Filip Ronning (right) in the low temperature nuclear magnetic resonance lab with his postdoctoral researchers Nick Wakeham (left) and Adam Dioguardi (center).

Photo by Sandra Valdez (NIE-CS)

“Pursuing materials studies that push the scientific agenda”

By Eileen Patterson, CPA-CAS

Physicist Filip Ronning (Condensed Matter and Magnet Science, MPA-CMMS) makes electrons nervous, specifically, the f-electrons of the actinides and lanthanides. Ronning is part of a DOE Basic Energy Sciences (BES) project that focuses on the f-elements and their electrons in a search for new materials that can reveal new physics. The project team—6 staff members, including Ronning and 5 postdoctoral researchers—finds about 20 new materials a year.

The f-elements hover between being magnetic and nonmagnetic, so the BES team designs compounds and experi-

continued on page 3
From Tanja’s desk...

Dear Colleagues,

In terms of infrastructure, we have had an eventful summer. A control board short at the magnet lab caused an AC unit to fail. In a similar incident—this time caused by water—the power to RC-1 was lost, which added to the woes with the aging AC unit and temperatures exceeding 90°F in the labs. Thanks to quick intervention by our FOD team, we were up and running again with rental units within days. I keep my fingers crossed that the CINT chiller will hang in there for another week. The installation of the new unit will take multiple days and we are shooting for the week of October 24, including the preceding weekend. It will not be convenient and all CINT staff need to be flexible to allow the installation to happen as expeditiously as possible. We also had a small flood in the basement of 03-34. These challenges are a reflection of our aging infrastructure requiring significant investments—there is no quick and easy solution, and we need to work the issues one bite at a time. Those of you in the MSC occasionally feel the buildings shake, as the old press building is being dismantled to create space for a new building. Research Park II is in the making … So gradually the infrastructure situation will improve. I am truly amazed by how our MPA staff is nevertheless tremendously successful. As a case in point, Jim Werner from CINT was just selected as APS Fellow. Congratulations, Jim!

Facility investments continue to operations at the NHMFL-PFF. We recently completed the installation of the new breaker system, which went amazingly smoothly thanks to the commitment of our outstanding staff who found on-the-spot solutions as stumbling blocks presented themselves. In FY17 investments at the PPF will continue with an upgrade of the outdated power supply regulators and UPS systems. Our cleanroom in SM-40 is also up and running, and we are hoping to make additional investments in FY17 to equip it with state-of-the-art instrumentation. We are encouraged by the institutional investments and excited about the future for both user facilities.

CINT is going through a leadership transition. I am happy to report that Alex Lacerda has been appointed deputy group leader and he is also serving in the role of acting group leader. Nate Mara and Jim Werner stepped up to share the duties of acting deputy group leaders. We have an ongoing search for the CINT group leader position, as well as a senior management position at Sandia-CINT. In the 10-year history of CINT, this is an unprecedented scenario: the CINT director and co-director positions are vacant at the same time. Therefore, the candidate who is better qualified to lead CINT first will take over the directorship. So our new CINT group leader will either become CINT director or co-director, which is reflected in the vacancy description IRC50715 through the use of a slash. This is an outstanding opportunity to lead one of the premier basic science organizations at LANL.

At the October EPS All Hands, Mary shared with us that FY16 was a very good year for LANL. The overall budget went up significantly, milestones were reached, and outstanding science conducted. Nevertheless, I am keenly aware that the uncertain fiscal climate on the science side causes a lot of anxiety, especially among our more junior staff. Federal science budgets have become increasingly tighter over the years, and LDRD is going through a refresh, with the outcome that LDRD funds will be used to invest in problems spanning a broader technology readiness level (TRL) range than in the past, creating new opportunities to collaborate with scientists in mission relevant areas through mission foundation research. These trends send a clear signal that times are changing, and it is more important than ever to sharpen our message in communicating “why at LANL” and how MPA’s basic research and user facilities play leading roles in identifying and solving important scientific challenges across the Lab. I welcome your ideas, suggestions, and creativity to ensure that MPA is more relevant than ever and continues to be LANL’s flagship organization for foundational science. I look forward to working with you.

MPA Division Leader Tanja Pietraß
ments that present the f-elements’ electrons with a magnetic dilemma. “We’re trying to make the f-electron uncomfortable,” said Ronning, “unable to decide what it wants to do. Does it want to be magnetic and stay in place, or nonmagnetic and itinerant, freely roaming throughout the solid?”

It’s in that uncomfortable place that new states of matter may emerge. To see if that will happen, the team tests a constantly changing selection of new materials in the form of crystals created from an f-element mixed with elements from other parts of the Periodic Table. The crystals are cooled by liquid helium in a cryostat and their properties measured as a function of temperature, magnetic field, and pressure.

The BES project has been ongoing at the Laboratory since the 1980s. Many groups have similar interests. But Los Alamos is one of the few groups working with the f-elements, which are a strength here because of the Lab’s historical interest in plutonium, along with the other actinides and by commonality, the lanthanides.

The f-elements also star in Ronning’s other project, an LDRD Directed Research study for which he is principal investigator. The project team—nine staff members and a handful of postdocs—studies topological materials, topology being a new way of classifying materials. “It’s a very hot field,” said Ronning. So hot in fact, that the 2016 Nobel Prize in Physics was just awarded to three British researchers for their groundbreaking work in topological phase transitions and topological phases of matter. “It’s wonderful to have the Nobel committee recognize both the foundational works of these great scientists and the exciting new field of study that they have enabled.”

Topological materials are classified according to discrete values determined by the material’s electronic structure. A mathematical analogy exists to the geometric classification in which the number of holes an object possesses defines the object’s topology. For example, a coffee cup and a donut are topologically equivalent because each has one hole. Beyond classification, the presence of a figurative “hole” in a material’s electronic structure guarantees certain physical responses in the material.

Ronning’s team tests samples made from f-elements to see if the magnetism associated with f-electrons affects the topology. If it does, researchers could potentially discover novel states of matter with unique properties, opening the door to new materials with applications for sensing, electronics, and computing.

Ronning earned his physics doctorate at Stanford University in 2001 and did postdoctoral studies at the University of Toronto. He came to Los Alamos in 2003 as a Director’s Postdoctoral Fellow and was a Reines Distinguished Postdoctoral Fellow before becoming a staff member in 2006. He has coauthored more than 200 publications, including in *Science, Nature, and Physical Review Letters*. He is a Fellow of the American Physical Society.

Ronning has earned the respect of his group and the international scientific community according to Laboratory Fellow Joe Thompson, who has led the BES project for more than 20 years. Thompson will be turning the lead over to Ronning in FY 2017.

He is also greatly appreciated by the postdocs he directs, as evidenced by his 2015 Laboratory Postdoctoral Distinguished Mentor Award. “Filip’s genuine interest in the career development of his postdocs goes well beyond what might normally be expected,” said Nicholas Wakeham, who finished his postdoctoral studies in April. “He valued my need to develop as a scientist on an equal footing with the need for CMMS to produce world-class work.”

Some of the postdocs who have worked with Ronning have become staff members. Others have taken positions in the United States or Asia and Europe, but they’ve stayed in touch. Said Ronning, “They are some of our strongest collaborators.”

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**Filip Ronning’s favorite experiment**

**What:** I’m always looking forward to the next one

**Why:** To answer an unresolved question

**When:** As soon as possible

**Where:** At Los Alamos, or if necessary at facilities with our international collaborators.

**Who:** I’ve had the privilege of working with many great people, and hope to continue my good fortune.

**How:** Work hard and ask for help when necessary.

**The “a-ha” moment:** That remains to be seen, but I hope it’s a good one...
Borup, Kim recognized with awards of merit for fuel cell efforts

Members of Los Alamos’s fuel cell program were recognized with 2016 Annual Merit Review Awards, presented at the annual Merit Review and Peer Evaluation Meeting of the Department of Energy’s Hydrogen and Fuel Cells Program.

Rod Borup (Materials Synthesis and Integrated Devices, MPA-11) was recognized for his outstanding role as director of DOE’s Fuel Cell Consortium for Performance and Durability (FC-PAD). Borup has been instrumental in setting up and leading the core team of five national laboratories and in reaching out to industrial developers to accelerate improvements in polymer electrolyte membrane fuel cell (PEMFC) performance and durability. He is the program manager of the fuel cell group at Los Alamos National Laboratory and has made extensive contributions to the fuel cell research community as a renowned expert in PEMFCs. He is a member of the U.S. DRIVE Fuel Cell Technical Team and co-chair of the DOE’s Fuel Cell Technologies Office Durability Working Group.

Yu Seung Kim (MPA-11) and collaborator Cy Fujimoto (Sandia National Laboratories) were recognized for their outstanding technical contributions and achievements in the development of alkaline exchange membrane (AEM) fuel cell technology. As a result of their work, this nascent technology is beginning to show promise for low-cost fuel cells and electrolyzers. Their continued collaboration since 2009 is an excellent example of how technology can be more effectively advanced through inter-lab partnerships. Working together these co-principal investigators investigated the degradation mechanism of AEM materials and subsequently developed novel AEMs that have shown unprecedented alkaline stability. The resulting membranes and membrane electrode assemblies have demonstrated good performance and durability under both fuel cell and electrolysis operating conditions, opening up opportunities in both fields.

Technical contact: Rod Borup

Los Alamos researchers survey current state of metasurfaces

Center for Integrated Nanotechnologies (MPA-CINT) scientist Hou-Tong Chen, together with his Laboratory colleague Antoinette Taylor (Chemistry, Life, and Earth Sciences, ADELCS), and his CINT user Nanfang Yu (Columbia University) published a review article in Reports on Progress in Physics highlighting recent progress in the physics of metasurfaces at wavelengths ranging from microwave to visible.

Metasurfaces are the two dimensional equivalent of metamaterials that consist of a single layer or a few layers of planar array of subwavelength metal/dielectric resonators arranged in a particular spatial profile to effectively manipulate electromagnetic waves. They possess many exotic properties of bulk metamaterials, which are a class of engineered effective media, but unlike metamaterials are much easier to fabricate, operate over a broader bandwidth and with lower losses, and are more compact and suitable for integration in many practical applications.

continued on next page
Metasurfaces cont.

Top panel is a photograph of a fabricated microwave metasurface that can redirect an incident beam into a refracted beam with nearly 100% efficiency. It is made of a stack of identical circuit board stripes, the top and bottom sides of which are printed with copper traces. Bottom panel: one unit cell of the metasurface consists of capacitively and inductively loaded traces to realize desired electric sheet reactance (on the top side of each stripe) and capacitively loaded loops to realize desired magnetic sheet reactance (on the bottom side of each stripe).

The article provided an overview of key metasurface concepts such as anomalous reflection and refraction, wavefront engineering and beam forming, polarization conversion, wave guidance and radiation control, dielectric metasurfaces, active and nonlinear phenomena, as well as opinions of opportunities and challenges in this rapidly developing research field.

Chen and his Los Alamos collaborators are designing and fabricating functional metamaterials to transform the technological world, with applications in integrated optics, renewable energy, sensing, imaging, and communications.

Chen was supported by the Laboratory Directed Research and Development program, and the work was in part performed at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences Nanoscale Science Research Center operated jointly by Los Alamos and Sandia national laboratories. The work supports the Laboratory’s Energy Security Solutions mission area and the Materials for the Future pillar through the examination of current and past research on metasurfaces. Reference: “A review of metasurfaces: physics and applications.” *Reports on Progress in Physics*, 79 (2016) 076401.

Technical contact: Hou-Tong Chen

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High-field magnetoresistance measurements of high-temperature superconductor suggest unusual resistivity-temperature relationship

A team of researchers that included Ross McDonald (Condensed Matter and Magnet Science, MPA-CMMS) has pinpointed a correlation between resistivity and temperature in the iron pnictide superconductor $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$, finding an unexpectedly simple scaling relationship between applied magnetic field and temperature dependences. Their results are an important clue towards future understanding of the strange metallic state in high-temperature superconductors and related strongly correlated metals, suggesting the possibility of a new route for the exploration of quantum criticality using high magnetic fields.

The resistivity of many exotic metallic systems, which is phenomenologically related to high-temperature superconductivity in both the cuprates and iron pnictides, varies linearly with temperature. Although this has attracted considerable attention, it has been unclear how the relevant physics is manifested in other transport properties, for example the response to an applied magnetic field.

The team investigated $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ using the National High Magnetic Field Laboratory’s Pulsed Field Facility (NHMFL-PFF) at Los Alamos, which provided magnetic fields of up to 92 T. These high fields enabled the researchers to destroy superconductivity, thereby revealing that the unconventional linear resistivity is simply set by the energy scale of the thermal energy and applied magnetic field added in quadrature. Furthermore, the scaling factor between

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Magnetotransport of $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ near optimal $T_c$. a) The magnetoresistance, $\rho(H,T) – \rho(0,0)$, (blue) is plotted as a function

$$\rho(H,T) = \rho(0,T) + aT^\alpha + bH^y$$

where $a/T^\alpha = 1$, approaches the same linear dependence as the zero-field resistance (pink). Lower panel shows the same data with the linear component (black dashed line) subtracted, and with the lowest temperature curves removed for clarity. The inset shows a schematic representation of the relationship between $T$ and $H$, expanded to illustrate the quantum critical plane as a function of temperature, field, and composition, in b).
Light-activated photocurrent degradation and self-healing in perovskite solar cells

A new study by Los Alamos researchers and collaborators has found both the cause and a solution for the tendency of perovskite solar cells to degrade in sunlight, a breakthrough potentially removing one roadblock to commercialization for this promising technology. The researchers determined this photo-degradation is a purely electronic process caused by charge accumulation without chemical damage to the crystal structure, and therefore can be circumvented, while the cells’ self-healing properties allow them to rebound in the dark.

The team is exploring organometallic halide semiconducting perovskite solar cells. They are promising due to their high power conversion efficiency (PCE) exceeding 20% and low fabrication costs; the perovskite material is synthesized via a low-temperature solution process using earth-abundant compounds. To move the material from proof-of-concept experiment to market-viable technology requires the device to operate at stability under continuous sunlight and in outdoor conditions. The sunlight-induced degradation undermines the commercialization of perovskite-based solar cells.

By performing extensive device and spectroscopy characterization, the team found that sunlight triggers the activation of metastable trap states at relatively low energy deep in the perovskite bandgap, which results in the trapping of photo-generated charge carriers. Over time, trapped carriers can further accumulate in the device, and thus reduce the photocurrent. Placing the solar cell devices in the dark for several minutes allows for “evacuation” of these trapped charges, thus leading to the recovery of the pristine device performance upon the next operation cycle. The team also found that these processes are strongly temperature dependent and that temperature control over a range of a few tens of degrees can either prevent the activation of the photo-degradation mechanisms or speed-up the self-healing process.

Joint experimental and theoretical investigations concluded that the most possible scenario is the creation of small polaronic states involving lattice strain and molecular reorientations of the organic cation present in the perovskite lattice.

Top: Photocurrent-degradation under sunlight and self-healing in the dark in organo-metallic halide perovskite solar cells. Bottom: Illustration of the light activation of metastable trap states during photo-degradation and curing of these traps during self-healing.

continued on next page
Light-activated cont.

Research is underway toward improvements and the long-term technological viability of perovskite-based photovoltaics.

Reference: “Light-activated photocurrent degradation and self-healing in perovskite solar cells,” Nature Communications 7 (2016). Los Alamos authors are Wanyi Nie (Material Synthesis and Integrated Devices, MPA-11), Jean-Christophe Biancon (Physical Chemistry and Applied Spectroscopy, C-PCS), Amanda Neukirch and Sergei Tretiak (Physics and Chemistry of Materials, T-1), Aditya Mohite, Hsinhan Tsai, and Gautam Gupta (MPA 11), and Jared Crochet (C-PCS). Collaborators are from Brookhaven National Laboratory, Rutgers University, Purdue University, Université de Rennes 1, France, and INSA de Rennes, France.

The Los Alamos portion of the work, done in part at the Center for Integrated Nanotechnologies, a DOE Office of Science User Facility, was supported by the DOE Office of Basic Energy Sciences and the Los Alamos Laboratory Directed Research and Development program. Computational and DFT calculations used resources provided by the Los Alamos Institutional Computing Program, supported by the U.S. DOE NNSA. This work supports the Lab’s energy security mission areas and the materials for the future science pillar.

Technical contact: Aditya Mohite

MPA students in the news

Ahn, Pound, and Ryter win Student Symposium achievement awards; many present during session

MPA student researchers Jung Ahn (Materials Synthesis and Integrated Devices, MPA-11), Benjamin Pound (Center For Integrated Nanotechnologies, MPA-CINT) and John Ryter (MPA-11), won awards for the work they presented at the Laboratory’s 16th Annual Student Symposium. A number of MPA student researchers also presented research at the August symposium.

The annual event is designed to provide students with the opportunity to present their research, thereby broadening their capabilities and preparing them for careers in science and nontechnical fields. It also lets presenters network and make professional contacts.

Jung Ahn (MPA-11), won an award for research on “Tuning and Assessing Ruthenium Catalysts for Self-Healing Applications.” Ahn worked to identify a ruthenium catalyst, which has already proven effective in ring-opening metathesis polymerization, that could be applied to self-healing materials. The proposed catalyst would also have a fast initiation rate, a modest propagation rate to widen the scope of viable monomers, and high catalyst stability in a solution to maintain its self-healing abilities. Ahn used UV-Vis spectroscopy and 1H-NMR to screen existing, commercially available catalysts for the aforementioned properties and to analyze the catalysts’ decomposition rates. He also modified the catalyst ligand system to tune catalyst stability and its kinetic properties. Ahn, a post-baccalaureate student from Cornell University, is mentored by Benjamin Davis (MPA-11). His research is sponsored by the DOE Office of Science.

Pound, a post-baccalaureate Utah State University student, was recognized for research on “Coherent Diffractive Light-activated cont. John Ryter (MPA-11) was recognized for “Advanced Sensor Arrays and Packaging.”
Imaging in the Near Field." This rapidly developing form of imaging, where the amplitude of the interference (or diffraction) pattern is directly imaged on a CCD and various algorithms reconstruct the phase of the diffraction pattern, offers improvements over other types of imaging and is especially useful for x-ray wavelengths. In deriving the relationship between light emerging from the sample (object plane) and arriving at the detector, a "necessary" condition arises, called the small angle number, An, that should be much less than one. In many envisioned experimental setups, however, this value could be much greater than one. Pound’s research sought solutions to overcome this limiting condition. The relationship is easier to probe with the distorted object method that allows imaging at any distance, and Pound’s work investigated where the distorted object approach fails in regards to An, demonstrating that good quality images can be acquired with An values of several thousand at visible wavelengths. This research is relevant to the Laboratory’s proposed MaRIE (Matter-Radiation Interactions in Extremes project), where experiments may need to be conducted in the near-field. Pound is mentored by

Richard L. Sandberg (MPA-CINT): his work was sponsored by the National Nuclear Security Administration.

Ryter, a Montana State University undergraduate student, was recognized for research on “Advanced Sensor Arrays and Packaging.” His presentation focused on advances in electrochemical sensors and application-specific packaging for automotive applications along with how this work has enabled real-world field trials testing of LANL safety sensor technology at commercial hydrogen vehicle filling stations in California. The Laboratory is developing multi-sensor arrays and working with Rutgers University to produce Bayesian mathematical models capable of deconvoluting signals produced by complex gas mixtures. Such powerful and robust systems have potential uses outside the automotive industry as well, including the detection and identification of explosives for global security applications. Ryter is mentored by Eric Brosha (MPA-11): his work was funded by Los Alamos’s Laboratory Directed Research and Development program, state and local governments, nonprofit organizations, and the Science Undergraduate Laboratory Internship program.

Other MPA student presenters included

- Quyen Nguyen (Condensed Matter & Magnet Science, MPA-CMMS), mentored by Doan Nguyen (MPA-CMMS), presented “Mechanical Interaction Between the Insert and Outsert Coils of 100T Magnet.”
- Emily Follansbee (MPA-CMMS), mentored by Chuck Mielke (MPA-CMMS), presented “Designing and Building a Cryogenic System for the Single Turn Project.”
- Shuprio Ghosh (MPA-CINT), mentored by Abul Azad (MPA-CINT), presented “Microfluidic Aspirators.”
- Joseph Roback (MPA-CINT), mentored by Quanxi Jia (MPA-CINT), presented “Toward Stoichiometry Controlled Magneto-Transport Behavior in LaMnO3 Thin Films.”
- Dennis Trujillo (MPA-CINT), mentored by Richard Sandberg (MPA-CINT), presented “Coherent Imaging via Ptychography in the Soft X-ray Domain.”
- Zachary Harrell (MPA-CINT), mentored by Quanxi Jia (MPA-CINT), presented “Tunable Strain and Functionality in Nanoparticle Arrays in Thin Film Matrix.”
- Erik Knall (MPA-CINT), mentored by Dmitry Yarotski (MPA-CINT), presented “Using SHG to Study Magneto-Electric Coupling in BTO with CFO Nanopillars.”
- Oscar McClain (MPA-11), mentored by Tommy Rockward (MPA-11), presented “Using a Film Applicator to Determine Platinum Loading for Fuel Cell Electrodes.”
- Aysha McClory (MPA-11), mentored by Rangachary Mukundan (MPA-11), presented “Durability of Catalyst Support in Proton Exchange Membrane Fuel Cells.”

continued on next page
CINT’s Quanxi Jia retires

In August close to 100 CINT staff and Los Alamos and Sandia national laboratories colleagues celebrated Quanxi Jia and his outstanding scientific career. The gathering was organized around Jia’s prolific and unparalleled scientific contributions to the materials community worldwide, including seminal publications in fabricating nanocomposite films and fibers. He is returning to his alma mater SUNY at Buffalo to lead their nanosystems R&D efforts.

MPA students cont.

• Raluchukwu Onwubuya (MPA-11), mentored by Tommy Rockward (MPA-11), presented “Study of Electrochemical Durability of Carbon-Supported Pt Catalysts for Fuel Cells.”
• Jared Borrego (MPA-11), mentored by Brian Scott (MPA-11), presented “Hydrophobic, Heat-Resistant, & Porous Filter Material for Safe Nuclear Waste Storage.”
• Courtland Brown (MPA-11), mentored by Tommy Rockward (MPA-11), presented “Using a Film Applicator to Determine Platinum Loading for Fuel Cell Electrodes.”
• Jonalyn Fair (MPA-11), mentored by Tommy Rockward (MPA-11), presented “Study of Electrochemical Durability of Carbon-Supported Pt Catalysts for Fuel Cells.”
• Stefan Williams (MPA-11), mentored by Tommy Rockward (MPA-11), presented “Using a Film Applicator to Determine Platinum Loading for Fuel Cell Electrodes.”

HeadsUP!

Lab safety, security programs showcased at national VPP conference

The Department of Energy highlighted Laboratory employee-driven safety and security initiatives from the 32nd Voluntary Protection Program national conference in Kissimmee, Fla.

Deputy Laboratory Director Rich Kacich, deputy principal associate director for Operations (PADOPS) Bill Mairson, and Associate Director for Environment, Safety, and Health (ADESH) Michael Brandt, along with several LANL employees, gave presentations on topics ranging from operational leadership and implementation of learning teams, to how ergonomic improvements have reduced risk of injury, improved productivity, reduced error rate, and improved the comfort of employees. Other Laboratory presentations included LANL Radio and the Lab’s workplace violence prevention program.

In 2014 the Laboratory received Voluntary Protection Program Star Status from the Department of Energy, the largest site in the DOE complex to attain this status.

MPA students cont.

• Raluchukwu Onwubuya (MPA-11), mentored by Tommy Rockward (MPA-11), presented “Study of Electrochemical Durability of Carbon-Supported Pt Catalysts for Fuel Cells.”
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Celebrating service

Congratulations to the following MPA Division employees celebrating service anniversaries recently:

Brian Scott, MPA-11 .................................................. 25 years
Peter Goodwin, MPA-CINT .................................... 25 years
Charles Mielke, MPA-CMMS ..................................... 20 years
Reginaldo Rocha, MPA-CINT .................................... 15 years
Jacob Spendelow, MPA-11 ..................................... 10 years
Benjamin Davis, MPA-11 ....................................... 10 years
Ricardo Martinez, MPA-CINT ................................... 5 years
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