

December 2012



SAS Student Awards and the FACSS Innovation Award Presented at SCIX 2012

Barbara Stull Graduate Student Award



Ruchira Chatterjee (on right with SAS President Mary Kate Donais) of Rensselaer Polytechnic Institute received the Barbara Stull Graduate Student Award at SCIX 2012. The award recognizes a graduate student for outstanding research in spectroscopy and was presented in honor of longtime SAS colleague Barbara L. Stull. Ms. Chatterjee is a doctoral student in the Department of Chemistry and Chemical Biology at Rensselaer Polytechnic Institute. She has been developing structural methods to directly probe the light-driven water oxidation reaction in the photosynthetic protein complex, photosystem II. Her research on understanding the fundamental principles of solar water oxidation in nature might enable the design of a new generation of cost-effective and highly efficient devices for solar energy conversion. Ruchira joined Rensselaer Polytechnic Institute as a doctoral student in 2007, after earning her

Bachelor's degree in Chemistry at St. Xavier's College (Calcutta, India) and a Master's degree in Physical Chemistry at the University of Delhi (Delhi, India). In early 2008, she joined the research group of Professor K.V. Lakshmi in the Department of Chemistry and Chemical Biology. Ms. Chatterjee's graduate research is focused on developing advanced multi-dimensional multi-frequency pulsed EPR spectroscopic methods to disentangle the individual steps that lead to solar energy conversion by photosystem II. The solar-water-splitting protein complex, photosystem II (PSII), catalyzes one of the most energetically demanding reactions in nature by using light energy to drive a catalyst capable of oxidizing water. Elucidating the water oxidation chemistry of photosystem II is of major importance in developing catalytic systems for solar fuels production. In addition to addressing important chemical problems related to energy conversion, her research also addresses the methodological void that exists in her field. She is exploiting the diverse potentials of EPR spectroscopy to interrogate the structure and dynamics of photochemical reaction intermediates. This approach brings new and otherwise unobtainable structural and functional insights to the problem.



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SAS Graduate Student Award



Nathan Gomer (on right with SAS President Mary Kate Donais) of the University of South Carolina was presented the SAS Graduate Student Award for outstanding research in spectroscopy. Mr. Gomer graduated from the University of Florida in May 2008 with a B.S. in Biochemistry. During his time at the University of Florida, he conducted undergraduate research with Dr. Richard Yost, analyzing polypeptides using mass spectrometry. Following his undergraduate studies, he has attended the University of South Carolina, where he currently studies spectroscopy under his research adviser, Dr. S. Michael Angel. His research has focused on the development of a spatial heterodyne spectrometer for Raman spectroscopy. Nathan first presented his results at FACSS 2010 and received first place in the FACSS Student Poster Competition. In 2011, he received a student award from the Coblenz Society, a Joseph W.

Bouknight Teaching Award from USC, as well as an Innovation Award at FACSS 2011. In 2012, he was given the USC Department of Chemistry's Guy F. Lipscomb Award for Excellence in Chemistry and Biochemistry and took second place in USC's Graduate Student Day oral presentation competition. His first paper, discussing the use of a spatial heterodyne spectrometer for Raman spectroscopy, received the 2012 William F. Meggers Award. He is also the recipient of the 2012 Tomas Hirschfeld Scholar Award.

SAS Student Poster Award Winners

SAS held the annual Sunday night student poster session at SCIX in Kansas City. Four students were recognized for the most outstanding presentations:

Changqi Xu (*below left*), University of Missouri-Kansas City School of Dentistry, for "Micro-Raman Spectroscopy to Evaluate the Effect of Oral Cancer Radiotherapy on Tooth Chemical Structure."



Joseph Swanstrom (*above right*), University of South Carolina, for "Measuring Phytoplankton Community Structure via Fluorescence Imaging Multivariate Optical Computing."

Kevin P. Pfeuffer (*below left*), Indiana University, for "Development and Characterization of a New Concentric-Geometry Flowing Atmospheric Pressure Afterglow."



Andrew Storey (*above right*), Indiana University, for "Glow Discharge Imaging Spectrometry with a Tilting Interference-Filter Spectrometer."

SAS Undergraduate Student Grant Recipients

Four students received SAS Undergraduate Student Grants to partially cover their travel expenses to present their research at SCIX 2012. Congratulations to the students and their advisors for their excellent work. The grant recipients were:

Priyanka Basnet of Hampshire College presented “Bioimaging of Trace Metal Distribution in Rice Seeds (*Oryza sativa*) by LA-ICP-MS.” Her advisor is Dr. Dulasiri Amarasiriwardena.

Kevin Higgins of Idaho State University presented “Assessment of Sample Selection Methods for Local Modeling.” His advisor is Dr. John Kalivas.

Jonathan Palmer of Idaho State presented “Localized Model Selection for Multivariate Calibration using Tikhonov Regularization with Net Analyte Signal.” His advisor is Dr. John Kalivas.

Catherine G. McKenas of Austin College presented “Using FT-IR to Investigate the Behavior of Carboxylate Based Monolayers on Titanium Dioxide at High Temperatures.” Her advisor is Dr. Karla McCain.

2012 FACSS Innovation Award

The Federation of Analytical Chemistry and Spectroscopy Societies is pleased to announce the winners of the 2012 FACSS Innovation Award. This is a juried prize awarded to the most innovative, creative, and outstanding work making its world debut at the FACSS-organized SciX conference. The winner is selected in a special oral session featuring five candidates selected from the many talks contributed to the program.

The 2012 Award Winner is **Rohit Bhargava**, *University of Illinois, Beckman Institute for Advanced Science and Technology*, for “**Advancing Infrared Microscopy Instrumentation by Theory and Computation**,” Rohit Bhargava, P. Scott Carney, Rohith Reddy, Kevin Yeh, Thomas van Dijk, Matthew Gelber, Matthew V. Schulmerich; University of Illinois, Beckman Institute for Advanced Science and Technology.

Dr. Bhargava presented a recently developed theoretical framework for understanding light propagation in microspectroscopic imaging systems that upends the widely held belief that vibrational spectroscopic imaging is a simple combination of spectroscopy and optical microscopy. This new theory and resulting modeling has allowed for the design and construction of instruments with new capabilities, enhancement and interpretation of spectral data, and the realizing of models for real-world samples. Fundamental understanding of light–matter interaction in complex systems recovery has also been advanced, allowing ultimate optimization of system performance for the first time.



Professor **Rohit Bhargava** is the Bliss Faculty Scholar and an Associate Professor, Engineering and Beckman Institute for Advanced Science and Technology, at the University of Illinois at Urbana-Champaign. Dr. Bhargava received dual B.Tech. degrees (in Chemical Engineering and Polymer Science and Engineering) from the Indian Institute of Technology, New Delhi, and his doctoral thesis work at Case Western Reserve University was in the area of polymer spectroscopy. Subsequently, he worked as a Research Fellow at the National Institutes of Health in the area of biomedical vibrational spectroscopy. Research in the Bhargava laboratories focuses on fundamental optical theory for vibrational spectroscopic imaging, developing new instrumentation, application of spectroscopic imaging to biomedical and polymer problems, and numerical analyses. Dr. Bhargava’s work has been recognized with several research and teaching awards, including *Applied Spectroscopy’s* Meggers Award, and he is routinely nominated to the list of teachers ranked “excellent” at Illinois.



Professor **P. Scott Carney** is an Associate Professor in the Department of Electrical and Computer Engineering at the University of Illinois. He is a theorist with research interests in inverse problems, imaging, coherence theory and other branches of optical physics and works closely with a number of great experimenters. Prof. Carney is widely respected for having written the seminal papers in the field of near-field inverse scattering. His current interests include problems in inverse-scattering, the statistical optics of fast pulses, and spectroscopy. Prof Carney holds a BS in Engineering Physics from UIUC (1994), and a PhD in Physics from the University of Rochester (1999, advisor: Emil Wolf).



Matthew Schulmerich joined Prof. Bhargava's laboratories at the Beckman in 2009 after a working at SABIC Innovative Plastics. Matthew received a B.S. in Chemistry(2004) and a B.A. in Biology (2004) from St. John Fisher College (Rochester, NY)and earned his Ph.D. in Chemistry (2008) from the University of Michigan where he used Raman Spectroscopy, novel optical probe configurations, and multivariate signal processing to noninvasively recover spectra of targets below several millimeters of light scattering material including plastics and tissue. His current research includes building instrumentation for spectroscopic mapping, imaging and tomography. Matthew's interests involve integrating IR and Raman methods in a multi model-approach to obtain accurate disease diagnosis of excised tissue. Towards this effort he has developed Dark Field Raman microscopy as a method for

rejecting signal from substrate fluorescence. He has also recently applied his expertise in transmission Raman spectroscopy to analysis of soybeans in a pilot study to assess the feasibility of using Raman measurements to quantify the concentrations of protein, oils, and amino acids in whole soybeans. Other research interests involve working with spectral basis sets to quantify tissue components by using multivariate signal processing towards noninvasive diagnostics.



Dr. Thomas van Dijk joined the University of Illinois as a Beckman Institute postdoctoral fellow in 2011 after receiving a Ph.D. in Physics at Vrije University in Amsterdam. His dissertation has a focus on theoretical and experimental studies in optical coherence theory, while his main areas of research include computed imaging, inverse problems, statistical optics and plasmonics. Thomas is interested in exploring the theoretical frontiers in bio-optics, which uses light to study, manipulate, and treat biological samples, toward advancing the design of experimental methods and analysis of results. He plans to concentrate his work on problems in the imaging and diagnosis of disease in order to meet both clinical and research needs.



Rohith Reddy received his Bachelor's degree in Electrical Engineering and a Master's degree in signal processing from Indian Institute of Technology (IIT), Chennai, India. His research in Prof. Bhargava's group is focused on creating and enhancing mid-infrared spectroscopic imaging techniques for biomedical applications. He has developed methods for prostate and breast cancer detection using FT-IR spectroscopic imaging. His latest work involves the conception and design of infrared instrumentation and entails a deep integration of theoretical, computational, and experimental aspects of optics. In recognition of his research in infrared imaging and spectroscopy, he has received several national and international awards including the Tomas Hirschfeld Award (2012), William G. Fateley Student Award (2011), Society of Applied Spectroscopy Student Award (2011) and Coblentz Student

Award (2011) among others.



Kevin Yeh received his BS in Biomedical Engineering from Johns Hopkins University and started as a graduate student in Prof. Bhargava's laboratories in 2011. His research interests involve developing technologies for mid-infrared spectroscopic imaging. His current work involves Fourier transform infrared (FT-IR) spectrometry and Quantum Cascade Laser (QCL)-based imaging systems.



Matthew Gelber received his B.S. in General Engineering from the University of Illinois at Urbana-Champaign in 2010 and joined Prof. Bhargava's laboratories as a graduate student in 2012. His research focuses on the development of high-throughput methods for both developing and imaging engineered 3D tissue. Using a combination of spectroscopic imaging and molecular biology, Matt hopes to enable better experimental characterization of the multi-dimensional interactions at play in degeneration, regeneration, and cancer.