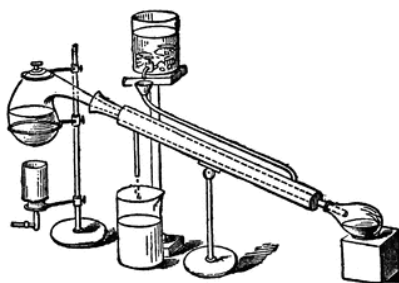




SOUTHWEST RETORT



SIXTY-NINTH YEAR

DECEMBER 2016

*Published for the advancement of
Chemists, Chemical Engineers
and Chemistry in this area*

published by

The Dallas-Fort Worth Section, with the cooperation of five other local sections of the American Chemical Society in the Southwest Region.

Vol. 69(4) DECEMBER 2016

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The Southwest Retort is published monthly, September through May, by the Dallas-Ft. Worth Section of the American Chemical Society, Inc., for the ACS Sections of the Southwest Region.



TABLE OF CONTENTS

Employment Clearing House.....	3
Fifty Years Ago.....	7

ARTICLES and COLUMNS

And Another Thing.....	9
Around the Area.....	12
Letter from the Editor.....	18

SPECIAL EVENTS

Save the Date! 2017 ACS DFW 4th Young Investigators Symposium.....	5
2016 Arkansas INBRE Conference.....	14

NEWS SHORTS

Toward opioid vaccines that can help prevent overdose fatalities.....	8
Could a seawater battery help end our dependence on lithium?.....	11
Urine test for fatigue could help prevent accidents.....	16
Mimicking bug eyes could brighten reflective signs and clothes.....	17

INDEX OF ADVERTISERS

Huffman Laboratories.....	4
Vance Editing.....	4
ANA-LAB.....	6
FWLSC meeting.....	10

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EMPLOYMENT CLEARING HOUSE

Job applicants should send name, email, and phone, along with type of position and geographical area desired; employers may contact job applicants directly. If you have an opening, send your list- ing, including contact info for your company, to retort@acsdfw.org. Deadlines are the 7th of each month.

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provide information required for analytical methods, contribute information for GMP related documentation such as investigations, batch records and reports and translate contract requirements for JenKem Technology departments.

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Previous working knowledge of cGMP manufacturing in the US or Europe, preferably polymer-related or pharmaceutical manufacturing.

Outstanding demonstrated interpersonal skills in English and Mandarin (Chinese) a must (both written and oral)

Proven aptitude for project management tools. Proficiency using project management tools to oversee all elements of project lifecycle including scheduling/planning, meeting coordination, tracking of costs and deliverables, reporting to stakeholders, and risk mitigation. Project Management Certification a plus.

Computer and software skills including MS Office Suite programs, Internet, email systems required.

Proven multi-tasking skills able to handle multiple projects simultaneously within a GMP environment; ability to motivate teams, work within aggressive timelines collaboratively with cross-functional departments

Demonstrated ability to work as a strong contributor in a team environment on complex projects.

Required skills include strong communication, leadership, decision-making, organizational and analytical skills. A candidate must be able to maintain customer focus, handle difficult discussions, build consensus, work independently and prioritize multiple tasks and adjust quickly, as needed. The ideal candidate must be willing to pursue tasks that may be required for projects but are not clearly defined within this job description.

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Save the Date!

2017 ACS DFW 4th Young Investigators Symposium

January Meeting

Date: January 28, 2017

Location: The University of Texas at Dallas

Time: 8:15am-3:30pm

Meet DFW's new young investigators and learn about exciting research in the DFW section! This is an excellent opportunity to network in the local section, meet local academic and industry leaders, and develop collaborative research projects. Oral presentations will be provided by young faculty in the DFW area. Postdoctoral research associates are invited to present a poster on their current research.

Tentative schedule:

8:15 Coffee and poster session setup

8:40 Opening remarks

8:45-10:45am Morning session

10:45am Coffee break

11:00-12:30 Afternoon session

12:30pm-2pm Lunch and Poster Session

2pm Tour of the new Bioengineering Science Building (BSB)

Registration and more info:

<https://goo.gl/forms/ORWN91XgkljMPd5n1>

Please contact Julia Chan (Julia.Chan@utdallas.edu) with any questions about the symposium or poster session.

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FIFTY YEARS AGO IN THE SOUTHWEST RETORT

The winner of the 1966 ACS Southwest Regional Award was Dr. Richard B. Turner of Rice University. He was born in 1916 in Minneapolis, and he attended Harvard, where he received the A.B. degree in 1938. He went on to receive the M.A. degree there in 1940, and he obtained the Ph.D. degree in 1942, working for Louis Fieser. He continued as a Research Associate at Harvard until 1943 and at the Mayo Clinic from 1943-45. He returned to Harvard as a Research Fellow during the 1946-1951 time period. He then joined Rice as an Assistant Professor of Chemistry. He became Associate Professor in 1953 and Professor in 1956. He was Chairman of the Chemistry Department from 1960-1963.

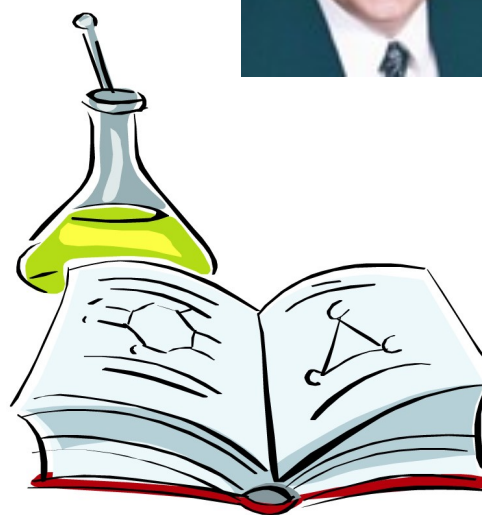
Turner has worked in all areas of organic synthesis with emphasis on reactions in which the course of the reaction might be controlled by stereochemical properties. He did early work on introducing carbon-14 into steroid ring systems as well as the more recent total synthesis of cassaic acid. He has also carried out a program to measure the heats of hydrogenation of olefins.

While he was Chairman of the Chemistry Department, the number of graduate students in chemistry more than doubled. Buildings and equipment were modernized and expanded, with the result that the Rice Chemistry Department was recognized as an outstanding research center.

He will receive his award at a luncheon meeting on Dec. 4 at the Southwest Regional Meeting in Albuquerque, New Mexico.

The keynote speaker at the Regional Meeting was Dr. Glenn T. Seaborg, current Chairman of the Atomic Energy Commission. Seaborg received his Ph.D. at the University of California at Berkeley working for G. N. Lewis. He then joined the Cal faculty. He was given a leave of absence in 1942 to head the plutonium work on the Manhattan project at the University of Chicago Metallurgical Laboratory. He was also the co-discoverer of a number of transuranium elements. He received the Nobel Prize in Chemistry in 1951.

Compiled by E. Thomas Strom



Toward opioid vaccines that can help prevent overdose fatalities

An Advance in Prescription Opioid Vaccines: Overdose Mortality Reduction and Extraordinary Alteration of Drug Half-Life

ACS Chemical Biology

In 2014, the number of deaths from opioid overdoses in the U.S. jumped to its highest level on record. The spike brought national attention to the epidemic and the awareness that new interventions are needed. Now researchers are developing opioid vaccines that could one day help protect people from dying of overdoses. Their study, which tested the vaccines on mice, appears in the journal *ACS Chemical Biology*.

The Drug Abuse Warning Network has reported that the prescription opioid pain-killers oxycodone and hydrocodone are associated with more than 200,000 emergency-room visits per year. Since 1999, more than 165,000 people have died from prescription opioid overdoses, according to the U.S. Department of Health and Human Services. To help prevent opioid-related fatalities, public health officials and practitioners have turned to naloxone, a drug that can be injected right after an overdose to reverse or block the opioid's effects. But naloxone — and someone trained to administer it — needs to be on hand. Kim D. Janda and colleagues wanted to devise a prophylactic approach to counter opioid-related deaths.

The researchers developed two compounds as potential vaccine candidates. They work by preventing opioids from entering the central nervous system, where the molecules induce their addictive euphoric and pain-relieving effects. Testing showed that oxycodone and hydrocodone remained in the bloodstream of mice given the vac-



To prevent fatal overdoses of prescription opioid pain-killers, scientists report progress on a new vaccine that was effective in mice.

Credit: Sherry Yates Young/ Shutterstock.com

cines, suggesting that the medicine effectively blocked the opioids from migrating into the central nervous system. Additionally, mice who received the vaccines survived oxycodone and hydrocodone overdoses at higher rates than unvaccinated mice.

The authors acknowledge funding from the National Institute on Drug Abuse. The authors acknowledge funding from the King's College London.

And Another Thing...

By Denise Merkle, PhD

A significant goal for the past couple decades of my life has been to focus on science and my career, and not on my contribution to survival of the species. Many colleagues know I experienced the miracle of cell-cell fusion, and some have even met my offspring, but I try, with varying degrees of success, to keep my professional life in a discrete packet, away from my personal life. So - I pick 2016 to actually write an article that acknowledges an overlap between professional and personal lives, and the reason I do this is to discuss an issue that really bugs me: Idiotic Behavior - NOT that my spawn is an idiot - far from it. (Do not write to complain about my referring to human offspring as spawn. It's not the editor's fault.) Anyway - it is incumbent upon parents to train their offspring to behave with compassion and decency. One might argue that grounding life in a religion is the mechanism by which this occurs. If this is what parents want for their issue, a religious background is what they should provide. Behaving with respect towards others and the surrounding world isn't based on any particular creed, however. It's a fundamental expectation of living on the planet with a lot of other beings. Respecting the environment is a part of this. Recent bizarre reports of hikers and park visitors vandalizing

natural attractions^{1,2} and actually being so unwise as to dissolve themselves in (very) hot springs³ are stark reminders that we're not Only Children. The world does not revolve around us as individuals. We have responsibilities to our planet and the people with whom we share it, regardless of whether or not we know them or if they can beat us up if we knock over their rocks. Surely, no parents set out to raise people who behave like idiots. Surely?

So, in case you were wondering, here is the point of all this, as well as the reason my offspring was introduced in print, in my professional life: After table manners are learned, please and thank you are instilled, Do Your Homework is ingrained, and Don't You Talk to Me in That Tone has been uttered (at least once), the only Rule is 'Don't Be An Idiot'. The rule is like etiquette - Use it, and you can't go wrong. Good situations, bad situations, happy days, sad days, experiments work, hypotheses are unsupported, hit the high notes or wobble in the aria - anything; one's offspring cannot go wrong if Don't Be An Idiot is the watchword of the ween. Amazingly enough, this phrase does work for others, too, although one might not know from reading the multiple sources of news lately.

So we send into adulthood the self-determining versions of what started out as gametes sharing cell membranes, and we hope that table manners, homework, and 'Don't Be An Idiot' will result in major positive contributions to our existence, and, really, to the beauty of the world. Don't Be An Idiot. And Call Your Maternal Parent.

1) <http://www.cnn.com/2016/09/06/us/oregon-rock-formation-duckbill-toppled-trnd/>

2) <http://www.dailymail.co.uk/news/article-3654897/Woman-banned-20-percent-land-including-national-parks-defacing-rock-formations-posting-evidence-crimes-Instagram.html>

3) <http://www.nydailynews.com/news/national/hiker-fell-yellowstone-hot-spring-dissolved-overnight-article-1.2877738>

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Could a seawater battery help end our dependence on lithium?

A Metal-Organic Framework Derived Porous Cobalt Manganese Oxide Bifunctional Electrocatalyst for Hybrid Na-Air/Seawater Batteries *ACS Applied Materials & Interfaces*

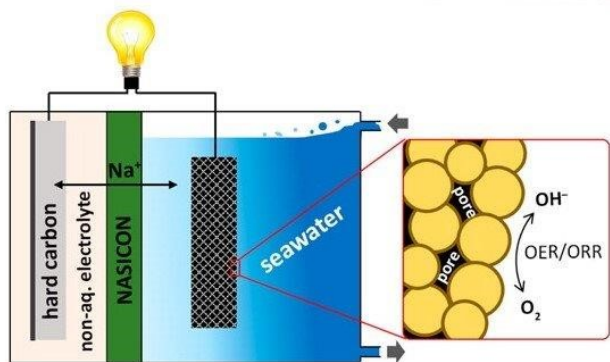
With the ubiquity of lithium-ion batteries in smartphones and other rechargeable devices, it's hard to imagine replacing them. But the rising price of lithium has spurred a search for alternatives. One up-and-coming battery technology uses abundant, readily available seawater. Now, making this option viable is one step closer with a new report on a sodium-air, seawater battery. The study appears in the journal *ACS Applied Materials & Interfaces*.

Sodium-air — or sodium-oxygen — batteries are considered one of the most promising and cost-effective alternatives to today's lithium-ion standby. But some challenges remain before they can become a commercial reality. Soo Min Hwang, Youngsik Kim and colleagues have been tackling these challenges, using seawater as the catholyte — an electrolyte and cathode combined. In batteries, the electrolyte is the component that allows an electrical charge to flow between the cathode and anode. A constant flow of seawater into and out of the battery provides the sodium ions and water responsible for producing a charge. The

reactions have been sluggish, however, so the researchers wanted to find a way to speed them up.

For their new battery, the team prepared a catalyst using porous cobalt manganese oxide nanoparticles. The pores create a large surface area for encouraging the electrochemical reactions needed to produce a charge. A hard carbon electrode served as the anode. The resulting battery performed efficiently over 100 cycles with an average discharge voltage of about 2.7 volts. This doesn't yet measure up to a lithium-ion cell, which can reach 3.6 to 4.0 volts, but the advance is getting close to bridging the gap, the researchers say.

The authors acknowledge funding from the Ulsan National Institute of Science and Technology (Republic of Korea).



Scientists have developed a battery that uses seawater as the catholyte.

Credit: American Chemical Society

Around the Area

University of Arkansas

Jie Xiao delivered an invited departmental seminar at the department of Materials Science and Engineering at University of Washington October 31, 2016. She discussed the interface challenges in battery research with the faculty members and students there.

Feng Wang gave an invited talk at the ACS meeting, "MP2 hydration free energy of simple salts predicted through adaptive force matching." ACS National Meeting, Philadelphia, PA, 10/21-25/2016.

Wei Shi gave several invited lectures during October and November. "Chemistry and Biology of Ipomoeassin Natural Products," Virginia Tech University, Blacksburg, VA, November 11, 2016, and at the Midwest Carbohydrate and Glycobiology Symposium, Mount Pleasant, MI, Oct. 14-15, 2016. "From Organic Chemistry to Biology" was delivered four different places: University of Toledo, Toledo, OH, Oct. 21, 2016; Michigan State University, East Lansing, MI, Oct. 19, 2016; Wayne State University, Detroit, MI, Oct. 18, 2016; and Central Michigan University, Mount Pleasant, MI, 10/17/16.

Matt McIntosh gave an invited talk, "Radical Chemistry of the Breslow Intermediate" at the Frontiers of Organic Synthesis symposium at the Southwest Regional Meeting in Galveston, TX,

on November 12. The talk was based on the work of two recent Ph.D. graduates, **Kola Ayinuola**, currently at Sealed Air Corp, and **Sefat Alwarsh**, currently an instructor in our department.

Nan Zheng gave a talk at ICIQ (<http://www.iciq.org>), Tarragona, Spain, October 14. "Development of Annulation Reactions of Cyclopropylanilines and Cyclobutylanilines by Visible Light Photocatalysis."

T.K.S. Kumar has been invited to present a Plenary Lecture and be a lead Panelist, "New Methods in the Over-expression and Purification of Recombinant Proteins," at the 16th Annual PEP TALK - Protein Science R & D to Therapeutics, January 9-13, 2017, in San Diego, CA.

Christian J. Goodnow and **Stefan Kilyanek**. "Electrochemical Reduction of Group VI Metal-Dioxo Complexes." Poster presented at 51st ACS Mid-West Regional Meeting, October 26-28, 2016, in Manhattan, KS.

Stefan M. Kilyanek gave a talk, "Deoxydehydration of Diols by d⁰ early-metal-oxo complexes." 51st ACS Mid-West Regional Meeting, October 26-28, 2016, Manhattan, KS.

Stefan M. Kilyanek gave an invited talk, "The Conversion of Polyols to Plastic Precursors: Deoxydehydration as a Route to a Green Chemical Economy" at The University of Memphis, November 11, 2016.

Around the Area

Mahsa Lotfi-

Marchoubeh, Mengjia Hu, Miguel Abrego, I. Fritsch, "Spatiotemporally-Distributed Electrochemical Signals at Microelectrode Arrays to Differentially Detect Catecholamines," Invited Talk in the symposium on Novel Electrode Materials & Architectures for Energy & Sensing Applications. 51st Midwest Regional Meeting of the American Chemical Society, Manhattan, KS, Oct. 26-28, 2016.

Jonathan C. Moldenhauer, Madeline Meier, David Paul, "Rapid Determination of Diffusion Coefficients using Electrochemical Time of Flight," Poster presented at 51st Midwest Regional Meeting of the American Chemical Society, Manhattan, KS, Oct. 26-28, 2016.

Publications

Ashley N. Martfeld, Denise V. Greathouse, and Roger E. Koeppe (2016) Ionization Properties of Histidine Residues in the Lipid-Bilayer Membrane Environment. *J. Biol. Chem.* 291, 19146-19156. <http://dx.doi.org/10.1074/jbc.M116.738583>.

Drew Marquardt, Fred A. Heberle, **Denise Greathouse, Roger Koeppe II**, R.F. Standaert, B. van Oosten, T.A. Harroun, J. Kinnun, J. Williams, Steve Wassall, and J. Katsaras (2016) Lipid Bilayer Thickness Determines Cholesterol's Location in Model Membranes. *Soft Matter* 2016, in press. <http://dx.doi.org/10.1039/c6sm01777k>.

T. Ryan Rogers, Kai-Yang Leong and Feng Wang (2016) Possible Evidence for a New Form of Liquid Buried in the Surface Tension of Supercooled Water. *Scientific Reports* 6, 33284.

Jicun Li and Feng Wang (2016) The Effect of Core Correlation on the MP2 Hydration Free Energies of Li⁺, Na⁺, and K⁺. *J. Phys. Chem. B*, 120, 9088.

Jicun Li and Feng Wang (2016) Replacing Water Models without Influencing Solute Properties by Decoupling Water-water and Water-solute Interactions. *J. Chem. Phys.* 145, 044501.

Jordana K. Thibado, Ashley Martfeld, Denise V. Greathouse, and Roger E. Koeppe II. Influence of High pH and Cholesterol on Single Arginine-Containing Transmembrane Peptide Helices. *Biochemistry* 2016, 55(45), pp. 6337-6343. This article was featured on Newswise <http://bit.ly/2fbpCZx> Jordana is now pursuing a doctoral degree in physiology, biophysics and systems biology at Weill Medical College, Cornell University's medical campus in NY City.

Fakharzadeh and **M. Moradi**, Effective Riemannian Diffusion Model for Conformational Dynamics of Biomolecular Systems. *J. Phys. Chem. Lett.* (2016, accepted).

2016 Arkansas INBRE Conference

The 2016 Arkansas INBRE Research Conference was hosted October 21-22 by the Departments of Chemistry and Biochemistry, Physics and Biological Sciences, with venues at the Chancellor Hotel, the Fayetteville Town Center and the University of Arkansas campus. Dr. Steven Harms, M.D., clinical professor at the University of Arkansas for Medical Sciences and radiologist at the Breast Center of Northwest Arkansas, delivered the keynote address on magnetic resonance imaging and medical diagnosis.

Invited faculty speakers included Dr. Mellissa Kelley, Professor of Chemistry at the University of Central Arkansas, Dr. Brett Lehmer, Assistant Professor of Physics at the University of Arkansas, and Dr. Tsunemi Yamashita, Professor of Biology at Arkansas Tech University. Invited undergraduate student speakers competed for awards. The full conference program is available at <https://inbre.uark.edu/>.

Congratulations to the undergraduate student award winners who are listed below:

Biological Sciences

Poster Competition

1st Place - John Short, Missouri State University

2nd Place - Christa Huber, Hendrix College

Honorable Mention - Dustin Brown (UALR), Julius B. Danquah (Philander Smith College), Alyssa Hoover (Harding University), Yuliya Kunz (Northeastern State University), Angeline Rodriguez (Missouri State University), Donnell White (UA Monticello), Taylor Winn (UA Monticello)

Oral Competition

1st Place - Gina Hauptman, UA Fayetteville

2nd Place - Brianna LaFerney, Harding University Chemistry and Biochemistry

Chemistry and Biochemistry

Poster Competition

1st Place - Samantha Jelinek, Rhodes College

2nd Place - Mercedes Winfrey, UA Pine Bluff

Honorable Mention: Alex Graves (Rhodes College), Jasmine Johnson (UA Pine Bluff), Madison Lee (University of Central Arkansas), Karli Lipinski (UA Fayetteville)

Oral Competition

1st Place - Tia'Asia James, UA Pine Bluff

2nd Place - Amanda Paz Herrera, University of the Ozarks

Honorable Mention - Madison Perchik (Rhodes College)

2016 Arkansas INBRE Conference

Physics

Poster Competition

1st Place - Christopher Oldfield, UA Fayetteville

2nd Place - Matthew Huber, Rhodes College

Honorable Mention - Chidubem Eg-bosimba (UA Fayetteville) and Hayley Heacox (UCA)

Oral Competition

1st Place - Jesse Underwood, Missouri State University

2nd Place - Joseph Matson, Hendrix College

Honorable Mention - Luke Fairbanks (Rhodes College)

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RETORT!

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Urine test for fatigue could help prevent accidents

Application of LC-MS-Based Global Metabolomic Profiling Methods to Human Mental Fatigue

Analytical Chemistry

Doctors, pilots, air traffic controllers and bus drivers have at least one thing in common: if they're exhausted at work, they could be putting lives at risk. But the development of a new urine test, reported in the ACS journal *Analytical Chemistry*, could help monitor just how weary they are. The results could potentially reduce fatigue-related mistakes by allowing workers to recognize when they should take a break.

The effects of fatigue have long been recognized and studied as a problem in the transportation and healthcare industries. In the early 2000s, studies published in scientific journals reported that fatigue-related mistakes were linked to thousands of vehicular crashes every year, and were a major concern in patient safety. Weariness can cause anyone on or off the job to lose motivation and focus, and become drowsy. Although very common, these symptoms come with biochemical changes that are not well understood. Zhenling Chen, Xianfa Xu and colleagues set out to determine whether a urine test could detect these changes.



Weariness on the job can put lives at risk, so scientists have devised a urine test to detect fatigue markers.

Credit: Daria Serdtseva/Shutterstock.com

The researchers analyzed urine samples from dozens of air traffic controllers working in civil aviation before and after an 8-hour shift on the job. Out of the thousands of metabolites detected, the study identified three that could serve as indicators of fatigue. Further work is needed to validate what they found, the researchers say, but their initial results represent a new way to investigate and monitor fatigue — and help prevent worn-out workers from making potentially dangerous errors.

The authors acknowledge funding from the National Natural Science Foundation of China and the Civil Aviation Administration of China.

Mimicking bug eyes could brighten reflective signs and clothes

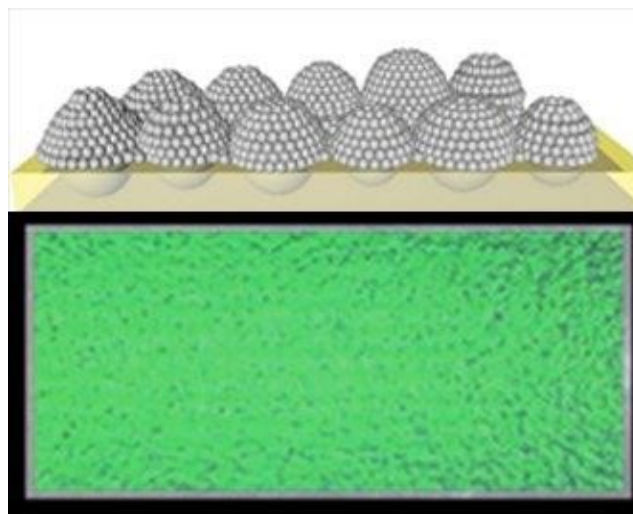
Self-Assembled Hierarchical Arrays for Colored Retroreflective Coatings

Langmuir

That bright, reflective coating used on road signs, bicycles and clothing is an important safety measure at night. They help drivers get to their destinations while avoiding bicyclists and pedestrians in low-light conditions. Now, inspired by the structure of insect eyes, scientists have developed new materials that could improve the color and effectiveness of these safeguards. Their report appears in the ACS journal *Langmuir*.

Retroreflective materials, including some tapes and road paints, work by bouncing light back toward the original source, such as a car's headlights, making them bright and easy to see. Existing retroreflectors are usually made with glass microbeads and microprisms. Dyes, pigments or plastic layers are often added for color; however, they tend to reduce the reflection of light, and the colors can fade over

time. Hongta Yang and colleagues turned to the compound eyes of insects for a new way to address these limitations.



The structure of bug eyes (top) has inspired bright, vividly colored reflective materials (bottom).

Credit: American Chemical Society

The researchers evenly coated an array of glass microspheres with smaller balls of silica. The result is a brilliantly colored, retroreflective material. The color can be adjusted by changing the size of the silica crystals, and

brightness can be boosted by adding layers. At 250 nanometers and 40 layers deep, the crystals appeared bright green and reflected more light than commercial coatings with no color. In addition to boosting the brightness of objects for safety reasons, researchers say that by reflecting rather than absorbing light, the material could be applied to buildings to reduce the urban heat-island effect.

The authors acknowledge funding from the Ministry of Science and Technology, Republic of China.

From the editor

December is always a quiet month for the **RETORT**, but we have January's DFW Section meeting already on the calendar. It will be on January 28 at UTD, the fourth annual Young Investigators conference, with oral and poster presentations; registration and info are at <https://goo.gl/forms/ORWN91XgkljMPd5n1>.

My favorite news release this month is the one on metabolic indicators of fatigue. Once you id the molecules in urine, the way is open to a dip test. This would seem to be a great aid for groups traditionally plagued by fatigue, like the air traffic controllers mentioned in the article.

Best wishes for the New Year,

*Best regards,
Connie*