

Society for Applied Spectroscopy Awards 2016

Society for Applied Spectroscopy Distinguished Service Award

Recognizing members for their long-time service to the Society for Applied Spectroscopy.



James A. de Haseth

James de Haseth received his B.S. in Chemistry from the University of Illinois at Chicago in 1972 and his Ph.D. in Analytical Chemistry from the University of North Carolina at Chapel Hill in 1977. Jim studied with Thomas L. Isenhour and his main interest of study was computerized information retrieval from spectrometric data. It was in graduate school that Jim became interested in Fourier transform infrared (FT-IR) spectrometry and decided to pursue further studies in vibrational spectrometry. This led to an eighteen-month postdoctoral research position with Gleb Mamantov at the University of Tennessee where Jim studied time-resolved FT-IR spectrometry involving fluorine-based reaction chemistry.

In 1979 Jim accepted a position as an Assistant Professor of Chemistry at the University of Alabama. He moved to the University of Georgia in 1983, where he was later promoted to Professor of Chemistry. Research interests have involved numerous projects in vibrational spectrometry, and include gas and liquid chromatographic interfaces as well as capillary electrophoretic interfaces to FT-IR spectrometers, vibrational circular dichroism, protein structure by infrared spectrometry, and the use of infrared fibers for the study of reaction kinetics. Research interests also focused on the design and development of field deployable spectrometers in the ultraviolet through mid-infrared spectral regions.

In 2009 Jim retired from the University of Georgia and co-founded a consulting group, Light Light Solutions, LLC, with three scientists from the Agricultural Research Service of the USDA (Franklin Barton, David Himmelsbach, and Dan Akin) as well as with Curt Marcott from Proctor and Gamble. In 2011 Jim and Franklin Barton spun off an instrument company, LLS Instruments, Inc., to develop a field-portable NIR spectrometer. The unit is designed to measure large areas to provide more accurate analyses of sample components. Commodities measured include living plants, bales, products on conveyor belts, and materials in vehicles, such as trucks, railroad cars,

and ship holds. Work with the instrument has been in the fiber, rubber, and sugar industries to name a few, in the US, Canada, and Australia.

Jim became a member of SAS in 1978 and has held several positions within the Society. He has been a member of the Coblenz Society since 1980 and was named an Honorary Member in 2011. Since 1974 Jim has been a member of the American Chemical Society and is also a member of the Council on Near Infrared Spectroscopy.

Jim remains active in teaching and is an instructor for IR Courses, Inc. That organization regularly conducts courses for the interpretation of infrared and Raman spectra. Three such courses were taught in 2016 in Texas, the United Kingdom and Maine. In addition, since 1982 Jim has taught numerous vibrational spectroscopy short courses for the Society for Applied Spectroscopy, FACSS, the Pittsburgh Conference, and for several overseas organizations. Jim is co-author with Peter R. Griffiths for the treatise "Fourier Transform Infrared Spectrometry," John Wiley & Sons, New York, 1986, and the second edition, 2007.

Society for Applied Spectroscopy Honorary Membership Award

Recognizing those individuals who have made exceptional contributions to spectroscopy.



Sanford A. Asher

Sanford A. Asher Distinguished Professor of Chemistry at the University of Pittsburgh received his B.A. in chemistry at the University of Missouri, St. Louis in 1971 and completed his Ph.D. in chemistry at the University of California, Berkeley in 1977. Dr. Asher was a Research Fellow in Applied Physics at Harvard University between 1977 and 1980, and in 1980 he became Assistant Professor of Chemistry at the University of Pittsburgh. Dr. Asher's research program at Pitt involves development of new materials and the development of new spectroscopic techniques. His group developed UV resonance Raman spectroscopy as a new technique for fundamental and applied structural and trace studies of molecules in complex matrices. His group is using UV resonance Raman to examine the first stages in protein folding. In addition, they are investigating

the use of UV resonance Raman for the detection of explosive molecules, especially for stand-off detection. They are working with others in developing a deep UV Raman instrument for NASA's 2020 Mars lander. In addition, Dr. Asher's research group develops new photonic crystal optical devices and chemical sensing devices from self-assembling colloidal particles. He pioneered the development of smart hydrogel materials for chemical sensing.

Dr. Asher received numerous awards. He is the recipient of the 2016 SAS Honorary Membership Award, 2016 Society of Analytical Chemists of Pittsburgh (SACP) Award in Analytical Chemistry, 2015 FACCS Charles Mann Award in Applied Raman Spectroscopy, the 2011 Charles E. Kaufman Award and the 2008 Pittsburgh Spectroscopy Award. He became a Fellow of the Society of Applied Spectroscopy in 2007, and received the Sigi Ziering Award from the American Society of Clinical Chemistry in 2005. The University of Missouri awarded him the 2004 St. Louis Distinguished Alumni Award. He won the 2002 ACS Pittsburgh Award, and the 2002 Ellis R. Lippincott Award from the Optical Society of America. He won the Pittsburgh Technology Council EnterPrize Award in 2000, the Coblenz Society's Bomem-Michelson Award in 1999, and the Society for Applied Spectroscopy's Lester W. Strock Award in 1998, the University of Pittsburgh's Chancellor's Distinguished Research Award in 1996, the American Chemical Society Award in Spectrochemical Analysis in 1994, the American Heart Association Established Investigator Award in 1984 and an NIH Career Development Award in 1984.

Professor Asher served as the Co-Director of the Materials Research Center of the University of Pittsburgh. He was the Chairman of the XV International Conference on Raman Spectroscopy held in Pittsburgh in 1996. He is Scientific Founder and Chairman of the Scientific Advisory Board of the startup company Vytrace Corp. (previously Glucose Sensing Technologies, LLC.), and is on the Scientific Advisory Boards of BioTools Inc. and Crystalplex Co. He consults for companies such as PPG Industries, ChemImage Corporation, Glucose Sensing Technologies, LLC, and ThermoFisher Co.

He is the author of greater than 295 publications and is the inventor in over 29 patents in the area of photonic crystals.

Society for Applied Spectroscopy Honorary Membership Award

Recognizing those individuals who have made exceptional contributions to spectroscopy.



Jaan Laane

Jaan Laane was born in Estonia in 1942 but fled with his family from the Soviets in 1944, winding up in a displaced persons camp in Germany. In 1949 the family immigrated to the USA, settling in the small town of Polo, Illinois. Jaan graduated high school as class valedictorian and then attended the University of Illinois as a Sloan Scholar and James Scholar. He graduated with Highest Distinction in Chemistry in 1964 receiving the Kendall Award as the top chemistry major. He then carried out graduate work at MIT with Richard C. Lord as a National Science Foundation and Woodrow Wilson Fellow, receiving his Ph.D. and the Kodak Award as the top graduate student in 1967.

Following a year at Tufts University, Jaan moved to Texas A&M University where he soon was promoted to Full Professor (1976). His research focused on the determination of vibrational potential energy surfaces in both ground and excited electronic states. He has contributed to the theoretical understanding of molecular vibrations and structures and to the experimental methodology in these areas. He has more than 300 publications and three books. He has been in the forefront of writing computer programs for analyzing potential energy surfaces. These have been widely distributed and utilized. Laane has supervised the research of more than 40 Ph.D. students, 60 undergraduates, and dozens of post-docs and visiting professors. He has received the Humboldt Award, a Texas A&M teaching award and the Lippincott Award among others. He was Chair of the Physical and Nuclear Chemistry Division for many years and Associate Dean of Science and Speaker of the Faculty Senate. Since 1994 Laane has been Editor for the Journal of Molecular Structure.

Society for Applied Spectroscopy Emeritus Membership Award

Recognizing those individuals who have who have contributed to spectroscopy and have been members of the Society for Applied Spectroscopy for 15 years, and now have retired from active scientific endeavor.



S. Roy Koirtyohann

S. Roy Koirtyohann was born Sept 11, 1930, the seventh of nine children by Earl and Carrie Koirtyohann. He was raised on their farm near Washington MO and graduated from Washington High School in 1949. He enrolled in the University of Missouri (MU) that fall, majoring in Agricultural Chemistry and became like the bad penny that could not be thrown away for MU. After graduation in 1953 he was on active duty in the army for two years before returning to MU for a Master's Degree under E. E. Pickett. He then worked at Oak Ridge National Laboratory for four years before returning to MU once more for the PhD and a faculty position.

His research activities resulted in nearly 100 publications in journals such as Applied Spectroscopy, Analytical Chemistry, and Spectro Chimica Acta as well many oral presentations at national and international conferences. Accomplishments include measurement of the free atom fraction for analytes in flames, identification of the cause for background problems in flames used for AA, and invention of continuum source background correction in AA.

He became active in the St. Louis SAS section while in graduate school. As his career progressed he became a very active participant and organizer for conferences such as FACSS which included SAS as a sponsor. He was SAS President in 1990.

He retired in 1995 after 32 years on the MU faculty. Roy and his wife, Laura, then moved to their 165 acre farm (Roy's playground) and started collecting, restoring, and showing antique agricultural equipment. Caring for the farm eventually got to be too much and they moved to a modest house on 5 acres a few miles North of Columbia, MO. Roy still tinkers with the remnants of his collection and does some gardening. Both he and Laura remain in good health for their age. On March 7th, 2016 they celebrated their 64th wedding anniversary.

Society for Applied Spectroscopy Lester W. Strock Award

Established by the SAS New England section to recognize an author(s) of an outstanding paper or series of papers.



Raymond Arvidson

Raymond Arvidson received a Ph.D. from Brown University in 1974. He is presently the James S. McDonnell Distinguished University Professor Washington University in St. Louis, where he focuses on teaching and research about current and past environments on the Earth, Mars, and Venus. He is a fellow of the McDonnell Center for the Space Sciences. He has been instrumental in development and implementation of both orbital and landed missions to the planets, including participation in the Magellan Radar Orbiter Mission to Venus, Team Leader for the Viking Lander Imaging System on Mars, member of the Project Science Group for the Mars Global Surveyor Mission, Deputy Principal Investigator for the highly successful Mars Rover Missions (Spirit and Opportunity), the Robotic Arm Investigator for the Mars Phoenix Lander Mission, Co-Investigator for the hyper-spectral mappers OMEGA (Mars Express orbiter) and CRISM (Mars Reconnaissance Orbiter), and a Science Team Member for the Mars Science Laboratory Curiosity Rover that landed on Mars in August 2012. He is the Director of the NASA Planetary Data System Geosciences Node, making available ~300 terabytes of NASA data to the worldwide research community. He is a Fellow of the Geological Society of America and the American Geophysical Union (AGU), received the AGU Whipple Award, has been honored as the Missouri Teacher of the Year, has been honored with three NASA Public Service Medals, and several dozen NASA citations for excellence. He has received several awards from Washington University in Saint Louis for research and teaching excellence.

Society for Applied Spectroscopy Barbara Stull Graduate Student Award
Recognizing a graduate student for outstanding research in spectroscopy and presented in honor of our longtime colleague Barbara L. Stull



Mustafa Unal

Mustafa Unal received his B.Sc. in mechanical engineering at Selcuk University in Turkey. He is currently a PhD candidate under the supervision of Prof. Ozan Akkus at Case Western Reserve University (CWRU). His current research focuses on Raman spectroscopic analysis of the changes in composition of bone and cartilage with diseases and aging. More specifically, he has focused on developing novel Raman spectroscopic techniques to assess the involvement of water and collagen matrix in bone and cartilage quality. He has recently developed Raman spectroscopy-based a novel nondestructive modality to assess the hydration status in bone and cartilage by developing a customized short wave infrared spectrometry system that is optimized to probe the water region in biological tissues. He was the first person to characterize OH-stretching bands of bone and cartilage to identify different water compartments as a novel tool to assess bone and cartilage quality. He has further worked on several side projects, including the novel use of Raman spectroscopic techniques for point of care testing such as diagnosis of microcrystals in urine for early detection of kidney stone and diagnosis of crystals-induced arthropathies. Since 2014, he has published 6 peer-reviewed articles, 1 book chapter, and presented 14 poster/oral presentations in scientific conferences. He has received several national and international prestigious awards, including FACSS Student Award, Coblenz Student Award, Baxter Young Investigator Award, ORS Osteoarthritis Young Investigator Award, The Victor M. Goldberg Award, and The George W. Codrington Charitable Foundation Student Research Award. He has also been selected as one of the ten finalists of 2016 CIMIT Student Technology Prize for Primary Healthcare.

Society for Applied Spectroscopy Meggers Award

Recognizing the author(s) of an outstanding paper appearing in Applied Spectroscopy

Presented for *“Probing Organometallic Reactions by Time-Resolved Infrared Spectroscopy in Solution and in the Solid State Using Quantum Cascade Lasers”*.
Applied Spectroscopy. 2015. 69(5): 519-524.



Michael George

Mike George received a PhD from the University of Nottingham under the supervision of Professor Martyn Poliakoff FRS and remained at Nottingham for 18 months where he began a very fruitful collaboration with Professor Jim Turner FRS in the area of using fast infrared spectroscopy for monitoring electron transfer in inorganic excited states. Fast infrared spectroscopy has continued to be a central feature of his research. He was awarded a Royal Society/STA of Japan postdoctoral fellowship to probe organic excited states with Professor Hiroo Hamaguchi. He returned to Nottingham as an Experimental Officer (1993) and was promoted to Research Officer (1996), lecture (1998), reader (2001) and professor (2003). Over the past two years he has taken a 50% secondment to be Vice-Provost for Research and Knowledge Exchange at the University of Nottingham Ningbo China. Many of his research interests combine photochemistry, fast time-resolved infrared spectroscopy (TRIR) and instrument development particularly focused at elucidating inorganic, organic and biological reaction mechanisms. He is particularly interested in the coordination and reactivity of small molecules such as CO₂ and alkanes and noble gases including studies focusing on the factors affecting C-H activation. He is currently working in a consortium applying time-resolved X-ray measurements at the Research Complex at Harwell. He was involved in the development of two national facilities (PIRATE and ULTRA) at the Rutherford Appleton laboratory, Oxford and the latter facility is currently underpinning a range of ultrafast science in the UK. He also works in a range of other areas of analytical chemistry particularly combining using vibrational spectroscopic studies with supercritical fluids ranging from phase measurements associated with Carbon Capture and Storage (CSS) to new ways synthesizing antimalarial drugs for the developing world. His work has been recognised by several awards including Royal Society of Chemistry Sir Edward Frankland Fellowship (2002/3); Corday-Morgan medal (2003), Photochemistry Award

(2005) and Inorganic Reaction Mechanisms Award (2013) together with Horiba award (2005); Seaborg Lectureship UC Berkeley (2010) and the Craver award (2011) from The Coblenz Society. He was Programme Chair for SciX in Milwaukee (2013) and ICAVS-8 (2015). He is on the Editorial Board of Applied Spectroscopy and he has also served on the committee of the Infrared and Raman Discussion Group (IRDG) since 1999.

**Bruce R. Kowalski Award in Chemometrics
administered by the Society for Applied Spectroscopy**

Presented in honor of the legacy of Professor Kowalski by recognizing outstanding young researchers in the field of chemometrics and by extension, for advanced mathematical and/or statistical methods in chemistry



Keshav Kumar

Keshav Kumar obtained his M.Sc. and Ph.D. from Department of Chemistry, Indian Institute of Technology-Madras, India, in year of 2008 and 2014, respectively. His PhD research work was focused on integrating the chemometric methods with Total Synchronous Fluorescence Spectroscopy (TSFS). He showed that TSFS data structure is intrinsically different and a better understanding is required for its integration with different chemometric techniques. One of his most significant contributions in this area is to prove that TSFS data set lacks the trilinear structure and must not be subjected to the parallel factor (PARAFAC) analysis. He has also successfully proposed a scheme that provides a computationally economical way of achieving trilinear decomposition of TSFS data sets using PARAFAC analysis. He has been successful in studying various aspects of performing Multivariate Curve Resolution Alternating Least Square (MCR-ALS) analysis of TSFS data sets. In a comparative study, he found that combination of chemometrics and TSFS provide quite a few significant analytical advantages over combination of excitation-emission matrix fluorescence (EEMF)-chemometrics for the analyses of dilute aqueous multifluorophoric mixtures.

He received the Best PhD and MSc Thesis award, from Department of Chemistry, Indian Institute

of Technology-Madras. He received KBC postdoctoral fellowship from Kempe Foundation, Sweden in 2015 and since then he is working as a postdoctoral researcher at the Department of Molecular biology, Umea University, Sweden. His current research mainly deals with the application of advanced chemometric methods on the chromatographic and mass spectrometry data sets to identify the novel bacterial cell wall targets.

Society for Applied Spectroscopy Fellows Award

Recognizes individual members for their outstanding service to the field of spectroscopy and the Society for Applied Spectroscopy.



Mike Angel

Mike Angel is a Professor of Chemistry at the University of South Carolina where he has held the Fred M. Weissman Palmetto Chair in Chemical Ecology since 2005. He received his PhD from North Carolina State University in 1985 and carried out Postdoctoral work with Tomas Hirschfeld at Lawrence Livermore National Laboratory. Angel's research group works mainly in the areas of remote and in-situ laser spectroscopy with a focus on deep-ocean, planetary, and homeland security applications of Raman and LIBS. Recent work includes developing the spatial heterodyne Raman spectrometer (SHRS) and exploring its use for deep UV Raman, standoff Raman and for use on future planetary landers and SmallSats.

Angel is a member of the Mars 2020 SuperCam science team and is an elected Fellow of AAAS. He has been a SAS Tour speaker, an A-Page Advisory Panel member for Analytical Chemistry and on the editorial advisory boards of Talanta and the International Journal of Spectroscopy, and a member of the scientific committee of NASLIBS and the International LIBS conference. Other honors include the 2015 Southern Chemist Award, 2012 Applied Spectroscopy William F. Meggers Award, 2012 ACS South Carolina Chemist of the Year Award, 2011 Federation of Analytical Chemistry & Spectroscopy Societies (FACSS) Innovation Technology Award, and

2006 Lawrence Livermore National Laboratory Physics and Advanced Technologies Directorate Award.



Jaan Laane

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Following a year at Tufts University, Jaan moved to Texas A&M University where he soon was promoted to Full Professor (1976). His research focused on the determination of vibrational potential energy surfaces in both ground and excited electronic states. He has contributed to the theoretical understanding of molecular vibrations and structures and to the experimental methodology in these areas. He has more than 300 publications and three books. He has been in the forefront of writing computer programs for analyzing potential energy surfaces. These have been widely distributed and utilized. Laane has supervised the research of more than 40 Ph.D. students, 60 undergraduates, and dozens of post-docs and visiting professors. He has received the Humboldt Award, a Texas A&M teaching award and the Lippincott Award among others. He was Chair of the Physical and Nuclear Chemistry Division for many years and Associate Dean of Science and Speaker of the Faculty Senate. Since 1994 Laane has been Editor for the Journal of Molecular Structure.



Barry Lavine

Barry K. Lavine is a Professor of Chemistry at Oklahoma State University where he both teaches and performs research in analytical and forensic chemistry. Lavine's research interests encompass many aspects of chemical analysis including vibrational spectroscopy (both infrared and Raman), infrared imaging, and the applications of pattern recognition, multivariate curve resolution, and multivariate calibration using genetic algorithms and other evolutionary optimization techniques to chemical analysis. Currently, Lavine's research activities are focused on the development of search algorithms for samples with similar IR spectra under sparse sample and data conditions. Lavine is also investigating the decantation of infrared image data of cross sectioned layers (prepared using a microtome) to obtain a pure IR spectrum of each layer. This methodology is currently being evaluated using automotive paints, which are well-suited to the exploration and application of concatenation-decantation methods because a large database of pure IR spectra from automotive paint systems exists.

Lavine has published more than 100 research papers, 20 book chapters, 16 review articles, and editor for 3 ACS monographs, is on the editorial board of several journals including the Journal of Chemometrics, Microchemical Journal, Chemoinformatics and Analytical Letters and has served as Chair of the Northern New York (1997-2004) and the Oklahoma (2006-2008) sections of the American Chemical Society. Lavine has been Program Chair and General Chair for several scientific meetings including Program Chair of FACSS (1992), Northeast Regional ACS Meeting (1999), and the Pentasectional Meeting of the local Oklahoma Sections of the American Chemical Society (2005).



R. Kenneth Marcus

R. Kenneth (Ken) Marcus, Ph.D., is Professor of Analytical Chemistry at Clemson University, beginning his tenure in 1986. His undergraduate education included BS degrees in Chemistry and Physics from Longwood College (now University) in Farmville, VA in 1982. He received his Ph.D. in Analytical Chemistry in 1986 from the University of Virginia, where he worked for Prof. W. W. Harrison. Professor Marcus' research program currently covers two very distinct lines of study: 1) use of capillary-channeled polymer (C-CP) fibers and films as platforms for protein separations, and) the development of liquid sampling-atmospheric pressure glow discharge (LS-APGD) microplasmas for spectrochemical analysis. The latter efforts are the subject of his awarding of the 2015 Society for Applied Spectroscopy's Lester Strock Award. His research program is currently funded by the National Science Foundation, DTRA, and the Pacific Northwest and Savannah River National Laboratories. His research group has published over 180 refereed journal articles, made over 550 conference presentations (>130 invited), and yielded over a dozen US patents. He serves on the editorial advisory boards of *Spectrochimica Acta B*, the *Journal of Analytical Atomic Spectrometry*, and *Analytical and Bioanalytical Chemistry*. Marcus takes great pride in the fact that over one-half of his 34 Ph.D. graduates are now employed in federal laboratories including NIST, the CDC, and the Savannah River, Oak Ridge, Sandia, Los Alamos, and Pacific Northwest National Laboratories. He has also been honored as a Fellow of the Royal Society of Chemistry and the American Association for the Advancement of Science.

Society for Applied Spectroscopy William J. Poehlman Award

Recognizing an outstanding SAS Regional Section that has met the goals and ideals of the Society over the past year.

SAS Cleveland Regional Section

The SAS Cleveland Section is being recognized as this year's outstanding section for maintaining a consistently high level of activity throughout the year and completing a large number of projects which furthered the mission and goals of SAS. These projects included the 59th annual May Conference, which included a full day of programming with three parallel sessions and several plenary/invited talks and award presentations. The conference fostered communications between members, students, and equipment vendors. The Section organized the event in conjunction with the local ACS and AVS sections and the Microscopy Society, and was able to obtain 28 (!) industrial sponsors. The latter achievement, in particular, is a strong example of the success that regional sections can have in finding financial support for projects.

Other Cleveland Section activities included seven monthly meetings, several of which featured speakers from outside the Section's boundaries, and a number of educational outreach presentations. Of the latter, one activity of note was the "Spectroscopy for Kids" program, which reached a total of ~1800 students (elementary to high school) at 10 different events, and included a teacher training workshop.