Sandia researchers have made the first measurements of thermoelectric behavior by a nanoporous metal-organic framework (MOF), a development that could lead to an entirely new class of materials for such applications as cooling computer chips and cameras and energy harvesting.

“These results introduce MOFs as a new class of thermoelectric materials that can be tailored and optimized,” says Sandia physicist François Léonard (8342). “This discovery brings us a step closer to realizing the potential of MOFs in practical applications.”

The results were published in “Thin Film Thermoelectric Metal–Organic Framework with High Seebeck Coefficient and Low Thermal Conductivity,” which appeared April 28 online in Advanced Materials. This work builds on previous research in which the Sandia team realized electrical conductivity in MOFs by infiltrating the pores with a molecule known as tetra-

(Continued on page 3)
That’s that

Over the past couple of years, there has been a lot of talk in the media about so-called “smart drugs.” Purportedly, these drugs can, as the name suggests, give you an edge by boosting your cognitive non-negotiations over your peers. The $64,000 question is, do they work? And if so, how? The answer to the first question is not as straightforward as it might sound. The answer to the second question is still a bit fuzzy.

As we know, Sandia is full of smart people. There aren’t many places in the world where performing at a super-high cognitive level is more important than here.

So here’s another question: For the sake of argument, let’s say that certain smart drugs do work. Let’s say they’re safe, at least as far as we know. Now let’s say you’re working on a project that demands every bit of your cognitive abilities. But it seems clear, too, that smart pills aren’t making anyone any smarter. As one navel article put it: “You aren’t going to turn Homer Simpson into Albert Einstein.” Or as another explained: “With smart drugs, all you’re doing is taking the brain you have and putting it in its optimal chemical state.”

There’s another factor to consider — and I think this has particular relevance for Sandians: It appears that the smarter you are to begin with, the less that smart pills will do for you. That is, smart people may be smart because they’re already using their brains at an optimal level.

The whole area of smart drugs is the subject of serious study and experiment, but researchers need to get a far better handle on what makes us smart before they can come up with a true cognitive enhancer. And then there’s the whole question of whether chemically enhanced intelligence is, in balance, a good thing. I think a case can be made either way.

But let’s say the ethical issues are resolved as the research moves forward. The current research understanding suggests that there won’t be a one-size-fits-all solution. What works for Homer Simpson probably won’t work for you. (On the other hand, it might work for me, in which case I could try to realize my long-pot-off ambition to be a Jeopardy champion.)

With or without smart drugs, it seems we’re all getting smarter. Or maybe I should say “smartier.” From the early 1900s to today, Americans have gained three IQ points per decade on two commonly used IQ tests and five points per decade on another. Across the developed world, the results are similar. No one disputes these numbers, but there is plenty of debate about the why and wherefore. Some argue that the rising IQ scores reflect an increase in our ability to reason abstractly, an ability fostered by the fact that we deal much more in abstractions than did our forebears 75 years ago. Some argue that better nutrition, more widespread education, and increased literacy explain the rising scores. No one knows for sure.

It’s also been argued that the factors cited contribute. But do the rising IQ scores actually mean we’re smarter? Or just better at taking IQ tests? After years of playing Trivial Pursuit with my now-grown kids, I think I know the answer.

See you next time.

— Bill Murphy (MS 1468, 505-845-0845, wtmurph@sandia.gov)

Mark Taylor receives highest award from DOE secretary

Mark Taylor (1446) has received DOE’s 2014 Secretary’s Honor Award — the department’s highest non-monetary employee recognition — for his work as chief computational scientist for DOE’s Accelerated Climate Modeling for Energy (ACME) executive council team.

The award recognizes the team’s work to unify the DOE’s climate modeling research community. Integration of DOE’s many efforts to develop atmosphere, land, ocean, and sea-ice models will enable coordination of a fully coupled-climate-system computational simulation with ultra-high resolution. This model will better serve the department’s energy and science missions.

Expected to be available in 2017, the ACME model will be used to address the most difficult questions that climate scientists face.

Says Mark, “Sandia will play a leading role by contributing our expertise in high-performance computing, uncertainty quantification, and software engineering best practices. I’m honored to be part of this exciting project.”

He shared the award with William Collins from Lawrence Berkeley National Laboratory and David Bader from Lawrence Livermore National Laboratory.

Secretary of Energy Ernest Moniz presented a plaque and certificate to Mark on May 7 in Washington, D.C.

— Neal Singer Lab News Reader Service

The Sandia Lab News is distributed in-house to all Sandia employees and on-site contractors and mailed to all Sandia retirees. It is also mailed to individuals in industries, academia, nonprofit organizations, media, and private life who request it.

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Thermoelectric behavior in ‘Tinkertoy’ materials

Guest@MOF concept described

Described as “molecular tinker toys,” MOFs have a crystalline structure that resembles molecular scaffolding, consisting of rigid organic molecules linked by metal ions. These organic molecules are the sticks and the metal ions are the balls. The hybrid of inorganic and organic components produces an unusual combination of properties: nanoporosity, ultralarge surface areas, and remarkable thermal stability, which are attractive to chemists seeking novel materials. The empty space framed by the organic molecules and metal ions is a truly unique realm of MOFs — empty space that can be filled with practically any small molecule a chemist chooses.

“We describe this concept as Guest@MOF, with the guest being practically any molecule small enough to fit in the MOF pores,” says materials scientist Alec Talin (8342). “The great thing about chemistry is you can synthesize a wide variety of molecules to be inserted inside a MOF to change its properties. In optimizing materials, this gives you a lot of knobs to turn.”

MOF-enabled efficient energy conversion

The researchers had to devise a method to measure the thermoelectric properties of TCNQ@MOF, where TCNQ was the guest molecule. MOFs are so new — they were discovered in 1999 — that researchers often find themselves on the frontier of science with few established tools or even a clear understanding of the material’s fundamental properties.

François, Alec, and Kristopher Erickson, a former Sandia postdoctoral fellow, created a thermoelectric device by connecting Peltier heaters and coolers to each end of a thin film of TCNQ@MOF to generate a tiny temperature gradient. They accurately measured the temperature gradient with an infrared camera while simultaneously measuring the generated voltage. From these data they obtained the voltage per unit of temperature change, known as the Seebeck coefficient.

Patrick Hopkins, an assistant professor of mechanical engineering at the University of Virginia, and his graduate student Brian M. Foley used a laser technique to measure the thermal conductivity. The resulting measurements showed great promise. TCNQ@MOF has a high Seebeck coefficient and low thermal conductivity, two important properties for efficient thermoelectricity. The Seebeck coefficient was in the same range as bismuth telluride, one of the top solid state thermoelectric materials.

“We were trying to understand the role of the guest molecule, TCNQ in this case, when it infiltrates the MOF pores,” says materials scientist Vitalie Stavila (8341), who grew the MOF thin films. “However, we believe the tric efficiency of TCNQ@MOF. One avenue is to change the MOF films from the polycrystalline structures used in the initial research to single-crystal.

“Another potential application is using temperature gradients in the ground to power sensors in remote areas,” says François. “Thermoelectrics could be quite ideal for this application, as you could set up a device and leave it to run for long periods of time.”

Future MOF work seeks to improve efficiency

The researchers are now improving the thermoelectric efficiency of TCNQ@MOF. One avenue is to change the MOF thin films from the polycrystalline structures used in the initial research to single-crystal.

Once thermoelectric MOFs realize sufficient energy conversion efficiency, they could begin replacing existing cooling methods in devices where compactness and weight are priorities. Cameras mounted on satellites, which require constant cooling to function properly, are one example. Replacing the fans in computer chips with thermoelectric MOFs could reduce the weight of laptop computers, smartphones, and other portable electronics and the number of moving parts that will eventually wear out.

Energy-harvesting thermoelectric devices capitalize on wasted heat to draw power. A thermoelectric device near a car engine or exhaust system could transfer that wasted heat into a power source for the car’s electronics. Thermoelectric devices are also used to provide localized cooling for passenger comfort.

“The next step is how do we make it better?” says Mark. “The energy conversion is not competitive yet with solid state materials, but we think we can improve that with better electrical conductivity.”

Measurements yield fundamental understanding of electronic structure

The TCNQ molecule changes the MOF’s properties to enable thermoelectric conductivity.

(Continued from page 1)
Bomb squads from across the country saddled up their robots and duked it out at the ninth annual Western National Robot Rodeo and Capability Exercise May 11-15 at Sandia. The five-day event offered a challenging platform for civilian and military bomb squad teams to practice defusing dangerous situations with robots’ help.

The rodeo was designed with elaborate props to model the atmosphere of real-life emergencies in a low-risk, competitive environment. Robots are life-saving tools for the nation’s hazardous device teams, providing a buffer between danger and first responders.

“Our underlying goal is that we want to make good robot operators into great robot operators,” says Jake Deuel (6532), a Robot Rodeo coordinator and Sandia manager. “We design problems and scenarios that take our state and local bomb squad teams way outside their comfort zones, outside the known techniques and procedures to see how they can handle it.”

UAVs introduced at Robot Rodeo

This year, Sandia introduced unmanned aerial vehicles (UAVs) into the competition. Sandia’s David Novick (6533), a pilot and robotics engineer, flew the UAVs at the event.

“It’s exciting to be able to show off a new technology to this group,” David says. “This technology is a game changer. It’s a stable, highly intelligent vehicle with controls similar to an airplane. Emergency responders can use these small, portable vehicles to get a bird’s eye view of a situation to help them get out of a tight spot.”

Scenarios at the rodeo change every year and grow in difficulty, which brings competitors back. The event prepares officers for the types of situations they may face on the job.

“The only time we get to simulate the level of complexity that we face in real life is at the Robot Rodeo,” says Albuquerque Police Sgt. Carlos Gallegos. “Robots are saving officers’ lives and have been critical to our SWAT teams.” Challenges have included managing suicide bombers, operating in darkened buildings, responding to roadside bombs, navigating obstacle courses, and rescuing first responders.

Sandia partners with Los Alamos National Laboratory on the annual event, which allows teams to practice emergency scenarios where robots are life-saving tools.

The winning bomb squad team was Doña Ana County Sheriff’s Office. Participants included the Albuquerque Police Department, Kirtland Air Force Base Explosive Ordnance Disposal Team, Holloman Air Force Base Explosive Ordnance Disposal Team, Los Alamos Police Department, Riverside County Sheriff’s Office from California, two US Army teams from Fort Carson, Colorado, and a team from the British army.

A TEAM MEMBER from the Albuquerque Police Department Bomb Squad controls a robot during the five-day competition.

NEW TECHNOLOGY allows members of bomb squads and other public safety organizations to review new products.

BOB SQUAD COMPETITORS from the Los Alamos Police Department prepare a robot before a scenario with an active shooter.

A ROBOT ENTERS a movie theater, in this case the old KAFB theater, to defuse a dangerous situation during one of the 12 challenging scenarios at the annual Robot Rodeo.

KIRTLAND AFB Explosive Ordnance Disposal Team debriefs with evaluators after one of the training exercises.
Employee death

A great and caring mentor, Don Gilbert passes away

For Don Gilbert, who passed away on May 10 in Albuquerque at age 60, it was “family first and mission always.” Oh, and there was the motorcycle, too.

According to an obituary published in the Albuquerque Journal, nothing made Don happier than riding a rough trail on his motorcycle — nothing, that is, except time with friends and family.

The Fort Worth native, who moved with his family to Albuquerque in 1958, was an engineering support technologist in Energetic Systems Research Dept. 5447.

He was hired on as a Sandia employee in 2013, but his association with Sandia goes back to 1997, when he started as a contract associate.

Don’s manager, Russ Maines, started working with him just a few months ago. But Russ says he was already familiar with Don’s work and was very happy to have him on his team.

“Don’s technical reputation always preceded him,” Russ says. “Folks in the nuclear business would call him and ask him to bring up his expertise because they had confidence in his work. They knew he’d never overlook the data that he generated, the diagnostics he ran, or tests he conducted. He was an honest man, who held scientific integrity and engineered reliability as the highest forms of serving our country.”

“Don was extremely resourceful and love for technology wasn’t limited to the workplace. According to the Albuquerque Journal obituary, ‘Don loved anything with an engine. If it was broken, he could fix it; if it moved fast, he could make it move faster.’ 

“Don had scientific integrity and engineered reliability as the highest forms of serving our country.”

“Don was always responsive to those who sought out hands-on knowledge and wisdom. ‘Don was always willing to share what he could, and took it upon himself to become an arbitrator for those who could not seem to come to a meeting of the minds,’ Russ says. ‘Don’s service to the national mission was not only mentionable, but exemplary. I only wish I had the chance to know him better. He will be sorely missed.”

The Albuquerque Journal obituary said, “Don’s true legacy lies with his family, friends, and colleagues. He believed his life’s most important work was being the best husband, father, uncle, friend, and mentor he could be. Don’s love and compassion improved countless lives and he has left the world a better place.”

He is survived by his wife, Cynthia; his sons, Travis and Brett; his sister, Linda Sexton; his step-brother, Maka Tolosa; several brothers- and sisters-in-law; and many nieces and nephews.

— Bill Murphy

Navy honors Jerry McDowell with achievement award

Jerry McDowell, who retires from his position as Sandia’s Deputy Labs Director and serves VP for National Security Programs on July 4, has been presented the Fleet Ballistic Missile Achievement Award, which recognizes significant personal contributions by FBM contractor personnel deemed pivotal to the success of the US Navy’s FBM Strategic Systems Program.

Jerry was honored for his significant contributions to national defense over the course of his 35-year career at Sandia. Major contributions by Jerry to the FBM program cited in the nomination package include his advocacy to the national security community, his contributions to technology development programs, and his management of projects and capabilities related to Sandia’s nuclear and

conventional weapon responsibilities.

US Navy Vice Adm. Jerry Benedict, who hosted the awards ceremony held in Washington, D.C., on May 7, recollected times he and Jerry had worked together over the years in their various positions within the Navy and Sandia, first on conventional weapons and, later, on the nuclear side.

“I was humbled to receive this award from Adm. Benedict and to be recognized by someone I respect and admire as a great leader,” Jerry says.

Special recognition to families

Benedict also paid special recognition to the families of awardees, noting that he deeply appreciated the team commitment to serving the nation. He invited Jerry’s wife, Tara, to join them on stage, where he presented her with a certificate and a personal note of thanks.

“It meant a lot to me that Adm. Benedict recognized the sacrifices Tara and my children made while I was away from home on Navy business,” Jerry says.

Over the years, Jerry’s program responsibilities have spanned the breadth and depth of national defense, including nuclear deterrence; conventional strike; missile defense; information operations; intelligence, surveillance, and reconnaissance; counterproliferation of weapons of mass destruction; nonproliferation technologies; and intelligence matters. In 2003, he served as a member of DoD’s Science Board summer study related to Strategic Strike. According to FBM nominators, this advocacy role — supporting senior DoD officials, such as US Strategic Command — produced significant positive impacts on the Navy’s Strategic Systems Program.

“A person in my position at Sandia can only be honored with an award like this because of the support and sacrifice of the hundreds of Sandians who work every day to meet the Navy’s mission,” Jerry said during his acceptance speech. “I accept this award on their behalf.”

The nomination states Jerry was critical to “shaping current and future national security missions and capabilities at Sandia, enabling important and unique deliverables for the Navy’s advanced conventional weapon development program, and supporting Sandia’s engineering and systems integration responsibilities.”

Jerry is the seventh Sandian to receive the Fleet Ballistic Missile Achievement Award. Other recipients include Mark Kozinthal (2600); Ron Hartwig (2200); Rick Kmadson (3535); Rich Holzhausen (3535); Charles Williams (ret.); and Dan Hardin (ret.).
MISCELLANEOUS

STEPPING STONES, 24, Flex stone, $70; black Champ golf travel bag, Masterful goblet vnt, $30. Weagley, 385-4039.

ELLIPSE, Machine, Nordic-Track Audiostrider 990 Pro, has ifi, great condition, sturdy, $150 OBO. Grogg, 505-980-2755.

STEEL CABINET, large, $60; maple woodworking bench, $450; maple workbench, $75; Iron Man spin bike, $330. Olbin, 275-2681.

DI EQUIPMENT, pair QSCK12 (140) powered speakers, strands, Yamaha mixer MCI124X2, mic stand, pair DJ lights, Fascinator. Louebriel, 268-1351.

LEATHER COUCH, burgundy/mahogany, good condition, $50. Naber, 918-637-6663.

HITCH, heavy-duty, w/stabilizer box frame, queen, good condition, $50. Naber, 268-1341.

DJ EQUIPMENT, pair QSCK12 (1-kW) powered speakers, strand, Yamaha mixer MC124X2, mic stand, pair DJ lights, Fascinator. Louebriel, 268-1351.

BED FRAME, loft, full size; cast iron wood-burning stove, $150 OBO. Moreno, 238-0494.

LATHES, 2, JET mini lathe model 1014, $300; Delta, full-size lathe, $1,425. Montoya, 880-8829.

GEOTRAX, child friendly train, 8 cars, $220. Gilliland, 505-306-1711.

HARLEY-DAVIDSON MAG WHEELS, '86 HARLEY-DAVIDSON FXSTC, 100K tune-up, outstanding, garaged, 92K miles, completed 10K tune-up, outstanding, $4,800. Bauck, 949-0999.

BICYCLE RACK, Thule, trunk-style, $125 ea.; car carrier, like new, $125. Jellison, 238-6079, call or text.

STEEL CABINET, large, $60; maple woodworking bench, $450; maple workbench, $75; Iron Man spin bike, $330. Olbin, 275-2681.

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And she says the award took her back to the commitment to education she made in war-torn Serbia. "It is a confirmation that years of hard work do pay off, and that in this country one does not need to be privileged to succeed," she says. "I immigrated to the United States to escape wars in the Balkans. I arrived with a diploma in math, two suitcases, and a desire to live a dignified life, working hard. I worked three jobs during my first year in the States. Over the years, I invested in furthering my education. I worked on what I am passionate about and expanded my personal and professional network. This award is the crowning achievement of that effort."