

USF Chemistry NEWS

News of Interest to
Friends of the Department of Chemistry
University of South Florida

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Introducing new Chemistry faculty members...

Dr. Wayne Guida joined as Professor of Chemistry (his biography appears below).

Dr. Xiao (Sheryl) Li, an analytical chemist, joined as Assistant Professor of Chemistry. She received her doctorate from the University of Illinois at Champaign-Urbana (2004) and was a post-doctoral fellow at the University of Texas-Austin.

Further information and pictures may be found in the Faculty section of our Webpage (http://chemistry.usf.edu).

Faculty Recognition

According to *in-cites*, from *Essential Science Indicators* $^{\text{TM}}$, **Dr. Mohamed Eddaoudi** is among the top 100 most-cited chemists in the world. He ranked 68 among 6,523 chemists.

Dr. Eddaoudi and **Dr. Peter Zhang** were among six faculty (campus-wide) who were given "Outstanding Research Achievement Awards" at the 2007 Faculty Honors & Awards Reception on November 7th. **Dr. Eddaoudi** was the first two-time recipient of this award.

Both **Dr. Eddaoudi** and **Dr. Zhang** are recipients of the coveted five-year NSF Early Career Development Awards

REU News

REU is a research experience for undergraduates and was initiated as an NSF-supported summer program with a three-year grant, as noted in previous issues of *News*. The program was adapted to the fall and spring semesters starting with the fall of 2005 and some 70 students.

This term the program is being coordinated by Mr. Greg McManus.

Faculty you should know

Dr. Wayne Guida wrote: "My story is perhaps a bit unique. I'm totally I was born, raised and homegrown. educated in Tampa. I went to high school in Tampa and received my B.A. and Ph. D. degrees in chemistry from USF in Tampa. At USF, Professors Jack Fernandez and Dean Martin were my undergraduate mentors, and I was very fortunate to have had the opportunity to do undergraduate research with Prof. Bob Whitaker under the auspices of an NSF funded Undergraduate Research Participation (URP) program, similar to today's REU initiative. My work with Bob, which led to two publications, involved the study of clathrates that form when the propeller-like substituted cyclotriphosphazatrienes crystallize from certain organic solvents. I can still vividly recall how thrilled I was to see our studies appear in print - in the Journal of Inorganic and Nuclear Chemistry (now named Polyhedron).



Dr. Guida in his office at CHE 202D

My Ph.D. studies were directed by Prof. Doug Raber (Prof. Terry Owen was Department Chair during that time) and our research involved both synthetic physical organic chemistry. One of our interests involved the use of oxonium salts in organic synthesis. It was Doug, however, who stimulated my interest in computational chemistry (Doug, himself, was a post-doc with Prof. Paul von Ragué Schleyer, who many consider to be one of the founders of the computational chemistry field). I must say that I was taught by many, many outstanding professors during my years in the Chemistry Department at USF, too many to mention all of them by name in this short discourse. Suffice it to say, though, that I received an exceptional education at USF, one that served me very well in my subsequent endeavors.

After leaving USF, I spent a year at Duke University as a Post-doctoral Fellow working with Profs. Steve Baldwin and Peter Jeffs. Our work was funded by the National Institute on Drug Abuse and involved the synthesis of cocaine labeled with tritium at various positions for metabolic studies. One of our starting materials was unlabeled Merck

pharmaceutical-grade cocaine of course, we had to account for each and microgram we used in our experiments. We lived in constant fear that some unsavory character might find out about our work and hold us up at gun-point for this substance, the bulk of which was locked in a safe at the teaching hospital at Duke. My stay at Duke served to enlighten me about pharmacological principles that, in addition to exposure I received at USF regarding the pivotal role chemistry plays in the drug discovery and development process, ultimately led to my long-standing interest in the discovery and design of novel therapeutic agents.

From Duke, I went to Eckerd College (for the first time) where I taught courses in organic chemistry and biochemistry and did research with undergraduates. Our studies involved both synthetic and computational One project involved the chemistry. synthesis of chiral crown ethers as catalysts for asymmetric synthesis. In retrospect, these (and other projects in our lab) were undertakings ambitious undergraduates. Fortunately, I was blessed with an abundance of extremely talented students and we made considerable progress. As expected, these former students have done extremely well and are now at the height of their careers in academic labs, pharmaceutical labs and in private medical practice.

After a few years at Eckerd, I longed to be more involved in research and after a one -year sabbatical leave at the University of South Carolina working in Prof. Jim Marshall's lab, I joined Prof. Clark Still's lab at Columbia University as a Senior Post-doctoral Associate, or maybe my title was Senior Research Fellow. Truthfully, I don't remember which it was but I was working with a group of post-docs and two computer

scientists and we were involved in producing the MacroModel molecular modeling software.

This was an extremely exciting time for us since we had funding from five pharmaceutical companies to actually produce a commercial product that would be used by their computational chemists and their synthetic chemists who might be interested in doing modeling as well. So, the software had to be accessible to the novice and expert alike and had to actually something useful! Clark alongside the rest of us, and we all worked very hard to ensure that the molecular mechanics calculations churned out by our code were reasonably accurate and that the user interface was as intuitive as possible. I guess I'd be dating myself if I mentioned that these calculations took place on a VAX computer that was the size of a very large refrigerator and that the best graphics terminal available to us was, well just that, a terminal that had to be tethered to the VAX computer to function. It had a dial box though - somebody should bring back the dial box! Now if you don't know what a dial box is, just ask me and I'll try to describe one.

In large part because of my involvement in the MacroModel project, I was invited to join the Pharmaceuticals Division of Ciba-Geigy Corporation in Summit, New Jersey. Ciba-Geigy, a Swiss company, eventually merged with Sandoz (also Swiss) to form Novartis Pharmaceuticals. I stayed at Ciba and then Novartis for almost 13 years and particularly enjoyed the many visits I made to Switzerland, which is a truly beautiful country.

While at Ciba/Novartis, our computational modeling group grew from a small group of two people (myself and a

post-doc) to a group of 30+ individuals engaged in molecular modeling, structural bioinformatics, X-ray crystallography, protein **NMR** spectroscopy, protein throughput biochemistry, and high screening. We made valuable contributions numerous drug discovery projects in inflammatory primarily and cardiovascular diseases. We also had considerable freedom to develop new computational methodology and publish our work, all of this without having to write a single grant application! Life was good.

After the formation of Novartis, and due to significant changes that were taking place industry-wide in the pharmaceutical business, it became increasingly more difficult to conduct novel research in computational chemistry in a pharmaceutical environment.

So, after a brief stint as President and CEO of Schrödinger, Inc., a company that was founded by Profs. Rich Friesner and Clark Still of Columbia along with Prof. Bill Goddard of Cal Tech and Dr. Murko Ringnalda (one of Rich's and Bill's students), I returned to the Tampa Bay area to teach once again at Eckerd College and do research with undergraduates. By the way, Schrödinger markets MacroModel and it is still in use in academic, government and industrial labs around the world. Upon returning to Florida, I fairly soon became affiliated with the Drug Discovery Program at the H. Lee Moffitt Cancer Center & Research Institute, where I still maintain a lab to this day.

I have now joined the Chemistry Department at USF and would have to admit that my career thus far has taken me down a number of unexpected paths. Some have said that I just never figured out what I wanted to do when I grew up. My good

friend, Greg Paris, at Ciba/Novartis and I used to laugh and tease each other about this since both of our careers have taken similar circuitous routes. Doug Raber, my Ph.D. mentor, shared with me that he once wrote in a letter of recommendation that at first glance my career path might appear to simply be a random walk, but upon closer inspection one can observe a well orchestrated quest. Yes, I suppose that is how I would prefer to think about it.

My wife, Natalie and I and our two boys, had returned home a few years ago to the Tampa Bay area, first living in St. Pete Beach and currently in Tampa. I have now returned to my academic home and am delighted to be back in the Chemistry Department at USF."

New Office Manager

Kimberly Read, B.A., M.B.A., joined the Department as Manager Fiscal and Business Administration on September 25th. **Dr Zaworotko** noted that "[she] is a manager with over 15 years experience: the last six years have been with USF. Through her previous experience in the Department of Psychology and the Enterprise Business



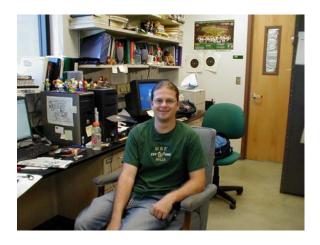
Ms. Kimberly Read, M.B.A.

Systems, she brings a detailed knowledge of the university business systems... as well as experience with University policies and procedures. In addition to her business background, Kimberly has also served as a journalist for About.com. She received her B.A. from USF and an M.B.A. through the University of Maryland."

The joy of our present, the hope of our future...

[a continuing series on current graduate students]

John J. Perry IV wrote: "I was born October 5th 1980 on MacDill AFB here in beautiful Tampa, Florida. I grew up in south Tampa where I attended local public schools (Dale Mabry Elementary and Coleman Schools) which was Middle pretty unremarkable. I tried my hand at a few different youth's sports such as T-ball, little league baseball, soccer, and cub scouts, but was equally terrible at all of them so I spent the majority of my childhood reading books and watching 'Saved by the Bell' and 'MacGyver.' By the time I was old enough to attend high school I thought I wanted to be a heart surgeon so I applied to a medical magnet high school, The Academy of Health Professions, located on the campus of Tampa Bay Technical H.S. (GO Titans!!!). I would often replace elective courses with additional Math, Science, and English classes (who needs drama anyway?) and in all I took 7 advanced placement courses and passed the national exams for 6 of them, the only exception being Chemistry, go figure." "During H.S. I was a member of the Cross Country and Track athletic teams, Mu Alpha Theta (competitive math league...nothing beats math tests on Saturday mornings), Society, National Honors Health America **Occupations** Students of



Mr. Perry in his laboratory

(competitions and elected offices), and held a part-time job. I graduated from T.B.T. as Salutatorian in 1999 and had performed well enough to qualify for Florida Academic Scholars, and since my mother was a single mom, and we had little money, I was destined to stay in Florida for a free college education. I started out still a pre-med in my naïve mind, but a mathematics major none the less and enrolled in the university's Honors Program (now the Honors College). I had been used to taking two math and two science classes in high school so I gave it a try in university as well, and it worked out okay. Since I needed to take all of the required courses for med school anyway, by the time I was a junior the Chemistry degree seemed doable, so I did it too. I graduated from the Honors College and the University with two degrees in four years (Mathematics and Chemistry)."

"In the summer after my junior year I was fortunate enough to be offered a chance to conduct research in Dr. Zaworotko's group working in the fields of coordination polymers and Supramolecular Chemistry and was immediately hooked. It was chemistry, which I had always found interesting and exciting (probably because I found it more challenging and rewarding

than other natural sciences), but it had a flair of mathematics to it as well, notably topology and crystallography. I continued on into the fall of my senior year and by now had changed my mind about the whole medical school thing.

I applied to and was accepted to USF graduate school for chemistry and choose to stay in Dr. Z's research group. In fact I choose to stay at USF because I wanted to work in those fields and for Dr. Z. I am beginning my fifth year in grad school working towards a Ph.D. and have been lucky enough to attend numerous local, state, regional, national, and international conferences to present my work and collaborate with peers. I have authored or co-authored two communications and three full papers, with several more in the pipeline. I expect to graduate within the next year at which time I hope to obtain a competitive post-doc position and eventually academic position at a research university."

New Project

A new project "Novel Porous Metal-Organic Frameworks for Hydrogen Storage," was recently funded by the U.S. Department of Energy. It is one of 13 projects that "will focus on fundamental science in support of hydrogen technologies," according to the Department's Office of Research.

Dr. Mohamed Eddaoudi is the principal Investigator with **Drs. Mike Zaworotko** and **Brian Space** as Co-Principal Investigators.

The project is funded at \$882,000 over a three-year period, according to **Dr. Zaworotko.** The project is one of seven in the area of novel materials for hydrogen storage. Additional information was found at: http://www.energy.gov/news/5064.htm

Martin Lecturer

Patrick H. Benz (Ph.D., '76), President, Benz Research and Development, Sarasota, presented the 2007 Martin Lecture on September 27th: "Contemporary Topics in Contact Lens and Intraocular Lens Materials."

News on Campus

The Marshall Student Center construction continues "on budget and on time" for the scheduled opening in Summer, 2008. See the progress at www.ctr.usf.edu

A new parking garage at the corner of Alumni Drive and Walnut (about a block from the Science Center) is scheduled to open in March 2008.

The student parking space to the east of the Science Center parking lot has been closed in preparation for construction of a dormitory.

Abe Stern, a doctoral candidate working with **Professor Brian Space**, is co-president of the Graduate Assistants United, an affiliate of United Faculty of Florida. He is the first chemistry student to hold this office.

A Message from the Chair...

As we approach the end of 2007 it is appropriate to reflect upon accomplishments of 2007 and our goals for However, given that my term as Chair will come to an end in August 2008, it is perhaps time to reflect upon what has happened since I came to USF in September 1999. The acknowledged centrality of chemical concepts towards the implementation of new technologies for

addressing societal problems continues to make the study of chemistry a critical academic component of all major research universities. The reason for this situation is simple: everything in the physical world can be delineated by understanding molecular matter at the intermolecular level. The broad relevance of chemistry has been the underlying theme that has facilitated the renewal and growth of the Department of Chemistry since 1999: 13 new research faculty (6 tenure track, 7 tenured); a new building (NES); renovation of existing infrastructure (CHE); increased research funding: greater impact (publications, prestigious citations, conference invitations, patents); growth in academic programs (doubling in size of Ph.D. program to ca. 100 students, > 85% increase in undergraduate SCH since 1999).

In this context, 2007 has been a watershed that makes predicting the future simple as we expect to see "more of the same": hire of new faculty [Drs. Xiao (Sheryl) Li and Wayne Guida joined in 09/07; see story above]; a proactive role for our three core areas of research application with cognate programs and/or industry:

- 1. Drug discovery (through the Center for Molecular Diversity of Drug Design, Discovery and Delivery: CMD⁵, http://chemistry.usf.edu/cmd5 a key component of the Florida Center of Excellence in Biomolecular Identification and Targeted Therapeutics);
- 2. Materials chemistry (through the interdisciplinary research group in Smart Metal-organic Materials Advanced Research and Technology Transfer, SMMARTT, http://chemistry.usf.edu/smmartt, that in 2007 has been awarded major peer-reviewed multi-year grants by the Departments of Energy and Defense; story above);
- 3. Chemical and science education (the Department has taken a leadership position

in STEM education research and curriculum development due to the contributions of Drs. Meisels, Potter, Lewis, and Caswell).

We will also continue to focus upon quality and outreach and 2007 has seen much in the way of tangible recognition: NSF CAREER Awards (the Department now has three awardees, Drs. Cardenas, Eddaoudi, Zhang); more JACS papers than ever before (7 and counting in 2007); citations (the Department is #1 in Florida in terms of citations per paper since 2000 and, most notably, Dr. Eddaoudi is now listed as one of the top 100 most cited chemists by the *Institute for Scientific Information*; story above).

In terms of outreach, there are numerous interactions with our community and with companies in terms of research contracts, consulting and patent licenses. A long term objective of the Department is to build the base of support for students. 2007 saw significant developments in the form of new endowed scholarships for graduate students (Barbara B. Martin Endowed Fellowship in Chemistry, the Martin Travel Endowment) and for undergraduate students (the Sally Everett Memorial Scholarship). In addition, each year, faculty and staff of Chemistry join others in raising funds scholarships and funds.

The 2006-2007 Faculty/Staff Campaign raised a record \$3.3 million dollars! We may take pride in knowing that Chemistry faculty and Staff donated over \$50,000 for worthy funds. In chemistry, funds of interest include those listed below together with the account numbers. Should you wish to participate in this year's campaign you may send checks "USF Foundation, Inc." with a note regarding the account of their choice to me, at the address on the last page.

Sadly, two long-serving faculty members, Profs. Jay Worrell (1938-2007) and George Wenzinger (1933-2007), passed away in 2007. One of the funds listed below is named in honor of Prof. Worrell.

Chemistry Operating Fund for general use (acct. # 42-0550)
Chemistry Scholarship Undergraduate
Awards (42-0700)
Barbara and Dean Martin Seminar Series
Fund (42-3014)
George Bursa Award in Chemistry for outstanding graduate students (42-3013)
Owen Chemistry Undergraduate Research
Fund (42-3030)
Worrell Memorial Scholarship (42-

35th anniversary

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2007 is the 35th anniversary of the awarding of the first USF chemistry doctoral degrees to **Anthony J. Girgenti** (Ph.D. '72) and **Craig Foreback** (Ph.D. '72).

News about...

Charles A. Asowata (B.S. '80), U.S. Army, was promoted to Lt. Colonel on October 16th in the Pentagon Hall of Heroes.

Had lunch with **Melissa Derby** (Ph.D. '02) at the Boston ACS meeting. She is enjoying life at Harvard University where she is a laboratory manager in Organismic and Evolutionary Biology.

We saw **Dr. Jack Fernandez** (Charter Faculty; 1960-95) and his wife **Mrs. Sylvia Fernandez** at the Faculty/Staff Club reception for new faculty members (August).

Dr. Fernandez has also served as a 2006-2007 Community Columnist for the Tampa **Tribune** and has contributed a personal column each month.

Dr. George Jurch (Faculty, 1966-98) and his wife, **Mrs. Molly Jurch**, attended the lecture by **Dr. Pat Benz** on September 27th. **Dr. George Wenzinger** (Faculty, 1963-99) helped introduce him.

Dr. Dean F. Martin (Faculty, 1964-06) was given the Honorary Membership Award of the Aquatic Plant Management Society, its highest honor. He has been a member of the Board of Directors, and held several offices including President.

He also served as a tour speaker for the American Chemical Society in September. He and his wife, Barbara Martin, visited sections in Texas (Houston, Lake Jackson, Victoria, San Antonio, and McAllen).

Brian Moulton (Ph.D. '03) said hello at the Boston ACS meeting. He was commuting from Brown University to present papers in the Inorganic Chemistry Division.

Jose Ors (Ph.D. '74) attended the lecture by given by Dr. Benz on September 27th.

Anil K. Patri (Ph.D. '99), an NCI scientist, gave a seminar to the Department Faculty and students on October 13. The title was "Cancer Nanotechnology: Preclinical Characterization".

William G. Sawyers (Ph.D. '99) is a field-based consultant for Applied Biosystems -/MDS-Sciex, and lives in Pasadena, MD on Chesapeake Bay, which he enjoys cruising around in his spare time.

Ralph Salvatore (Ph.D. '01), Professor and Chair, Department of Chemistry, Lehman College was among those attending the

"Symposium on Molecular Diversity in Drug Design, Discovery, and Delivery," October 24-26, organized by **Dr. Ed Turos**.

At the recent SERMACS 2007, we saw a copy of the 9th edition of *Organic Chemistry* by **T.W. Graham Solomons** (Faculty, 1960-1990) and C. B. Fryhle. It has a 2008 copyright.

News and feedback

Chair's Address: Dr. M. J. Zaworotko Department of Chemistry-CHE 205 University of South Florida 4202 East Fowler Avenue Tampa, FL 33620-5205

For additional information on faculty, staff, students, awards, fellowships, and programs, please look at our Department Home Page: http://www.cas.usf.edu/chemistry

For past issues you may have missed, please see the Home Page.

News for us or comments? Please write to dmartin@cas.usf.edu