



**USF** UNIVERSITY OF  
SOUTH FLORIDA



**Department of Chemistry**

*College of Arts and Sciences*

## Graduate Faculty/Research Interests

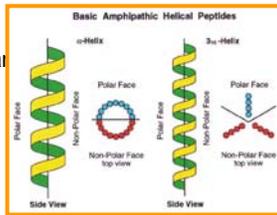
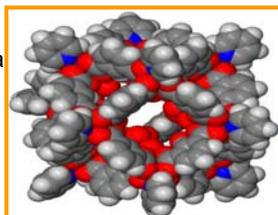
<http://chemistry.usf.edu/>



### **About USF and the Department of Chemistry**

The University of South Florida is a comprehensive multi-campus research university serving more than 45,000 students and is the largest metropolitan research university and the second largest in total enrollment in the State University System of Florida. In FY2006/2007, USF generated \$308 million annually in sponsored research. Its endowment exceeds \$244 million and includes 55 endowed chairs. USF is classified as a Doctoral/Research University-Extensive, which is the highest classification by the Carnegie Foundation. According to the latest (2006) annual National Science Foundation Survey of R&D expenditures in Science and Engineering, USF ranked 42nd in public universities and 33rd in R&D expenditures in medical sciences. USF faculty members are making national and international contributions in their fields, and their commitment to quality education is central to the University's teaching, research, and service mission.

The Department of Chemistry at USF is home to 27 tenured and tenure-track faculty members and over 130 graduate students (both M.S. and Ph.D.) with the faculty bringing in over \$8 million in external funding, with \$6 million being from the National Science Foundation (NSF), NIH, DoD and DoE over the past five years. The Department of Chemistry has also developed state-of-the-art instrument facilities including both high field NMR spectroscopy core and mass spectrometry/protein synthesis core facilities. The Chemistry Department is home to research centers: *Center for Molecular Diversity in Drug Design, Discovery and Development* (CMD<sup>5</sup>) and *Smart Metal-organic Materials Advanced Research and Technology Transfer* (SMMARTT). With strengths in materials chemistry, biophysics/computational chemistry, drug discovery/synthesis, and biochemistry our graduate students have excellent opportunities for inter-disciplinary degrees in a rapidly growing department.



## USF Department of Chemistry Graduate Faculty/Research Interests

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**M. Acevedo-Duncan, Assistant Professor:** *Biochemistry*- Research in Dr. Acevedo-Duncan's laboratory investigates signal transduction pathways involved in cell cycle control in high-grade gliomas, one of the most radioresistant forms of cancer for which there is no current successful therapy.

**Jon Antilla, Assistant Professor:** *Organic- Chiral Organocatalysis, Metal-Catalysis, New Stereoselective Reaction Methodology, Marine Natural Products, Drug Discovery.* We have begun initial studies into a new area of organocatalysis that utilize chiral Brønsted acids in a number of interesting synthetic transformations. We have also initiated a project whereby marine natural products are being transformed into analogues that are expected to provide increased bioactivity versus a number of disease types. Recently, we have begun a collaboration with the medical center to develop drugs for post-stroke treatment.

**Bill Baker, Professor:** *Organic-* Biosynthesis of alkaloids in Floridian tunicates; Chemical Ecology of shallow-water antarctic marine invertebrates; Chemotherapeutic agents from marine invertebrates; Natural products from marine microorganisms; synthesis, semi-synthesis and lead optimization of bioactive marine natural products.

**Kirpal Bisht, Associate Professor:** *Organic-* Efficient and environmentally friendly synthetic routes towards synthesis of polymers for biodegradable applications; Stereo controlled synthesis/modification of molecules that serve as precursors to biologically active molecule, i.e., unnatural amino acids, sugars, etc.; Regio and stereo-selective synthesis of multi-arm dendrimers by chemo/enzymatic routes.

**Jianfeng Cai, Assistant Professor;** *Bioorganic Chemistry, Medicinal Chemistry, Biophysics* - The research in our laboratory is focused on the expansion of interdisciplinary research at the interface of chemistry and biology to discover novel peptidomimetics and other small molecules that modulate protein-protein interactions involved in critical cellular processes. Understanding how these compounds interact with proteins will help to reveal mechanisms governing cell activities. We are particularly interested in developing compounds that lead to the design of novel therapeutics potentially targeting cancer, HIV, and Alzheimer's disease, etc

**Mohamed Eddaoudi, Associate Professor:** *Inorganic/Materials-* Students to be involved in this interdisciplinary program will be exposed to a variety of techniques including solid state synthesis, organic and inorganic chemistries, Solvo/Hydro thermal synthesis, characterization techniques (UV-visible, Gas chromatography, solid and solution NMR, Infra-Red (IR), Fluorescence, X-ray powder diffraction (XRPD), Single X-ray diffraction, Thermogravimetric Analysis, and Circular Dichroism spectroscopy) and other physical methods to characterize porous materials.

**Steve Grossman, Professor:** *Biochemistry/Biophysics-* Protein folding, structure/function of the phosphagen kinases, modulation of arginine kinase in insects.

**Wayne Guida, Professor:** *Computational/Organic/Biochemistry-* The Guida group uses computational chemistry for the structure-based design of new therapeutic agents. The lab performs in silico screening of chemical databases to identify novel compounds that bind to specific biomolecular target molecules and performs molecular modeling studies in collaboration with medicinal chemists for lead optimization studies that ultimately allows for the discovery of new drugs that can be tested in a clinical setting.

**Julie Harmon, Professor:** *Polymer/Physical Chemistry-* Vinyl polymerizations; polymer processing; carbon nanotube composites; optical fiber materials; polymer structure-property relations; radiation effects on polymers; thermal analysis - dielectric analysis, dynamic mechanical analysis, differential scanning calorimetry; mechanical properties.

**Milt Johnston, Professor:** *Computational Chemistry-* Molecular Spectroscopy (in particular, NMR), Physical Chemistry (that is, the science of anything which is interesting), Molecular Orbital Theory, Monte Carlo Calculations and Simulations, Density Matrix Theory and Computational Simulations of Real Systems.

**Randy W. Larsen, Professor and Chair:** *Biophysical Chemistry-* Protein structure/function, time-resolved optical spectroscopy. We are interested in time-resolved conformational changes and thermodynamics associated with ligand binding to heme proteins, biological electron transfer, protein folding and bacterial signal transduction. We utilize both traditional time resolved optical spectroscopies (nanosecond transient absorption/fluorescence) together with novel photothermal methods (photoacoustic calorimetry and photothermal beam deflection).

**Jennifer Lewis, Associate Professor:** *Chemical Education-* Conceptual Change, Assessment Issues, Qualitative Methods, and Evaluation

**Xiao (Sheryl) Li, Assistant Professor;** *Analytical Chemistry-* Bioanalytical Chemistry, Drug Effect and Development, Optical Spectroscopy, Scanning Electrochemical Microscopy (SEM), Nanoparticle, Electrochemistry

**Abdul Malik, Associate Professor:** *Analytical chemistry-* Analytical separations including Column Technology for Analytical Micro-separations, Sol-gel Chemistry-based Separation Systems, Capillary Zone Electrophoresis (CZE), Capillary Electro-chromatography (CEC), Capillary Gas Chromatography (CGC), Micro-column Liquid Chromatography (micro-LC), Supercritical Fluid Chromatography (SFC), Chiral Separations, Biomedical and Environmental Applications of Micro-separation Techniques. Sample Preparation Techniques include Solid-phase Micro-extraction (SPME), Capillary Micro-extraction (CME), Supercritical Fluid Extraction (SFE), SPME-GC, CME-GC, CME-HPLC, CME-CEC, CME-CE.

**Roman Manetsch, Assistant Professor:** *Organic-* The research interests represent a well-balanced blend of organic and biological chemistry, addressing in particular modern aspects of medicinal chemistry. The conducted research includes development of new drug/target discovery methods and organic synthesis of new biochemical tools, as well as their application to biologically relevant processes.

## USF Department of Chemistry Graduate Faculty/Research Interests Continued

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**Dean F. Martin, Emeritus Distinguished University Professor:** *Analytical / Environmental* -- Applications of coordination chemistry currently focusing on IMLIGs (immobilized ligands) for the removal of arsenic and other species from water supplies. Historical aspects of chemistry.

**Mark McLaughlin, Professor:** *Organic*- We are synthesizing amphipathic helical peptide mimetics with anticancer activity and constrained dipeptides that enforce an extended conformation for use in the synthesis of stable beta-sheet-like peptide structures with applications to age-related disease such as Alzheimer's and Parkinson's disease. We are developing a new class of HIV protease inhibitors based on related constrained dipeptide-like units using a structure-based approach. We are also synthesizing cell-permeable peptide nucleic acids as anticancer therapeutics and as early cancer diagnostic aids.

**David Merkler, Professor:** *Biochemistry*- Long term plans for the laboratory will be to build on our experience with peptidylglycine  $\alpha$ -amidating enzyme to work on other enzymes catalyzing post-translational modifications of proteins and peptides, such as tyrosylprotein sulfotransferase, acyl-CoA:glycine N-acyltransferase, peptidylarginine deiminase, and other oxygenases, such as tyrosinase. Other projects in the lab deal with the biosynthesis of cell signaling fatty acid amides, the discovery of novel peptide hormones, and the synthesis of reactive CoA analogs for proteomic profiling.

**Li-June Ming, Professor:** *Inorganic/Biochemistry*- Hydrolytic chemistry, metal-DNA chemistry, chemical modeling, detoxification of toxic phosphoesters like pesticides and nerve agents, NMR of paramagnetic compounds. *Biochemistry* - Metalloproteins, Metalloproteases, Metalloantibiotics, peptides and proteins as "natural model systems", Magnetic Resonance Spectroscopies. Structure, activity, and inhibition of Alzheimer's disease-related amyloid-beta peptides.

**Rebecca O'Malley, Professor:** *Physical Chemistry*- Mass-Spectrometry. Laser desorption, time-of-flight, FTICR, HPLC MS/MS. Physical and analytical applications of mass spectrometry to interesting research problems. Characterization of structural/stereo isomers by MS/MS. Isolation, separation and characterization of physiologically active compounds from natural sources. Chemical Education.

**Bob Potter, Professor:** *Biochemistry/Science Education*- Protein Chemistry/Structure Function, Spectroscopic Analysis of Blood and Blood Products, Mechanisms of Biological Signal Transduction, Regulation by Mono-Glycosylation and Protein Phosphorylation-Dephosphorylation

**Brian Space, Professor:** *Theoretical/Computational Chemistry*- Our group is concerned primarily with computer simulation of condensed phase phenomena. A main research thrust is the development and application of instantaneous normal mode and time correlation function methods to model liquid state vibrational spectroscopy. These (semi)classical methods can be successfully applied in a complimentary fashion to understand intramolecular vibrations in the condensed phase. We also develop new and improved semi-classical approaches. We are also interested in the low frequency portions of the spectrum where there is still uncertainty as to what information these ever changing low frequency modes might relinquish!

**Santiago Sandi-Urena, Assistant Professor;** *Chemical Education*- Our research revolves around the assessment and development of metacognition use, and its impact on chemistry problem solving. We are also interested in designing strategies to evaluate the effectiveness of learning environments (such as research experiences) in promoting intellectual skills associated with scientific development. Our research uses both quantitative and qualitative inquiry approaches, as well as mixed-methods designs

**Ed Tuross, Professor:** *Organic*- Our research group is focusing on the synthesis and evaluation of new antibacterial and anticancer agents, as well as development of nanoparticle polymers as drug delivery vehicles and biomedical plastics.

**Arjan van der Vaart, Assistant Professor;** *Biophysical/Computational Chemistry* - Computer simulations of biomolecular systems. We are particularly interested in coupled binding - folding processes of DNA-binding proteins and in the conformational dynamics of kinases and bacteriological toxins. We also develop new computational methods to push simulations to longer time scales and larger system sizes.

**H. Lee Woodcock, Assistant Professor;** *Computational Chemistry/Biophysical Chemistry* - My research focuses on the development and application of molecular simulation techniques to solve interesting problems that exist at the interface of chemistry, biology and medicine. I currently have two main areas of interest: (1) Examination of structure, dynamics, and mechanism by simulation. Specifically, this focuses on two main areas; examination of antibiotic and inhibitor resistance mechanisms with hybrid quantum mechanical and molecular mechanical (QM/MM) methods and elucidation of carbohydrate structure and dynamics as related to energy production. (2) Development of new simulation and analysis techniques. This area primarily focuses on multi-scale modeling methods, techniques for computing free energies of enzymatically catalyzed reactions, and methods for probing the normal modes of complex systems.

**Mike Zaworotko, Professor:** *Inorganic/Materials/Pharmaceutical Chemistry*- *Crystal engineering, nanotechnology, supramolecular chemistry, x-ray crystallography.* Design, synthesis and application of network solids; molecular recognition; nano-porous adsorbents for environmental, pharmaceutical and materials applications; crystal structure analysis and prediction; drug design; supra-molecular synthesis of solids; solid phase synthesis; coordination polymers; nano-composite structures.

**Peter Zhang, Associate Professor:** *Organic*- The primary research interests of our group are in the areas of organic and organo-metallic chemistry. The research program involves the design and synthesis of new organic and organo-metallic compounds, and the exploration of their applications in areas of catalysis, medicine, biomimics and materials. The specific applications include 1) the development of catalytic systems for selective organic reactions including asymmetric synthesis; 2) discovery of new therapeutic agents for cancer and neurodegenerative diseases; 3) the construction of functional models for metallo-enzymes that can mediate important chemical and energy transformations; and 4) the synthesis and study of novel transition metal-containing inorganic-organic hybrid materials.