, Dan C.; Civis, Svatopluk; Jordan, Kenneth D. January 23, 2014. Mechanism of Oxygen Exchange Between CO_2 and TiO2(101) Anatase, *J. Phys. Chem. C*, 118 (3), 1628-1639.
7.	Cheng, Tian-Le; Wen, You-Hai; Hawk, Jeffrey A. January 16, 2014. Diffuse-Interface Modeling and Multiscale-Relay Simulation of Metal Oxidation Kinetics-With Revisit on Wagner's Theory, *J. Phys. Chem. C*, 118 (2) 1269-1284.
8.	Velaga, Srinath C.; Anderson, Brian J. January 16, 2014. Carbon Dioxide Hydrate Phase Equilibrium and Cage Occupancy Calculations Using Ab Initio Intermolecular Potentials, *J. Phys. Chem. B*, 118 (2) 577-589.
9.	Braun, Fernando, Tarditi, Ana M.; Miller, James B. January 15, 2014. Pd-based Binary and Ternary Alloy Membranes: Morphological and Perm-Selective Characterization in the Presence of H_2S, *J. Membrane Science* (450) 299-307.
10.	He, Hongkun; Li, Wenwen; Lamson, Melissa, et al. January 14, 2014. Porous Polymers Prepared via High Internal Phase Emulsion Polymerization for Reversible CO_2 Capture, *Polymer*, 55 (1) SI 385-394.
11.	Levine, Jonathan S.; Goldberg, David S.; Lackner, Klaus S.; et al. January 7, 2014. Relative Permeability Experiments of Carbon Dioxide Displacing Brine and Their Implications for Carbon Sequestration, *Env. Science & Technology*, 48 (1) 811-818.
12.	Monazam, Esmail R.; Spenik, James; Shadle, Lawrence J. January 2014. CO_2 Desorption Kinetics for Immobilized Polyethylenimine (PEI), *Energy & Fuels*, 28 (1) 650-656.
13.	Lekse, Jonathan W.; Natesakhawat, Sittichai; Alfonso, Dominic; et al. 2014. An Experimental and Computational Investigation of the Oxygen Storage Properties of BaLnFe(2)O(5+delta) and BaLnCo(2)O(5+delta) (Ln = La, Y) Perovskites, *J. Materials Chemistry A*, 2 (7) 2397-2404.

Recent NETL Publications

14.	Chen, Ting; John, Hendrik; Xu, Jing; et al. January 2014. Influence of Surface Modifications on Pitting Corrosion Behavior of Nickel-Base Alloy 718, Part 2: Effect of Aging Treatment, *Corrosion Science*, 78, 151-161.
15.	DeGeorge, V.; Shen, S.; Ohodicki, P.; et al. January 2014. Multiphase Resistivity for Magnetic Nanocomposites Developed for High Frequency, High Power Transformation, *J. Electronic Materials*, 43 (1) 95-108.
16.	Ohodnicki, P.R. Jr.; Sokalski, V.; Baltrus, J.; et al. January 2014. Structure-Property Correlations in CoFe-SiO_2 Nanogranular Films Utilizing x-Ray Phooelectron Spectroscopy and Small-Angle Scattering Techniques, *J. Electronic Materials*, 43 (1) 142-150.
17.	Mitrano, Peter P.; Zenk, John R.; Benyahia, Sofiane; et al. January 2014. Kinetic-Theory Preductions of Clustering Instabilities in Granular Flows: Beyond the Small-Knudsen-Number Regime, *J. Fluid Mechanics*, 738 (R2).
18.	Dogan, O. N.; Song, X.; Palacio, D.; et al. January 2014. Coherent Precipitation in a High-Temperature Cr-Ni-Al-Ti Alloy, *J. Materials Science*, 49 (2) 805-810.
19.	Lebarbier, Vanessa M.; Dagle, Robert A.; Kovarik, Libor; et al. January 2014. Sorption-Enhanced Synthetic Natural Gas (SNG) Production From Syngas: A Novel Process Combining CO Methanation, Water-Gas Shift, and CO_2 Capture, *Applied Catalysis B-Environmental*, 144, 223-232.
20.	Lamont, Justin A.; Ekkad, Srinath V.; Alvin, Mary Anne. January 2014. Effect of Rotation on Detailed Heat Transfer Distribution for Various Rib Geometries in Developing Channel Flow, *J. Heat Transfer-Transactions of the ASME*, 136 (1) Article 011901.
21.	Kaneko, Tetsuya Kenneth; Zhu, Jingxi; Howell, Nathan; et al. January 2014. The Effects of Gasification Feedstock Chemistries on the Infiltration of Slag Into the Porous High Chromia Refractory and Their Reaction Products, *Fuel*, 115, 248-263.

Patents Issued This Quarter

1.	Gas Sensing System Employing Raman Scattering. Steven D. Woodruff (NETL); Joel Faulk (University of Pittsburgh); Peng Kevin Chen (University of Pittsburgh); Michael Paul Buric (University of Pittsburgh); **8674306**, Issued March 18, 2014.
2.	Layered Solid Sorbents for Carbon Dioxide Capture. George A. Richards; Henry W. Pennline; Daniel J. Fauth; McMahan L. Gray (NETL); Bingyun Li (West Virginia University); Bingbing Jiang (West Virginia University); **8658561**, February 25, 2014.
3.	Plasmonic Transparent Conducting Metal Oxide Nanoparticles and Nanoparticle Films for Optical Sensing Applications. Paul Ohodnicki, Jr. (NETL); Mark A. Andio (ORAU/ORISE); Congjun Wang (URS); **8638440**, January 28, 2014.

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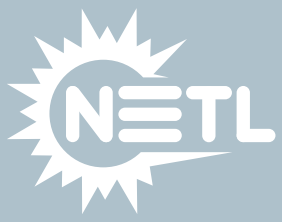

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