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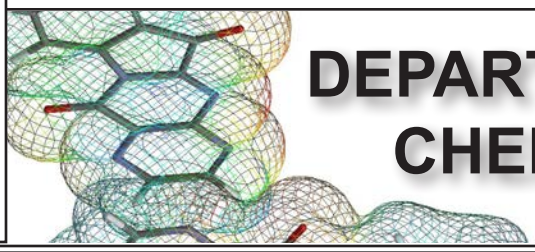
Panther Chemist Newsletter No 3. Spring 2017



DEPARTMENT OF CHEMISTRY

Welcome New Faculty: Drs. Peverati and Schoedel

The Chemistry Department welcomed two new faculty in the fall of 2016.

Hired as a replacement for Dr. Baum, Dr. Peverati is a physical chemist and a native of Italy who earned his Ph.D. from Universität Zürich, Zurich, Switzerland in 2010, after which he was a postdoctoral fellow at the University of Minnesota and the University of California at Berkeley. His research is in computational chemistry, where he develops new functionals for density functional theory (DFT).

Dr. Schoedel is an inorganic chemist who was hired to bolster the department's needs after the retirement of Dr. Babich in 2014. A native of Germany, Dr. Schoedel earned his Ph.D. in Chemistry in 2014 from the University of South Florida, Tampa. He then went on to a postdoctoral fellowship at the University of California at Berkeley. Dr. Schoedel is an inorganic chemist who specializes in materials chemistry; his research is focused on developing novel low-density metal-organic frameworks (MOFs).

We are excited to see new faces in the department, and we wish great success for these new Panther Chemists.

Editors: J.A. Olson, jolson@fit.edu and K. Winkelmann, kwinkel@fit.edu

Dr. Baum Retires

Florida Tech and the Chemistry Department bid a fond (partial) farewell to Dr. J. Clayton Baum, who officially retired last spring (2016). With a career spanning nearly four decades, Dr. Baum has been an institution within the department, beloved by colleagues and students alike.

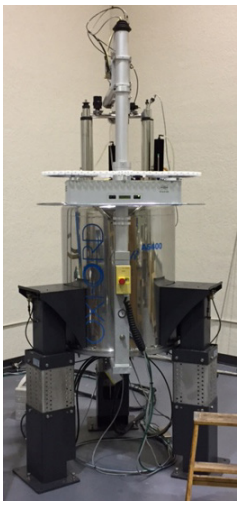
Dr. Baum began his career with Florida Tech in 1979, when the Chemistry Department did not yet exist (it was established as a separate department in 1988). He served the university as a faculty member for 37 years. Alumni remember him as the professor who taught Physical Chemistry (lectures and lab) with a balance of rigor and compassion. And his colleagues have been supremely blessed by his mentorship and collegiality, from advising help to providing a seldom-used, obscure tool.

Dr. Baum's research has involved molecular spectroscopy and the application of computational chemistry methods. He co-developed a novel fluorescence-based chemical sensor with Dr. Brown; this is still an active line of inquiry. Additionally, he co-developed a novel computer-aided drug design method (patent pending) with Dr. Olson and Dr. Novak (currently with South Dakota School of Mines and Technology, Rapid City, SD).

Now as an Emeritus Professor of Chemistry, he can still be seen in the department from time to time working on an NSF-funded research project, the grant for which was awarded to him and Dr. Liao shortly before his official retirement. In addition to continuing his research with a more relaxed schedule, Dr. Baum plans to spend some time travelling, especially via rail.

We wish him all the best on his continued work in chemistry, and on his enjoyment of a well-earned retirement.

New Instrumentation



Florida Tech's Chemistry Department has recently benefited from new instrumentation acquired from support by the university. Led by Dr. Brown, The NMR facilities were expanded with a new 400 MHz NMR spectrometer with autosampler. In addition, the department recently purchased a new powder X-ray diffractometer, improving our materials analysis capabilities. Dr. Schoedel is in charge of the new diffractometer. Finally, through the efforts of Dr. Knight, we also purchased an LC-MS which greatly enhances our analysis capabilities, complimenting our GC-MS facilities. The department is very thankful to the university administration for their support.

New Panther Chemists 2015-2016

Ph.D.

-2015-

Mahmoud M. Saleh (Wehmschulte): *Synthesis, Structure and Reactivity of Cationic Organoaluminum and -gallium Species.*

Raymond J. Terryn III (Baum): *Density Functional Theory Applications to Potential Energy Barrier Maps via Scanning Tunneling Microscopy Simulations, Ab Initio Docking of Specific DNA Intercalators, and Charge Dependent Ferrate Oxidation Kinetics.*

-2016-

Rafaela Nita (Knight): *Catalytic Degradation Of Organophosphate Esters Using Gold Nanoparticles, Supported Copper(II) Bipyridine Caomlexes and Plasomonics.*

M.S.

-2015-

Afef Al Taleb, Hussam Alhamza, Justin Damon, James DiBella, Junxiao Gan, Moustafa Hamaad, Adam Ibrahim, Shahad Khomeis, Qinyi Li, Khalid Osman, Saad Rfaish, Shiyu Sun, Yishu Wang, Chengju Yang, Keng-Chih Yeh, Eric Ziegler.

-2016-

Anad Afhaima, Hibah Alharbi, Leonard Bernas, Zhuo Li, Shon Neal, Mshari Rajab, Anthony Starett, Yangyang Sun, Shuqi Xiao.

B.S.

-2015 -

Leonard Bernas (*Magna Cum Laude*), Grace Holcomb (*Cum Laude*), Carolina Nascimento (*Magna Cum Laude*), Clint Price.

-2016-

Everett Cooper, Will Henderson, Jian Ma (*Summa Cum Laude*), Nathaniel Price (*Cum Laude*), Shukun Yang (*Magna Cum Laude*), Flavia Zisi Tegou (*Cum Laude*).

We congratulate all our new chemistry alumni on their achievements!

⌘ CHEMISTRY DEPARTMENT NEWS ⌘

The Chemistry Department currently includes 45 undergraduate students, as well as 50 M.S. and Ph.D. graduate students. The department also currently manages over $2.2 M in external contracts and grants.

Al Brown's group was visited from January to July 2016 by postdoctoral fellow Essmat El-Sheref, who was sponsored by the Egyptian Ministry of Higher Education. He worked on a synthesis of a new sensor compound, for the long-running collaboration with the Baum group. Also continuing are collaborations with biologist Drew Palmer on quorum sensing, and with Ashraf Aly's group on NMR of heterocycles. Al spoke on the latter topic, at the 2016 Florida Heterocyclic and Synthetic Conference; the group published two papers in 2015, two so far in 2016, and has three more in press.

The **Freund** group continues their NSF funded research on solar fuels. This work on membranes for artificial photosynthesis involves a collaboration with researchers at Caltech, MIT and Simon Fraser University as part of the larger NSF Center for Chemical Innovation – Solar Fuels. Projects are also being developed on electrocatalytic reduction of carbon dioxide in collaboration with Jonathan Mbah (FIT-CHE) as well as a project on artificial olfaction with Anthony Smith (FIT-ECE) and researchers at the University of Manitoba. During the past year, his group has published 7 articles in high impact journals including *Scientific Reports (Nature)* with 3 articles under review.

Dr. Rafaela Nita, a former graduate student in Professor **Andy Knight**'s group, has received a postdoctoral associate award from the National Research Council. Dr. Nita has joined the research group of Dr. Jake Fontana, Center for Bio/Molecular Science and Engineering at the Naval Research Laboratory in Washington DC where she is studying new plasmonic materials for catalytic reactions, an extension of the work she pursued with Professor Knight. Professor Knight spent the previous academic year as an Office of Naval Research Sabbatical Fellow at the Naval Research Laboratory and has now returned to Florida Tech. Professor Knight was named the 2015 Outstanding Chemist of the Year by the Orlando Section of the American Chemical Society.

Dr. **Yi Liao** and his group have continued their research on photochemistry and photoresponsive materials. The photoacid developed by the Liao Group was recently applied to controlling the formation of polymer nanoparticles using visible light. Dr. Liao is collaborating with Dr. Baum to understand the fundamentals of the photoacid. He is also collaborating with Dr. Bashur to incorporate a photo-CORM (carbon monoxide releasing molecule) in a tissue scaffold and study the effects of carbon monoxide on cell growth. Professor Yang from Hebei University of Technology visited the Liao group and spent a year at Florida Tech working on photoresponsive materials.

Gordon Nelson, Dean of the College of Science (1989-2010), Vice President for Academic Affairs (2011), and University Professor of Chemistry since 2011. Dr. Nelson was elected as an ACS Fellow in 2015. Dr. Nelson co-chaired and gave a paper at the Fire and Polymers Symposium at the ACS National Meeting in Philadelphia, August 2016. As ACS Past-President, Dr. Nelson continues as a member of the ACS Council. Drs. Nelson and Feng Yang were awarded a $125k NASA STTR Phase I grant, a $700k Phase II grant, and a $350k Phase IIE grant on highly flame retardant flexible polyurethane foams for energy absorption applications. The Phase II grant was one of only 14 awarded nationally, and the only one at a Florida university. Phase IIE is half industry funded. Phase III funding is in discussion.

Nasri Nesnas continues his research activities primarily in vision and neuroscience. The latter project was awarded an NIH grant. Nesnas lab has a group of 5 PhD, 3 MS, 1 post-baccalaureate and 2 undergraduate students, as well as a high school scholar. Nesnas has active collaborations in neuroscience with Columbia University; in vision research with the University of Arizona; and in synthetic method development with Caltech. Nesnas hosted Professor Brian M. Stoltz of Caltech to present the A. H. Blatt Seminar at Florida Tech in March 2016. At the invitation of one of his first students, Professor Mariana P. Torrente (B.S. '05) of City University of NY, Brooklyn College, Dr. Nesnas presented a lecture about vision and neuroscience. Nesnas was also awarded the 2016-17 Kerry Bruce Clark Award for Excellence in Teaching.

Joel Olson's research group continues to build on the breakthrough they achieved last year in collaboration with Dr. Baum and Dr. Mark Novak at South Dakota School of Mines and Technology. They submitted an application for a U.S. patent (15/194115) for their novel computer-aided drug design (CADD) quantum descriptor. Papers published include: X. Guo, F. Marrucci, N. Price, E.L. Stewart, J.C. Baum, J.A. Olson, *J. Phys. Chem. C*, **2015**, *119*,

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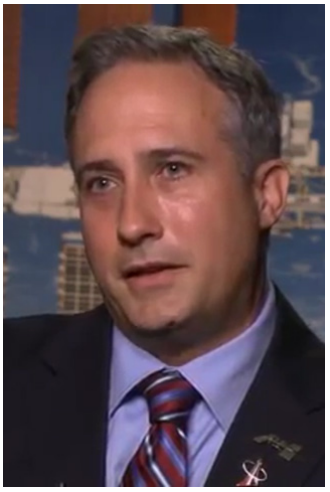
Alumni Focus – Trent Smith, M.S.

Trent M. Smith (B.S. Chemistry, 2001, M.S. Chemistry 2005) is the project manager for Veggie, the Vegetable Production System, which received international attention as astronauts aboard the International Space Station harvested their first ornamental flowers and NASA-approved food grown in space. Trent previously was the strategic communications manager for NASA's Commercial Crew Program (CCP) at Kennedy Space Center. In this role, he coordinated efforts to demonstrate progress to key stakeholders and inform the public on the value of competition for transporting NASA astronauts to the space station. He has served as a NASA technical advisor to the US Senate Committee on Commerce, Science and Transportation, providing recommendations and guidance to policy makers about NASA operations and space issues. After joining NASA in 2003, Trent used his knowledge of polymer chemistry gained in Dr. Gordon Nelson's research lab to lead parts of the investigation of damage caused by foam and ice related to the Space Shuttle Colombia disaster. He has also served as a vehicle processing engineer for the Ares I-X test rocket, and led the transition of KSC facilities as the Space Shuttle retired and the Constellation program began. During his 13 year career, NASA has honored Trent with numerous awards, including a Spaceflight Awareness Award, a KSC Certificate of Commendation for Outstanding Leadership, two NASA Superior Accomplishment Awards for Leadership, and over a dozen Space Act Awards for Inventions and Innovations. Trent remains an active scientist, having written two book chapters, more than a dozen patents granted or pending, and many more government reports and scientific articles.



Chemistry Department News
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24804; K. Sriraman, R.J. Terryn III, X. Guo, M.J. Novak, J.C. Baum, J.A. Olson, *J. Phys. Chem. C*, **2016**, *120*, 3420; and R.J. Terryn III, K. Sriraman, M.J. Novak, J.A. Olson, J.C. Baum, *J. Vac. Sci. Tech. A*, **2016**, *34*, 051402-1. An additional manuscript has recently been submitted to *J. Med. Chem.* Finally, we launched an entirely new Olson Group Webpage, which can be found at **research.fit.edu/olson/**. Check out the web page to see what's been happening in the group, and to update information on group alumni.

Roberto Peverati's research group focuses on the development of computational techniques to tackle outstanding problems in the calculation of the electronic structure of molecules. Electronic structure theory is broad in scope with connections to many branches of experimental chemistry. Research in our group is along three main areas of electronic structure theory. Software development: involves students in the development of large collaborative quantum chemistry computer programs. Theory improvement: expands the applicability of our equations to problems where electron correlation is dominant, which are currently very hard to treat. Applications: working in collaboration with other Faculty within the Chemistry Department and from outside, to try to elucidate the atomic and molecular mechanisms behind their chemistry through our calculations.

Dr. **Mary Sohn**'s group has been focusing on the analysis of organic components in cores taken from Chukchi Sea sediments after recently completing a project on Antarctic benthos. Collaborating with Dr. Aronson in Biological Sciences on the Antarctic project and with Dr. Trefry in Oceanography on Arctic sediments has provided interesting samples for graduate and undergraduate research projects.

With the research funding from NSF, Dr. **Norito Takenaka**'s group continues to develop new synthetic methods that selectively provide novel organic molecules with desired properties. Such methods are a key to access superior analogs of drug candidates found in nature. Recently, graduate students in his group found an efficient way to selectively construct all-carbon quaternary stereocenters, the most complex motif found in molecules of nature.

Rudi Wehmschulte's group is finishing a project dealing with the synthesis of low oxidation state gallium and indium compounds which is funded by the Petroleum Research Fund ($100k). Some results were reported in *Inorganic Chemistry* (**2016**, *55*, 10617). Current work focuses on the synthesis of very strong Lewis acids stabilized by polydentate phenoxide substituents for applications in catalysis.

Dr. **Kurt Winkelmann** recently handed over the reins of the General Chemistry program to Dr. **Jessica Smeltz**. He is now devoting more time to studying the environmental impact of nanoparticles and he continues his nanotechnology and chemistry education research. Mr. Leonard Bernas (B.S. '15, M.S. '16; currently at Harris Corp., Palm Bay, FL) completed his M.S. thesis describing the effect of silver cations and silver nanoparticles on the growth of common water plants. Dr. Winkelmann will expand this project to study different nanomaterials and collaborate with Dr. Drew Palmer in the Biological Sciences Department to study the impact of these nanomaterials on biological functions within plant cells. He is collaborating with faculty in the Mechanical and Aerospace Engineering Department and scientists at Vencore Services and Solutions Inc., a NASA contractor, to test a wire repair method in low-Earth orbit. This is both an educational and a research project. Students will learn project management, engineering design, and microscopy as they design the payload, experiment, and analysis methods. This study is of interest to Vencore for their development of self-healing materials for space flight. Dr. Winkelmann co-edited the book *Global Perspectives of Nanoscience and Engineering Education* published in summer 2016 and he is co-author of a book chapter about nanotechnology education around the world in the upcoming edition of the *Handbook of Nanotechnology*, both published by Springer International.

Give to the Chemistry Department Directly via Endowments.

The Paltzik Endowment: Endowed by the family of Alan Paltzik and alumni. Supports outstanding incoming graduate students.

The Baum Endowment: Endowed by alumni. Provides scholarship award(s) for the outstanding junior undergraduate student(s).

The Johnathan B. Zung Family Scholarship Endowment: Endowed by Dr. Johnathan Zung (B.S. '86). Provides support for a freshman undergraduate student.

Chemistry Endowment (Blatt Seminars): Endowed by Organic Syntheses and alumni. Provides funds to host a world-famous speaker in organic chemistry research.

Sharma Endowment: Endowed by New York Community Trust Funds. Supports research in environmental remediation and Fe chemistry.

Mrs. Krishna Devi Sharma Fellowship Endowment: Endowed by Dr. Virender Sharma. Provides support for a Ph.D. graduate student.

Martin Zung Memorial Chemistry Award: Endowed by Dr. Jonathan Zung (B.S. '86). Supports a junior/senior undergraduate student.

For more information contact Dr. Michael Freund at msfreund@fit.edu

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Florida Tech Chemistry Alumni are on FACEBOOK!
Just search for the Facebook group: Florida Tech Chemistry Alumni and Friends

From the Department Head

Greetings:

Since our last newsletter, the Department has been very active with the arrival of two new Assistant Professors, new instrumentation, new funding and continued research productivity. We encourage you to check our webpage (cos.fit.edu/chemistry) often for updates of new happenings and highlights related to our students and faculty. We have included a "latest publications" link to give a current snapshot of recent publications (31 in 2016!)

We have been incredibly fortunate to add Dr. Roberto Peverati and Dr. Alexander Schoedel to our faculty ranks (see story p. 1). I encourage you all to peruse their departmental websites to learn more about them and their research. We are also very happy to have Dr. Andy Knight back from his sabbatical at the Naval Research Laboratory. Dr. Clayton Baum remains with us after retirement, flush with NSF funding secured jointly with Dr. Yi Liao to continue their collaborative research (see the story on Dr. Baum's retirement on p. 1).

In addition to our "software" improvements we have had major hardware upgrades with the additon of new NMR, LC-MS, and X-ray diffraction instruments (see story, p. 1).

As we continue to transition and grow, our connection with alumni will be as important as ever. We are looking forward to interacting with you and hearing about your careers and families (*c.f.* Alumni Focus, p. 2). Whenever possible we hope that you will visit the Department to see what is going on and to meet the new additions. We are looking forward to your involvement. All the best in your continued success.

--Dr. Michael Freund

Editor's Corner With the retirement of Dr. Clayton Baum, I have now been promoted to senior editor of *The Panther Chemist* (see story on p. 1). I aspire to show the same dedication that Clayton did for his students and for Florida Tech. Our alumni define our department. As such, we are always interested hearing from you. So please keep in touch, especially with regard to changes of email or physical addresses. And look for annual installments of *The Panther Chemist*, to be issued each spring.

--Dr. Joel A. Olson