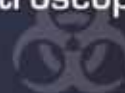


FACSS PRESENTS

# SCIX2017

National Meeting of:  
Society for Applied Spectroscopy (SAS)  
and

North American Society for  
Laser-Induced Breakdown Spectroscopy  
(NASLIBS)



## FINAL PROGRAM

**OCTOBER 8 - 13**

Grand Sierra Resort - Reno, NV

[SciXconference.org](http://SciXconference.org)

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*Attention Presenters: Check this final program to verify the schedule of your talk or poster.  
Changes may have occurred since the preliminary program.*

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## WELCOME TO SciX 2017

On behalf of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) it is our pleasure to welcome you to Reno for SciX 2017. We are excited to be back in Reno for what we know will be the ultimate opportunity for learning, networking and socializing with your SciX (new and long term) friends.

We now have (a lucky number) 13 FACSS sponsoring societies working together to host a “right sized” conference. SciX 2017 is the National Meeting for the Society for Applied Spectroscopy and for the North American Society for Laser-Induced Breakdown Spectroscopy (NASLIBS). As in the past, the focus of SciX 2017 is the technical program organized under the leadership of the Program Chair, Matthieu Baudelet. The Sunday Keynote speaker is our opening event and features Janie Dubois discussing the current challenges of maintaining food safety.

Throughout the SciX program and every morning, we honor our award-winning colleagues. Award winners, their presentations and sessions are prominently identified throughout the program and the SciX mobile app (download the app for the most up-to-date information). Equally important are the poster sessions that feature students, early-career professionals and seasoned scientists that allow for more in-depth, but relaxed discussions. Under the guidance of the Program Chair, the Section Chairs, and Session Chairs have worked hard to organize symposia across many interesting topics and applications within the analytical sciences. The chairs also secure financial support from our sponsoring industrial partners. These funds go directly into the program to help bring in the best and brightest as our presenters. We also are pleased to honor the finalists in the competitive FACSS Innovation Award session on Thursday afternoon. We close out the technical program on Friday morning with a more casual discussion of the new vision for analytical science in the world.

A major goal for SciX is to support networking opportunities for every SciX attendee. Please be sure to check the program for all the networking opportunities that range from coffee breaks, lunch, poster sessions, and evening events. Everyone at SciX is welcome to the Wednesday night “It’s a 3-Ring Circus” all-inclusive event (food, drinks, entertainment).

SciX is here to meet your needs – please let us know how we did and how we can improve by filling out the survey after the conference ends. Also, many volunteers are required each year – if you want to join the team, please contact FACSS, SciX, or your member society and volunteer! In addition, the SciX 2017 team is indebted to Marin Walker, Jennifer Watson and Lola Priest at the FACSS / SciX International Office.

Becky Dittmar, 3M - SciX General Chair 2017

Matthieu Baudelet, University of Central Florida– SciX Program Chair 2017

Mike Carrabba, Hach – SciX Exhibits Chair 2006 - 2020

Mark Henson, Shire Pharmaceuticals – SciX Workshops Co-Chair

Rob Chimenti, Innovative Photonic Solutions – SciX Workshops Co-Chair

John Wasyluk, Bristol-Myers Squibb – SciX / FACSS Marketing Chair 2014-2019

Steven J. Ray, SUNY Buffalo, Governing Board Chair, 2016-2017



**General Chair, SciX**  
**Becky Dittmar**

3M

beckydittmar@gmail.com



**Program Chair, SciX**  
**Matthieu Baudelet**

University of Central Florida  
baudelet@ucf.edu



**Exhibits Chair, SciX**  
**Mike Carrabba**

Hach Company  
mcarrabba@hach.com



**Workshops Co-Chair, SciX**  
**Robert Chimenti**

Innovative Photonic Solutions  
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**Workshops Co-Chair, SciX**  
**Mark Henson**

Shire  
mhenson@shire.com



**Marketing Chair, FACSS & SciX**  
**John Wasyluk**

Bristol-Myers Squibb  
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**SciX Conference and FACSS International Office**  
2019 Galisteo Street, Building I-1, Santa Fe, NM 87505

(505) 820-1653 ○ (505) 820-1648 ○ [facss@facss.org](mailto:facss@facss.org) ○ [www.scixconference.org](http://www.scixconference.org) ○ [www.facss.org](http://www.facss.org)

## FACSS and SciX CONFERENCE ORGANIZATION

### Member Organizations of FACSS

#### MEMBER ORGANIZATIONS OF FACSS

AES Electrophoresis Society  
American Chemical Society, Division of Analytical Chemistry  
American Society for Mass Spectrometry  
ANACHEM  
Austrian Society of Analytical Chemistry  
The Coblentz Society  
Council for Near Infrared Spectroscopy  
The Infrared and Raman Discussion Group  
International Society of Automation-Analysis Division  
North American Society for Laser-Induced Breakdown Spectroscopy  
Royal Society of Chemistry Analytical Division  
Society for Applied Spectroscopy  
The Spectroscopical Society of Japan

### 2017 FACSS Executive Committee



**Governing Board Chair**  
**Steven Ray**, *SUNY Buffalo*  
sray2@buffalo.edu

Governing Board Chair Elect  
Past Governing Board Chair  
Second Past Governing Board Chair  
Secretary  
Treasurer

**Fred LaPlant**, *3M*  
**Greg Klunder**, *LLNL – Forensic Science Center*  
**Ian R. Lewis**, *Kaiser Optical Systems, Inc.*  
**Glen Jackson**, *West Virginia University*  
**Mark Druy**, *Galvanic Applied Sciences USA*

### SciX 2017 Program Section Chairs

Awards  
AES Electrophoresis  
  
Atomic Spectroscopy  
Biomedical and Bioanalytical  
Chemometrics  
Contemporary Issues in Analytical Science  
Laser-Induced Breakdown Spectroscopy  
Mass Spectrometry  
  
Molecular Spectroscopy  
Nanotechnology  
Pharmaceutical Analysis  
  
Process Analytical Technology  
Raman Spectroscopy  
  
Security and Forensics  
SPSJ - Frontiers of Deep- and Far Ultraviolet Spectroscopy  
Surface Plasmon Resonance  
Surface Science

**Karen Esmonde-White**, *Kaiser Optical Systems, Inc.*  
**Jason Dwyer**, *University of Rhode Island*  
**Darwin Reyes-Hernandez**, *NIST*  
**Jorge Pisonero**, *Universidad de Oviedo*  
**Karen Esmonde-White**, *Kaiser Optical Systems, Inc.*  
**Peter Harrington**, *Ohio University*  
**Rebecca Airmet**  
**Mattheiu Baudelet**, *University of Central Florida*  
**Glen P. Jackson**, *West Virginia University*  
**Yu Xia**, *Purdue University*  
**Curt Marcott**, *Light Light Solutions and University of Delaware*  
**Wei Zhao**, *University of Arkansas at Little Rock*  
**John Wasyluk**, *Bristol-Myers Squibb*  
**Anna Luczak**, *Bristol-Myers Squibb*  
**James Rydzak**, *Specere Consulting*  
**Duncan Graham**, *University of Strathclyde*;  
**Ian R. Lewis**, *Kaiser Optical Systems, Inc.*; and  
**Pavel Matousek**, *Rutherford Appleton Laboratory*  
**Greg Klunder**, *Lawrence Livermore National Laboratory*  
**Yukihiro Ozaki**, *Kwansei Gakuin University*  
**Jean-Francois Masson**, *Université de Montreal*  
**Kateryna Artyushkova**, *University of New Mexico*



## GENERAL INFORMATION

**LOCATION** All plenaries, symposia, short courses, workshops and the exhibits are located at the Grand Sierra Resort.

**NEW THIS YEAR** Additional recognition of student poster winners, where the winning posters will be displayed in the plenary room throughout the conference. Student poster award winners will receive additional details upon notification of their award.

**SPEAKERS *New this year!*** Prepare your slides and save to a USB stick (flash drive). Arrive at your session room 30 minutes prior to the session start to connect your USB stick to session room laptop (PC running Windows 10 and MS Office 2016 with PowerPoint). There is a Speaker Practice Room in the registration area where speakers may preview presentation slides on a PC laptop (identical to session room PC laptops). Speakers will NOT be able to present from their own laptop.

### POSTER SESSIONS

**Sunday SAS Student Poster Session, Reno Ballroom**

7:15–9:00 pm SAS Poster Session & SciX Welcome Mixer

**Monday Poster Session – Reno Ballroom**

Posters remain up all day.

Set up posters between 7:30 – 9:30 am and remove by 5:00 pm

9:45 – 10:45 am – Poster Session

3:10 – 3:50 pm – Poster viewing and break

**Tuesday and Wednesday Poster Sessions – SciX Exhibit Hall**

Posters remain up all day on their designated day. Set up posters between 9:00 – 10:45 am and remove Tuesday posters by 4:30 pm and Wednesday posters by 3:50 pm.

11:00 am – 12:00 noon – Poster Session

3:10 – 3:50 pm – Poster viewing and dessert break

**Thursday Poster Session – Grand Salon**

Posters remain up all day.

Set up posters between 9:00 – 10:45 am and remove at 3:50 pm

11:00 am – 12:00 noon – Poster Session

3:10 – 3:50 pm – Poster viewing and break

*Poster presenters are required to be present at BOTH morning and afternoon sessions. This will extend the time for discussions and judging for student awards.*

**SHORT COURSES / WORKSHOPS** A list of workshops begins on page 31. You must register for a SciX workshop at the conference registration desk

**EMPLOYMENT BUREAU/ INTERNET CAFE** Available in the Grand Salon conference registration area. See page 5

**EXHIBITS** The exhibition is located in the Exhibit Hall (Summit Pavilion) and will be open as follows. See page 27 for details.

Monday (Opening Reception) 5:30 pm – 7:30 pm

Tuesday 10:00 am – 4:30 pm

Wednesday 10:00 am – 4:00 pm

### WHAT'S HOT VENDOR PRESENTATIONS

Sunday, 4:10 – 6:00 pm, *Tahoe Ballroom*

Tuesday, 11:30 am – 1:20 pm, *Exhibit Hall*

Wednesday, 11:30 am – 1:20 pm, *Exhibit Hall*

**BREAKS** A complimentary lunch will be served at noon in the exhibit hall on Tuesday and Wednesday for all registered conferees. Must be present to participate. Ticket required.

Monday morning and afternoon breaks.

9:45 am – 10:45 am & 3:10 – 3:50 pm – *Reno Ballroom*

Tuesday and Wednesday morning and afternoon breaks.

11:00 am – 12:00 pm & 3:10 – 3:50 pm – *Exhibit Hall*

Thursday morning and afternoon breaks.

11:00 am – 12:00 pm & 3:10 – 3:50 pm – *Grand Salon*

**INTERNET ACCESS.** Free Wi-Fi is available in all meeting space

**COMPANION REGISTRATION** Does not include access to symposia. Cost is \$75 and includes the following: **Sunday** - Evening Welcome Mixer. **Monday** - coffee/pastries 9:00 am and Exhibit Hall Opening Reception. **Wednesday** – Conference All Inclusive Event

### SPECIAL EVENTS

#### SUNDAY

6:15 pm **SciX 2017 Welcome.** Becky Dittmar

**Keynote Lecture.** The Analytical and Economic Challenges of Maintaining Food Safety in a Global Supply Chain; **Janie Dubois**, University of Maryland, JIFSAN. *Tahoe Ballroom*

7:15 – 9:15 pm **Welcome Mixer and SAS Sponsored Student Poster Session.** SAS, Coblenz, and FACSS Student Award Presentations, *Reno Ballroom*

#### MONDAY

All Plenary Lectures will be held in Tahoe Ballroom

7:45 am **Opening Address**, Matthieu Baudelet

8:00 am **Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award Plenary**  
Russ Algar, *University of British Columbia*

8:30 am **Ellis R. Lippincott Award Plenary**  
Roberto Merlin, *University of Michigan*

9:00 am **Sir George Stokes Award Plenary**  
Tony Cass, *Imperial College London*

11:30 am **Coblenz Speed Mentoring**, Nevada 8

5:30 pm **Reception for Exhibit Opening** (wine, beer, light hors d'ouvres) *Exhibit Hall*

#### TUESDAY

All Plenary Lectures will be held in Tahoe Ballroom

8:00 am **FACSS Charles Mann Award for Applied Raman Spectroscopy Plenary**  
Duncan Graham, *University of Strathclyde*

8:30 am **Coblenz Society Craver Award**  
Martin Zanni, *University of Wisconsin – Madison*

12:00 pm **Complimentary lunch in the Exhibit Hall.**  
Attendee must be present. Ticket required.

2:30 pm Raffle Drawing in the Exhibit Hall

6:00 pm **Raman Reception** Invitation Only. *Reno Ballroom*

7:30 pm **Society for Applied Spectroscopy Wine and Cheese Awards Reception.** *Tahoe Ballroom*

#### WEDNESDAY

All Plenary Lectures will be held in Tahoe Ballroom

8:00 am **Applied Spectroscopy William F. Meggers Award Plenary**  
Naoto Nagai, *Industrial Research Institute of Niigata Prefecture*

8:30 am **Lester W. Strock Award Plenary**  
Frank Vanhaecke, *Ghent University*

12:00 **Complimentary lunch in the Exhibit Hall.**  
Attendee must be present. Ticket required.

2:30 pm Raffle Drawing in the Exhibit Hall

6:00 pm **Wednesday Evening All Inclusive Event**,  
Conference badge required. *Reno Ballroom*

#### THURSDAY

All Plenary Lectures will be held in Tahoe Ballroom

8:00 am **ANACHEM Award Plenary**  
Jennifer Brodbelt, *University of Texas at Austin*

8:30 am **AES Mid Career Award Plenary**  
R. Scott Martin, *Saint Louis University*

3:50 pm **Plenary Session**  
FACSS Distinguished Service Awards  
FACSS Innovation Award Session

#### FRIDAY

7:50 am **Closing Session.** *Tahoe Ballroom*

**Announcement of Innovation Award**

8:30 am **New Vision of Analytical Science by the World**

10:00 am **Preview of 2018 Conference**

## EVENTS OF SPECIAL INTEREST TO STUDENTS

### SUNDAY EVENING, *Reno Ballroom*

- Welcome Mixer: 7:15 – 9:15 pm
- SAS Sponsored Poster Session: 7:15 – 9:15 pm
  - SAS and Coblenz Student Award presentations
  - FACSS Student Award and Tomas Hirschfeld Scholar Award presentations

### MONDAY through THURSDAY

- FACSS Student Poster Awards will be presented daily. Winners announced at 7:50 each day before the Plenary Session.
- Coblenz Speed Mentoring, 11:30 am – 1:30 pm (seating is limited), *Nevada 8*

### MONDAY through THURSDAY

- Employment Bureau (Monday through Thursday), *Registration Area*

### SHORT COURSES

This year we are offering a wide variety of introductory and fundamental short courses geared to toward students. Visit the SciX website or conference registration desk to register. Special discounted rates available for students.

**NEW THIS YEAR** Additional recognition of student poster winners, where the winning posters will be displayed in the plenary room throughout the conference. Student poster award winners will receive additional details upon notification of their award.

## EMPLOYMENT BUREAU / INTERNET CAFÉ

The Employment Bureau is located in the Registration Area in conjunction with the internet café Monday through Thursday. Computers and printers will be available in the Grand Salon

**EMPLOYERS:** Bring either hard copy or print an electronic copy of job opportunities and display on poster board in the employment area. There will be copies of resumes for you to review or to take with you.

**JOB SEEKERS:** Bring copies of your resume to be made available for prospective employers to review.

A message board will be available for employers and job seekers to communicate.

## CONFERENCE REGULATIONS AND CODE OF CONDUCT

The following regulations are in the best interest of the conference. FACSS/SciX reserves the right to revoke anyone's conference badge and attendance to the meeting.

#### General:

1. There is no smoking in any conference areas.
2. An official name badge is required at all times.
3. No advertising may be placed in the conference areas.
4. Only official exhibitors may display in the Exhibit Hall.
5. No demonstration of instrumentation or distribution of any type of literature is allowed outside the Exhibit Hall.

#### While in Sessions:

1. All devices including cell phones must be silenced.
2. No talking during oral presentations and awards ceremonies.
3. No Photography of PowerPoint presentations or Posters.
4. No distribution of product/meeting literature.

#### Expected Behavior throughout the Conference:

1. Be respectful and considerate of others and the facilities.
2. Be mindful of your surroundings and of your fellow participants.
3. Alert a SciX volunteer if you notice a dangerous situation or someone in distress.

#### Unacceptable Behavior:

1. Harassment, intimidation or discrimination in any form will not be tolerated.
2. Physical or verbal abuse of anyone attending or involved with the conference is not tolerated.
3. Alert a SciX volunteer if you witness or are the subject of unacceptable behavior.

SciX is the Annual North American Meeting of FACSS

National Meeting of:  
Society for Applied Spectroscopy (SAS)  
and

North American Society for Laser-Induced Breakdown Spectroscopy (NASLIBS)

## PROGRAM and CONFERENCE SPONSORS

SciX 2017 and FACSS greatly appreciate the support it receives from its sponsors.

### Platinum Sponsors

**Bristol-Myers Squibb ♦ Kaiser Optical Systems**  
**Pfizer ♦ Spectroscopy Magazine**

#### GENERAL CONFERENCE AND MEDIA SPONSORS

Applied Sciences MDPI  
Bristol-Myers Squibb  
HORIBA Scientific  
Necsel  
Texere Publishing (*The Analytical Scientist*)  
Wasatch

#### ACS

ACS Division of Analytical Chemistry

#### ATOMIC SPECTROSCOPY

Agilent Technologies  
Applied Spectra  
HORIBA Scientific  
IonSense  
ISAS  
LECO  
Meinhard – Elemental Scientific Glassblowing  
Postnova Analytics  
Tofwerk

#### CHEMOMETRICS

CAMO Smart Software  
Eigenvector Research  
Ohio University Center for Intelligent Chemical Instrumentation

#### CONTEMPORARY ISSUES IN ANALYTICAL SCIENCE

Society for Applied Spectroscopy  
*Spectroscopy Magazine*  
Waters Corporation

#### FORENSIC

Applied Spectra  
Bruker Optics  
Pittcon 2018  
Thermo Scientific

#### INFRARED SPECTROSCOPY

Anasys Instruments  
Andor Technology  
CNIRS  
Light Conversion  
Pike Technologies  
Princeton Instruments

#### LASER-INDUCED BREAKDOWN SPECTROSCOPY

Continuum, Amplitude Laser Group  
LLA Instruments  
LTB-Berlin  
OPOTEK

#### MASS SPECTROMETRY

American Society for Mass Spectrometry  
Bruker Optics  
IonSense  
JEOL USA  
Prosolia  
PurSpec Technologies  
Thermo Scientific

#### NANOTECHNOLOGY

Anonymous  
HORIBA Scientific  
Renishaw

#### PHARMACEUTICAL

Bruker Optik  
HORIBA Scientific  
Metrohm USA  
Ondax  
Oxford Instruments

#### PROCESS ANALYTICAL

ABB  
B&W Tek  
CPACT  
Ocean Optics  
Viavi Solutions

#### RAMAN

B&W Tek  
Cobalt Light Systems  
HORIBA Scientific  
Innovative Photonic Solutions  
Kaiser Optical Systems  
Ocean Optics  
Ondax  
Pfizer  
Pittcon 2018  
Renishaw  
Royal Society of Chemistry  
Wasatch  
Wiley-Blackwell

#### RSC

Royal Society of Chemistry

#### SPECIAL SESSIONS

##### Art and Archaeology

Glass Expansion  
Meinhard – Elemental Scientific Glassblowing  
TSI

##### Modern Techniques in Microscopy

Electron Microscopy Sciences  
Mad City Labs  
Nikon Instruments

##### Stand-Off Sensing

Continuum, Amplitude Laser Group

#### SPSJ

Spectroscopical Society of Japan

#### STUDENT SPONSORS

Mary and Mike Carrabba  
Meinhard-Elemental Scientific  
Society for Applied Spectroscopy

#### SURFACE SCIENCE

SPECS Surface Nano Analysis  
WITec Instruments

## FACSS AWARDS

### DISTINGUISHED SERVICE AWARD

*Awarded to an individual(s) for recognition of exceptional, long-term service to the FACSS organization.  
The 2017 recipients have served with excellence in many different capacities and contributed to the continuing success of FACSS through consistent dedication and sacrifice.*

Award will be presented Thursday, 3:50 pm, Tahoe Ballroom



**Diane Parry**  
*Procter & Gamble*

**Diane Parry** is currently a Research & Development Associate Director for the Procter & Gamble Company, managing an organization dedicated to modeling and simulation and upstream projects. In her 28 years at Procter and Gamble, she has led many disciplines within Research & Development. She is a passionate champion of breakthrough, applied innovation. She holds over a dozen international patents for her work.

After working for P&G for a couple of years with her undergraduate degree, Diane quit to pursue her Ph.D. in Physical and Analytical Chemistry from the Joel Harris group at the University of Utah, graduating in 1989. She completed Post-Doctoral work with Physicists at IBM's Almaden Research Center, San Jose, before re-joining P&G in 1991.

Diane is currently the Treasurer and Past Past President of the Society for Applied Spectroscopy. She has served FACSS, SciX, SAS and science for more than twenty years, including as:

- Workshop co-presenter or presenter to undergraduate and graduate students, "Professional Analytical Chemists in Industry". FACSS/SciX Meeting, annually, in the city hosting the meeting, 1995 to 2015; Also, co-presenter of the same Short Course at the Eastern Analytical Symposium and various Universities by invitation, since 1997.
- ACS Analytical Section delegate to the Governing Board of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS), 2003.

- FACSS renewal participant 2004-2005. Participated as equity design Facilitator in 2005. Facilitated separation and capture of SciX/FACSS equities for the FACSS LRP in 2013 and 2014.
- Acting role of FACSS Metrician. Diane tracked FACSS progress against equity objectives from 2004 to 2015, until the position had an official name.
- FACSS Governing Board Chair, 2006. Completed GB Chair Elect, GB Chair, Past Chair, and Past Past Chair annual terms.
- Society for Applied Spectroscopy Parliamentarian 2009-2011.
- FACSS Long Range Planning Committee member, 2010 to present.
- Program Special Section Creator/Organizer, Analytical Chemists Easing World Poverty, (ACEWP) FACSS Program 2011, PittCon Program 2013, SciX 2014. Organized double-session for the 2013 SciX meeting in Milwaukee; gave a talk and chaired the session. Diane successfully transferred the job of organizing sessions to Rebecca Airmet in 2015, but remains an ardent supporter. Diane and Rebecca recently co-authored a chapter on ACEWP, which has been accepted for the upcoming ACS Book "Mobilizing Chemistry Expertise to Solve Humanitarian Problems" edited by Dr. Ronda Grosse (Chemists Without Borders).
- 2015 President for the Society for Applied Spectroscopy. Contributed on a number of SAS Committees as part of this role.

### PREVIOUS DISTINGUISHED SERVICE AWARDEES

1993 Edward Brame and Syd Fleming  
1994 L. Felix Schneider  
2001 David Coleman  
2003 Jeanette Grasselli Brown  
2009 Paul Bourassa and Mike Carrabba  
2010 Scott McGeorge and Alexander Scheeline

2011 Jon W. Carnahan and Patricia B. Coleman  
2012 Bruce Chase and O. Karmie Galle  
2013 Mark A. Hayes and Cynthia M. Lilly  
2014 Ron Williams and Edward J. Havlena  
2015 Michael Blades, Gary Brewer and Keith L. Olson  
2016 John Chalmers, John Graham and Jim Rydzak



## FACSS AWARDS

*The FACSS Student and the Tomas Hirschfeld Scholar Awards recognize outstanding contributions by individual who are Ph.D and M.Sc candidates.*

### FACSS STUDENT AWARD



**Nicholas Riley**

*University of Wisconsin-Madison*

**Oral Presentation: Thursday, 2:50 pm, Room Nevada 7**

**Nick Riley** is originally from Louisville, KY and earned his B.S. degree in Chemistry and Psychology from the University of South Carolina with Honors from the South Carolina Honors College, where he was a Robert C. McNair Scholar. He conducted undergrad research in forensic analytical chemistry with Dr. Stephen L. Morgan and developed a fascination for the instrumentation he used while in the Morgan lab. Following graduation, he moved to Madison, WI to join the lab of Joshua J. Coon as an analytical chemistry graduate student at the University of Wisconsin. In his tenure there, Nick has conducted research in the field of bioanalytical mass spectrometry with a focus on developing instrumentation and methodologies to improve characterization of protein post-translational modifications in complex systems. The majority of his work has centered on improving the efficacy of electron transfer dissociation (ETD) and related tandem MS techniques. Through the use of infrared photo-activation concurrent with ion-ion reactions, Nick has significantly enhanced the capabilities of ETD to sequence peptide and protein ions in high-throughput proteomic experiments, and the scope of this exciting technology is just beginning to be explored. Throughout his

graduate career Nick has worked on globally characterizing protein acetylation and phosphorylation, but his most recent efforts have focused on protein glycosylation, a chemically complex and analytical challenging modification involved in a wide array of intra- and inter-cellular functions. Nick's work with ETD and hybrid tandem MS methods is among the first to characterize thousands of glycosites via intact glycopeptides, providing crucial site-specific biological context at an unprecedented scale. He is now continuing to develop this technology to investigate glycosylation profiles in models of cancer aggressiveness to understand cancer cell metastasis. In all, Nick has published 17 peer-reviewed papers (10 first author) and has presented 26 oral/poster presentations at scientific conferences up to this point. He has also been honored with several distinctions, including a National Science Foundation Graduate Student Fellowship, the American Society for Mass Spectrometry Student Award, the Marg Northcott Student Award, the Roger J. Carlson Memorial Award for Research Excellence, and a National Cancer Institute Predoctoral to Postdoctoral Fellow Transition Award (F99/K00) via the National Institutes of Health.

## FACSS AWARDS

### FACSS STUDENT AND TOMAS HIRSCHFELD SCHOLAR AWARDS – Call for Applications for 2018

The Tomas Hirschfeld Scholar and the FACSS Student Awards recognize the most outstanding papers submitted to FACSS by a graduate student. Recipients will receive financial support to help them attend the SciX 2018 conference in Atlanta, Georgia (October 21-26).

In 2017 one FACSS Student Award and two Tomas Hirschfeld Scholars are being presented. In order to have your presentation considered for a Tomas Hirschfeld Scholar Award or FACSS Student Award, students should submit their abstracts using the SciX website submission form and indicate on the dropdown menu on the form their interest in these awards.

**The submission process involves submitting an abstract, completing the website submission form, and submitting the following electronically to [facss@facss.org](mailto:facss@facss.org)**

- the form, available on the SciX website
- a 250 word abstract of the work to be reported
- two letters of nomination, one by the student's mentor. An explanation of the inventive contributions by the student to the work should be given. Creativity was a primary characteristic of Tomas's work, and thus should be a characteristic of the awardee
- a copy of the candidates resumé
- a copy of the candidate's graduate transcript
- Copies of reprints and/or preprints of research accomplished.

The recipients will be included in either a session highlighting young scientists and their work or in an appropriate topic area. The SciX website will begin accepting abstracts and applications for FACSS student awards in January 2018.

Go to [www.scixconference.org](http://www.scixconference.org) to submit an application.

## FACSS AWARDS

The FACSS Student and the Tomas Hirschfeld Scholar Awards recognize outstanding contributions by individual who are Ph.D and M.Sc candidates.

### TOMAS HIRSCHFELD SCHOLAR AWARDS



**Ebrahim Aboulizadeh**

*University of Wisconsin-Milwaukee*

**Oral Presentation: Thursday, 10:35 am, Room Carson 1**

**Ebrahim Aboulizadeh** : While studying Quantum Gauge Theory and cosmology during his Master's program in 2009, Ebrahim learned of the University of Wisconsin-Milwaukee through the work of the Professor Leonard Parker. But exposure to a broad array of disciplines at UWM led him into a biomedical vibrational spectroscopic field with potential impact in the health sciences. As a Physics Ph.D. student under the supervision of Prof. Carol Hirschmugl, the central premise of his research was to determine the novel mechanistic insight into the pathogenesis of diabetes in the mouse retina at different duration of diabetes. Ebrahim started his doctoral research at the most advanced infrared beamline, IRENI, at the Synchrotron Radiation Center in Wisconsin, which enabled him to develop a better understanding of the relationship between structure and function of individual retinal cells. He pioneered the development of infrared spectrochemical imaging of diabetic retinal tissue engaged with chemometric tools to determine highly localized diabetes-induced alterations and oxidative stress damage in distinctive layers of retina, which has never been achieved. He has further worked on several side projects including the novel use of spectroscopic techniques and computational analysis for quantifying the activity of adipose tissues, revealing the interaction between blue-light and MRSA, and three-dimensional imaging of live cells. In recognition of his efforts, he received spectroscopy research award from the Society for Applied Spectroscopy, best poster award and travel award from Midwest Microscopy and Microanalysis Society, Distinguished Dissertator Fellowship, Distinguished Graduate Student Fellowship, and David Lichtman Scholarship for outstanding performance in experimental physics. Up to now, he has published 8 peer-reviewed journal papers and 1 book chapter, and presented 12 poster/oral presentations in national and international conferences. In addition, his paper that addresses the retinal oxidative stress at the onset of diabetes determined by synchrotron FT-IR imaging has made the cover of *Analyst*. His innovative paradigm for detecting the temporal-dependent biomarkers of diabetes in individual retinal layers, shed light on the mechanisms leading to vision loss at cellular level. He is currently working as a postdoctoral associate in Dr. David Williams team, at the Advanced Retinal Imaging Alliance, at the University of Rochester, exploring three different approaches to vision restoration: preserving photoreceptors with gene therapy, replacing lost photoreceptors using stem cells, and genetically re-engineering cells other than photoreceptors to respond to light.



**Santosh Paidi**

*Johns Hopkins University*

**Oral Presentation: Wednesday, 10:35 am, Room Nevada 7**

**Santosh Paidi** is a graduate student in the Department of Mechanical Engineering at Johns Hopkins University. His current research efforts in Dr. Ishan Barman's lab are directed towards application of Raman spectroscopy and multivariate data analysis to develop novel quantitative approaches for addressing unmet needs in the molecular study of cancers. His recent work in this area has resulted in the creation of a new landscape for spectroscopic monitoring of stromal adaptations in the lungs of animals bearing breast tumor xenografts, prior to the arrival of metastatic cancer cells. He demonstrated this by exploiting the unique Raman markers stemming from the stromal modifications (induced by factors secreted from the primary tumor) to develop a decision algorithm for accurate differentiation of pre-metastatic lungs in mice bearing high metastatic tumor xenografts from those in mice with low metastatic tumor xenografts and normal controls. He is currently working towards extending the developed approach to delineate the events that unfold at the pre-metastatic secondary sites and enable identification of stage specific molecular markers in a label-free fashion. In addition to applications in cancer, a major focus of Santosh's graduate study is the development of a detection framework based on label-free plasmon-enhanced Raman spectroscopy for rapid identification of closely related human and murine antibody drugs during their manufacturing, with the ultimate goal of translation to fill-finish sites. Prior to commencing doctoral study at Johns Hopkins, Santosh graduated from Indian Institute of Technology (IIT) Bombay in 2014 with a B.Tech in Mechanical Engineering and a minor in Aerospace Engineering. As an undergraduate, his research was directed towards understanding the effects of inert gas dilution on the characteristics of hydrogen combustion. Overall, his research efforts have resulted in 9 peer-reviewed publications in journals such as Cancer Research, Analytical Chemistry and Scientific Reports. He has been awarded the Whiting School Doctoral Fellowship and Mechanical Engineering Departmental Fellowship by Johns Hopkins University, Molecular Medicine Tri-Conference Student Fellowship and Undergraduate Research Award by IIT Bombay in recognition of his work.

## FACSS INNOVATION AWARD

The FACSS Innovation Award will be given for the most innovative and outstanding new research advancements debuted at the SciX Conference. All program areas are included. Only research findings presented for the first time in the public domain qualify for entry (work based on submitted papers not yet published electronically or in print at the time of abstract submission also qualify). Papers submitted for SciX will be considered for these awards – authors can check the appropriate box for their papers to be entered. Finalists will be selected for presentations at the SciX conference in special award sessions. Award winner(s) will be selected after the award sessions are concluded. Each award includes: A cash prize of \$1,500; a plaque; and publicity.

### 2016 INNOVATION AWARD WINNER:

An Inexpensive Medical Device for Barrett's Esophagus Screening; **Rohith Reddy**; *Harvard Medical School; Massachusetts General Hospital*

**Thursday, 3:50 pm, Tahoe Ballroom**  
**2017 FACSS INNOVATION AWARD SYMPOSIUM**  
Organizer and Presider: Karen Esmonde-White

- 3:50 PM (847) **Probing Cancer by Exploiting Spontaneous and Stimulated Raman Scattering**; Ji-Xin Cheng<sup>1</sup>, Chien Sheng Liao; <sup>1</sup>Boston University
- 4:10 PM (848) **Effective Light Directed Assembly of Building Blocks with Microscale Control**; Chia-Hung Chen<sup>1</sup>; <sup>1</sup>National University of Singapore
- 4:30 PM (849) **Optical Reflection and Waveguiding of Sound in Free Space**; Daniel Kaza<sup>1</sup>, Ellen Holthoff<sup>2</sup>, Brian Cullum<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore County; <sup>2</sup>Army Research Laboratory, Adelphi, MD
- 4:50 PM (850) **Dried Blood Spheroids: A Versatile Paper-Based Biofluid Sample Collection Platform for Improved Analyte Stability**; Abraham Badu-Tawiah<sup>1</sup>, Deidre Damon<sup>1</sup>; <sup>1</sup>The Ohio State University

## It's a 3-Ring Circus at SciX 2017



### **Wednesday Evening** **6:00 pm, Reno Ballroom**

Step right up! Come one, come all!

In the first ring, watch the transformation of ordinary balloons into an unusual variety of animals and hats! In ring two, be prepared for a special surprise! And, featured in the center ring, delicacies that will take you back to your very first trip to the circus.

Challenge your colleagues to a carnival game or dress up like a (scary) clown. After dinner, put on your dancing shoes and boogie the night away!

**An All Inclusive Event**  
(SciX 2017 conference badge required for entry)



## FACSS CHARLES MANN AWARD

*For Achievements in the Field of Applied Raman Spectroscopy*

**Duncan Graham**  
University of Strathclyde

**Presentation: Tuesday, 8:00 am, Tahoe Ballroom**



**Duncan Graham** is the Research Professor of Chemistry and Head of Department for Pure and Applied Chemistry at the University of Strathclyde in Glasgow. He obtained his BSc Honours in Chemistry from the University of Edinburgh in 1992 and his PhD in Bioorganic Chemistry in 1996 under the direction of Prof. Tom Brown investigating the use of modified oligonucleotides to inhibit HIV. He then moved to the University of Strathclyde where he joined the group of Prof. Ewen Smith as a postdoctoral fellow to examine the use of surface enhanced resonance Raman scattering (SERRS) for DNA analysis with Zeneca Diagnostics. Breakthroughs during that period of research led to the award of a five-year David Phillips fellowship from the BBSRC to examine the area of DNA analysis by SERRS. In 2002 he won the RSC's Analytical Grand Prix Fellowship which provided funding for another period of five years to further develop his chosen area of using synthetic chemistry to create and develop new methods of bioanalysis using optical spectroscopy. In 2004 he was awarded the SAC Silver medal for the 'Innovative synthesis of new analytical reagents for sensitive and selective analysis' and in 2005 he was presented with the Nexxus Young Life Scientist of Year award. In 2007 he was elected to the fellowship of the Royal Society of Edinburgh (Scotland's National Academy) and is a cofounder and director of Renishaw Diagnostics Ltd (formerly D3 Technologies Ltd) which formed in 2007. He has published over 200 papers with 16 patents and has supervised or co-supervised over 55 PhD students and 30 postdoctoral researchers. He was appointed as a lecturer in 2002 and promoted to professor in 2004. He was awarded the Corday Morgan prize of the Royal Society of Chemistry in 2009 for 'outstanding and pioneering contributions to nanometrology in support of molecular manipulation and chemical and biological systems' and a Royal Society Wolfson Merit Award in 2010. In 2012 he was awarded the Craver Award of the Coblenz Society 'in recognition of his pioneering work in surface enhanced Raman scattering (SERS) to generate ultra-sensitive and highly selective methods of detection for a range of analytes, especially bio-analytical targets' and a Fellows Award from the Society of Applied Spectroscopy. In 2016 he was recipient of the RSC's Theophilus Redwood award for 'innovation and leadership in exploiting surface enhanced Raman spectroscopy in the analytical community.' He is chair of the editorial board of Analyst and serves on the advisory boards of Chemical Society Reviews, Chemical Science, Analytical Methods, Journal of Raman Spectroscopy, Journal of Biomedical Spectroscopy and Imaging and the new Cell press journal, Chem. He is president elect of the analytical division of the Royal Society of Chemistry, assuming the presidency in July 2017 and represents the RSC on the FACSS governing board. He is currently co-chair of the Raman programme at SciX with Ian Lewis and Pavel Matousek who share his love of cheese and stage musicals. His scientific interests are in using synthetic chemistry to produce nanosensors that respond to a specific biological species or events as measured by SERS and collaborating with scientist from different disciplines to exploit these approaches.

## WILEY RAMAN STUDENT AWARD

*The Wiley Raman Student Award is given at the annual SciX conference presented by FACSS. The awardee is selected from research submissions for the annual SciX meeting by a panel of Raman subject matter experts and is awarded to an outstanding graduate student and is open to students in any area of Raman spectroscopy research. The student will present their research during the SciX Raman Symposium and will be presented with the award comprising a presentation piece, a certificate, and a book voucher at the annual Raman reception held on Tuesday evening.*

**Fay Nicolson**  
**Oral Presentation Monday 4:30, Carson 4**



**Fay Nicolson** graduated from the University of Strathclyde in 2014 with a First-Class honours degree in Chemistry with Drug Discovery. She undertook a 12-month industrial placement with Reckitt Benckiser working on formulation science. Fay was awarded the JLS Allan Memorial Prize for the best research thesis submitted to The Department of Chemistry for work exploring the metabolic chemistry of polyunsaturated fatty acids.

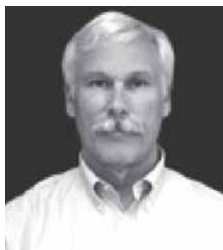
Following her undergraduate degree Fay joined the Centre for Nanometrology at the University of Strathclyde to begin a PhD in Surface Enhanced Spatially Offset Raman Spectroscopy (SESORS). Working under the supervision of Profs Karen Faulds and Duncan Graham at the University of Strathclyde and Prof. Neil Shand from DSTL, Fay's work focuses on the use of a handheld SORS spectrometer, with a back-scattering geometry, for through barrier detection in the fields of defence and biomedicine. This approach demonstrates the potential of SESORS, particularly in a

biomedical setting, where the more common transmission geometry may not always be feasible. Fay has developed a multiplex system where SERS nanotags have been tracked to depths of 20 mm with a view to demonstrate this in vivo.

In 2016 Fay secured WestCHEM funding to visit Prof. Rohit Bhargava's lab at the University of Illinois – Urbana Champaign to gain experience in the use of microscale manufacturing devices. She delivered an oral presentation at SciX 2016 and has presented posters at the IRDG 14th Martin and Willis Prize Meeting; Faraday Discussion on SERS as well as ARF, where she was awarded the Analyst poster prize.

**DISTINGUISHED SERVICE AWARDS**

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



**Geoffrey Coleman**

In 1976, **Geoff Goleman** was awarded a Ph.D. in chemistry at Colorado State University for working with Rod Skogerboe, esteemed mentor, humorist, and friend. He has M.A. (1972) and B.A. degrees in chemistry from DePauw University. After a brief postdoctoral with David F.S. Natusch, he began his academic career at the University of Georgia. In 1983, he moved to the University of Alabama. His research interests centered on applications and fundamentals of plasma emission spectrometry. Geoff considers himself very fortunate to have worked with more than a dozen M.S. and Ph.D. students during his academic career and is pleased that most are still speaking to him in polite, if not entirely gentle terms.

Geoff left academia in 1988 for greener pastures at Leeman Labs, then Fisons (ARL and VG), and Thermo, working first as an applications chemist and eventually as a product line manager. In 2002, he moved back to Colorado to join Meinhard where he is responsible for manufacturing, research and development, and sales and marketing.

Geoff has been active in SAS since the mid-1970s. Working with Rick Browner, Scott Goode, Ivan Glaze and others, he was involved in the formation of the Piedmont Section of SAS and briefly served as its Treasurer. He has been a tour speaker, has chaired the Program Committee and the Honorary Membership Committee. Geoff has been a member of the Editorial Board of Applied Spectroscopy, the Publications Committee, the Nominating Committee, and the SAS Governing Board.

In retirement, he will most likely be found sailing on the Great Lakes or near Chair 6 at Breckenridge.



**Brian Perry**

**Dr. Brian Perry** is Senior Staff Scientist at LORD Corporation in Erie, Pennsylvania. Dr. Perry joined LORD Corporation in 1989 as a Senior Chemist and has spent his entire professional career, 28 years, at LORD in the Analytical Services Department. His specialization in FT-NMR and FT-IR characterization of polymers enables him to apply a multidisciplinary approach to solving complex problems, in support of LORD's business developing highly reliable adhesives, coatings, and motion management devices.

Dr. Perry has been a member of the Cleveland section of the Society for Applied Spectroscopy (SAS) since 1986. He served as vice president of the SAS Cleveland section in 2002, before becoming president in 2003, a position he still holds and has served continuously for a tenure of 14 years.

Under Brian's direction, the Cleveland section has been awarded the William J. Poehlman Award for outstanding local section nine times, more than any other SAS section. Brian also coordinates the Cleveland section's annual May Conference, a one day conference attracting 200 attendees, 35 oral presentations, and 40 student poster presentations. He has strengthened the May Conference significantly by partnering with other local professional societies and by offering significant student awards; 2017 heralds the 61<sup>st</sup> annual May Conference. Another activity which Brian has grown as president of the Cleveland section is the popular outreach program "Spectroscopy for Kids," which has now reached 20,000 students. In addition, the Cleveland section annually bestows the prestigious Earnest B. Yeager Award to an undergraduate student, and multiple John Bell Memorial Awards to grade 7-12 students, for the utilization of spectroscopy. Over the years, Brian's visionary leadership of the Cleveland section has been anchored in efforts to increase student involvement in the local section.

Brian earned with a B.A. in Chemistry from The College of Wooster, where he was also lettered in football for three years. He subsequently earned M.S. and Ph.D. degrees in Macromolecular Science and Engineering from Case Western Reserve University under the direction of Professor Jack L. Koenig, Honorary Member of the Society for Applied Spectroscopy and recipient of the SAS Fellows Award.

Dr. Perry also serves as a director of the Andy Nowacki Foundation, which provides scholarships for men and women in pursuit of careers in service to their communities as members of the safety forces.

Perhaps most significantly, Brian has been married to a member of the Society for Applied Spectroscopy for 28 years



## SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

### HONORARY MEMBERSHIP AWARD

*Recognizing those individuals who have made exceptional contributions to spectroscopy.*



**Terry Miller**

**Terry Miller** obtained his undergraduate degree in chemistry from the University of Kansas. After receiving his Ph.D. from Cambridge University on a Marshall Scholarship, he went to Bell Laboratories where he became a Distinguished Member of Technical Staff before leaving. He moved to The Ohio State University as the first Ohio Eminent Scholar Professor. He has held visiting faculty appointments at Princeton University, Stanford University, and the Institute for Molecular Science in Japan. Dr. Miller's research centers on the spectroscopic identification, characterization and monitoring of reactive and/or trace chemical species. He has developed numerous highly sensitive, spectroscopic techniques spanning frequencies from the microwave to the ultraviolet. Presently, his work focuses upon laser induced fluorescence and cavity ringdown spectroscopy of reactive intermediates, which play critical roles in a variety of important processes, including combustion, atmospheric chemistry, and plasma processing of electronic devices. The spectra of these species serve as diagnostics to monitor their chemical reactions and characterize their geometric and electronic structures. He is author of more than 350 scientific publications. His research has been recognized with the Meggars Award (Optical Society of America), the Bomem-Michaelson Award (Coblentz Society), the Bourke Medal (Royal Society of Chemistry), the Broida Prize and Plyler Prize (American Physical Society), the Morley Prize (Cleveland Section of the American Chemical Society) and the Ioannes Marcus Marci Medal (Czechoslovak Spectroscopic Society). He has been granted the recognition of Fellow by the American Chemical Society, American Physical Society, Optical Society of America and American Association for the Advancement of Science. He presently serves as Editor-in-Chief of the Journal of Molecular Spectroscopy and for 22 years was Chair of the International Symposium on Molecular Spectroscopy which annually attracts approximately 500 conferees. He currently chairs the Advisory Committee for the International Free Radicals Symposium.

### LESTER W. STROCK AWARD

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



**Frank Vanhaecke**

*Presentation: Wednesday, 8:30 am, Tahoe Ballroom*

**Frank Vanhaecke** (1966, Ostend, Belgium) received a PhD from Ghent University (Belgium) in 1992. Currently, he is Senior Full Professor in Analytical Chemistry at Ghent University, where he leads the 'Atomic & Mass Spectrometry – A&MS' research group that is specialized in the determination, speciation and isotopic analysis of (trace) elements via ICP-mass spectrometry (ICP-MS). His group studies fundamentally-oriented aspects of the technique and develops methods for solving challenging scientific problems in an interdisciplinary context. Nowadays, specific topics of research include the direct bulk and spatially resolved analysis (including depth profiling and 2- and 3-dimensional elemental mapping) of solid materials by means of ICP-MS using laser ablation (LA) for sample introduction, the development of speciation strategies based on HPLC-ICP-MS for ADME (absorption, distribution, metabolism and excretion) studies in cooperation with the pharmaceutical industry and isotopic analysis using multi-collector ICP-MS. Methods for high-precision isotopic analysis are developed for applications in, among other, the fields of archaeometry, geo- and cosmochemistry and medicine ("isotopic diagnosis"). So far, Frank's scientific research has resulted in ca. 350 publications in peer-reviewed journals with >8000 citations, resulting in an h-factor of 45 (according to ISI's Web of Science). He is a member of the Advisory Boards of JAAS – Journal of Analytical Atomic Spectrometry, ABC – Analytical and Bioanalytical Chemistry and SAB – 'Spectrochimica Acta B and acted as chair of the Editorial Board of JAAS from June 2012 to June 2016. At the 2011 Winter Conference on Plasma Spectrochemistry (Zaragoza, Spain) in February 2011, Frank received a 'European Plasma Spectrochemistry Award' for his group's contributions to this research field. In 2013, he was designated 'Fellow of the Society for Applied Spectroscopy – SAS'.

## 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

## SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

### 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*



**David A. Bryce**

**David A. Bryce** is currently a Ph.D candidate at the University of Utah, working in the Joel M. Harris research group. David received a Bachelor's of Science degree in chemistry from Central Washington University in 2012. During his undergraduate studies, David worked with Prof. Dion Rivera, utilizing ATRFTIR methods for investigating polyelectrolyte adsorption to oxide films. After graduating, David worked as a post bachelor's research assistant at Pacific Northwest National Lab, developing infrared spectroscopic methodology for in situ study of the partitioning of contaminants between water and supercritical CO<sub>2</sub>. Following this post bachelor's appointment David moved to the University of Utah to pursue a graduate degree in analytical chemistry, working for Joel Harris. At present, David is the Society for Applied Spectroscopy student representative. David's work in the Harris research group has focused on developing and utilizing confocal Raman microscopy methods for analysis carried out within individual chromatographic particles. David's work in the Harris group initially focused on the measurement and modeling of accumulation kinetics of polyaromatic hydrocarbons in reversed-phase chromatographic silica. More recent work has focused on the preparation and characterization of supported phospholipid bilayers throughout the pore-network of chromatographic silica particles, and use of these pore-confined bilayers for label-free confocal Raman microscopy experiments to detect membrane partitioning of small molecules, specific protein binding to membrane localized ligands, and detection of signaling peptide accumulation. This work provides both quantitative and structural information about these molecular interactions with phospholipid membranes.

### 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*



**Joseph P. Smith**

*Award Session: Wednesday 3:50 pm, Crystal 1*

**Joseph P. Smith** is originally from Wallingford, PA. He earned his B.S. in Chemistry in 2012 from the Pennsylvania State University, where he worked under the advisement of Dr. Mary E. Williams performing analytical chemistry research on nanoparticles and nanomaterials. He earned his Ph.D. in Analytical Chemistry from the University of Delaware under the advisement of Dr. Karl S. Booksh in 2017. At the University of Delaware, Joseph developed and applied innovative analytical methodologies utilizing Raman microspectroscopic imaging and multivariate analysis to investigate novel geological and planetary materials. Moreover, he investigated a high-pressure,  $\alpha$ -PbO<sub>2</sub>-structured polymorph of titanium dioxide, termed TiO<sub>2</sub>-II, for geochemical applications, and enhanced the search for life on Mars for applications in the upcoming NASA and ESA rover missions to Mars. His research resulted in a NASA-funded graduate fellowship, in which he directly collaborated with the NASA Johnson Space Center to study lunar, martian, and asteroidal meteorites using chemical imaging and chemometrics. Joseph then joined Merck & Co., Inc. in 2017 and is currently a Senior Scientist in the Analytical Research and Development Department. Joseph has published 12 peer-reviewed manuscripts in journals that include *Analyst*, *Applied Spectroscopy*, *Advanced Energy Materials*, *ACS Nano*, *ACS Catalysis*, *Carbon*, and *Geology*. He has received a variety of awards, including the Glenn S. Skinner Memorial Award for distinction in scholarship, research, teaching, and service, the Eastern Analytical Symposium Graduate Student Award for research in analytical chemistry, and the University of Delaware's Excellence in Teaching Award. Joseph has also been the President of the University of Delaware's SAS Student Chapter and a mentor in the Science and Engineering Leadership Initiation Research Experience for Undergraduates (SELI-REU).



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## SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

### WILLIAM F. MEGGERS AWARD

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

**Presented to Naoto Nagai, Yuta Kijima, and Makoto Okawara**

*“Infrared Response of Sub-Micron-Scale Structures of Polyoxymethylene: Surface Polaritons in Polymers Applied Spectroscopy”, Vol 70, Issue 8, pp. 1278 – 1291*

**Presentation: Wednesday, 8:00 am, Tahoe Ballroom**



**Naoto Nagai** received a Master's degree from Niigata University under the supervision of Professor Shin-ichi Katayama in the field of theoretical solid state physics. He worked at Toray Research Center, Inc. (TRC) after graduation. He was a leader of the infrared spectroscopy team in TRC and received his PhD from Tohoku University under the supervision of Professor Aritada Hatta while

working at TRC. His main work was to resolve problems in the production processes or complaints from the large companies in Japan using spectroscopic techniques such as infrared spectroscopy, photoluminescence, spectroscopic ellipsometry and terahertz spectroscopy. His main interests were the point defect analysis of semiconductor materials, characterization of dielectric films, analyzing polymer surfaces, and feasibility study of the application of the terahertz spectroscopy. When he moved to Industrial Research Institute of Niigata Prefecture (IRI-Niigata), which is one of the research centers organized by the local government in Japan, he helped small companies in Niigata Prefecture to deal with manufacturing problems, using Raman spectroscopy and X-ray photoelectron spectroscopy. However, the central feature of his research is the development of new analytic methods in infrared spectroscopy. With Daipla Wintes Co., Ltd, he produced the “Nano Catcher”, which is an original instrument to prepare very thin surface layers of samples. He is now a research director of Ken-ou Technical Support Center in IRI-Niigata. He received the Advanced Analytical Technology Award from The Japan Society for Analytical Chemistry in 2005.



**Yuta Kijima** received a Bachelor's degree from the University of Electro-Communications (Tokyo). He joined Industrial Research Institute of Niigata Prefecture (IRI-Niigata) after graduation. His main work was to resolve problems in the small companies in Niigata Prefecture using electrical characterization techniques and improvements of software



**Makoto Okawara** received a Master's degree from Niigata University. He worked at Honda Automobile R&D Center after graduation. He received his PhD from Niigata University under the supervision of Professor Tomiichi-Hasegawa in the field of fluid dynamics (rheology) in 2008. After he worked at Seiko Epson co., Ltd., he joined Industrial Research Institute of Niigata Prefecture (IRI-Niigata). His main work was to resolve problems in the small companies in Niigata Prefecture using mechanical characterization techniques and SEM image analysis.



## SAS

### Student Poster Showcase and Awards

Please join us in celebrating the future of spectroscopy as SAS students showcase their research and compete for the annual SAS Student Poster Awards.

Sunday, October 8, 2017, 7-9 p.m. *(during the SciX mixer)*

Sponsored by  
The Society for Applied Spectroscopy and SciX

**SAS FELLOWS AWARD**

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



**Franklin E. (Woody) Barton, II** received his B.S. in Chemistry from North Georgia College in 1964 and his Ph.D. in Chemistry from the University of Georgia in 1969. He entered active duty and served as a Field Artillery Battery Commander in Vietnam and returned to do Post-Doctoral research at the University of Georgia in 1970-1971. He accepted a position with the U.S. Department of Agriculture's Agricultural Research Service in Athens Georgia at the Russell Research Center from which he retired in 2008. During those years he was the Research Leader of a multidisciplinary research group for over 25 years. He served as Location Coordinator/ Center Director for his last 4 years and earlier as an Acting Area Director for the South Atlantic Area (VA to Puerto Rico). He continued his military service in the U.S. Army reserves by teaching quantitative management course for the Command and General Staff College and retired from the YSAR in 1995. After retirement from the USDA in 2008 he became a partner in Light Light Solutions, LLC and as a senior officer in LLS Instruments, Inc. He is still active in solving analytical problems in the Agricultural and food industries.



**Richard Crocombe** has been active in SAS's New England Section for many years, including being its chair twice, and its regular delegate to the Governing Board. With Mark Drury, he was the guest editor for *Applied Spectroscopy* in May 2016, an issue concentrating on portable spectroscopy. Richard's education was in chemistry and spectroscopy at Oxford University, and then the University of Southampton, where he did his Ph.D. with Prof. Ian Beattie, followed by a postdoctoral fellowship with Prof. Gleb Mamantov, working on FT-IR spectroscopy, infrared laser photochemistry, time resolved spectroscopy and gas chromatography/FT-IR.

His industrial career has focused on product development and commercialization of new technologies and applications, and for the past 15 years, on handheld and portable spectroscopy.

At Bio-Rad Digilab Division this included applying digital signal processing techniques to step-scan applications, and commercialization of mid-IR FT-IR spectroscopic imaging. At Axsun Technologies, he took their chip-sized near-infrared tunable laser module into analytical and process spectroscopy. He then joined Thermo Fisher Scientific's handheld x-ray fluorescence business, and this led to the acquisitions of Ahura Scientific and Polychromix. He then moved to PerkinElmer to integrate the just-acquired Torion Technologies portable GC/MS technology, and left in 2017 to set up his own spectroscopic consulting company.

He was previously secretary of the Coblenz Society, and is a current board member. In addition, he is co-chair of SPIE's 'Next-Generation Spectroscopic Technologies' conferences, and co-editor of the resulting conference proceedings publications. He received the Williams-Wright Award for Industrial Spectroscopy in 2013.



**Karen Faulds** is a Professor in the Department of Pure and Applied Chemistry at the University of Strathclyde and an expert in the development of surface enhanced Raman scattering (SERS) and other spectroscopic techniques for novel analytical detection strategies and in particular multiplexed bioanalytical applications. She has published over 100 peer reviewed publications and has filed 5 patents. She has been awarded over £10M in funding as principal and co-investigator from EPSRC, charities, industry and governmental bodies. In 2009 she was presented with the *Nexus Young Life Scientist of the Year* award and in 2011 was elected to the *Royal Society of Edinburgh Young Academy of Scotland*, the first such Academy amongst the national academies in the UK and was elected *Fellow of the Royal Society of Chemistry* in 2012. She was awarded the *2013 RSC Joseph Black Award*, the *2016 Craver Award* from the Coblenz Society and was also recently named as one of the *Top 50 Women in Analytical Science* by The Analytical Scientist. She has given over 50 invited talks at national and international conferences. She is the Strathclyde Director of the Centre for Doctoral Training in Optical Medical Imaging, serves on the editorial board of *RSC Advances* and the editorial advisory board for *Analyst* and *Chemical Society Reviews* and is the current Chair of the UK's Infrared and Raman Discussion Group (IRDG).



**Dr. Kathleen M. Gough** is currently a Professor in the Department of Chemistry and a Core Member of the Biomedical Engineering Graduate Program at the University of Manitoba, Winnipeg MB, Canada. She is an expert in vibrational spectroscopy (infrared and Raman), having done her PhD research on gas phase overtone spectroscopy with Professor Bryan Henry, then postdoctoral experience in Raman trace scattering intensities with Dr. William Murphy and Dr. Henry Mantsch at the National Research Council of Canada, Ottawa and an NSERC post-doctoral fellowship under the late Professor Richard Bader, applying the Theory of Atom In Molecules to model Raman scattering intensities of small hydrocarbons. Since joining the Chemistry faculty at the University of Manitoba in 1995, she has turned her attention to spectrochemical imaging, initially with synchrotron source IR at the Synchrotron Radiation Center, WI, and with Raman microscopy, thermal and synchrotron source FTIR with focal plane array. Most recently she has been imaging with near field infrared techniques at the nanoscale. Her research subjects range from biological (mammalian tissues, fungi, arctic sea ice diatoms) to novel materials (synthetic spider silk, polyacrylic hydrogels for wound dressings, self-disinfecting materials). She is also working on the development of thermal source FTIR tomography to enable visualization of the 3D composition of microscopic targets. She served as Vice-Chair and Chair of the Division of Physical, Theoretical and Computational Chemistry, Canadian Society for Chemistry, 2008-2014. She is a long time member of the Society for Applied Spectroscopy, and has served on the Editorial Advisory Board of *Applied Spectroscopy* since 2011. She is a founding member of the International Society for Clinical Spectroscopy (2016) and was co-organizer of the SPEC 2016 conference, the flagship meeting of that society. She organized a CLIRSPEC symposium at SCIX 2016, co-sponsored by the Royal Society for Chemistry, UK. She loves mentoring, teaching, research, and dancing.



## SOCIETY FOR APPLIED SPECTROSCOPY AWARDS

### SAS FELLOWS AWARD

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



**Terry Miller** obtained his undergraduate degree in chemistry from the University of Kansas. After receiving his Ph.D. from Cambridge University on a Marshall Scholarship, he went to Bell Laboratories where he became a Distinguished Member of Technical Staff before leaving. He moved to The Ohio State University as the first Ohio Eminent Scholar Professor. He has

held visiting faculty appointments at Princeton University, Stanford University, and the Institute for Molecular Science in Japan. Dr. Miller's research centers on the spectroscopic identification, characterization and monitoring of reactive and/or trace chemical species. He has developed numerous highly sensitive, spectroscopic techniques spanning frequencies from the microwave to the ultraviolet. Presently, his work focuses upon laser induced fluorescence and cavity ringdown spectroscopy of reactive intermediates, which play critical roles in a variety of important processes, including combustion, atmospheric chemistry, and plasma processing of electronic devices. The spectra of these species serve as diagnostics to monitor their chemical reactions and characterize their geometric and electronic structures. He is author of more than 350 scientific publications. His research has been recognized with the Meggars Award (Optical Society of America), the Bomem-Michaelson Award (Coblentz Society), the Bourke Medal (Royal Society of Chemistry), the Broida Prize and Plyler Prize (American Physical Society), the Morley Prize (Cleveland Section of the American Chemical Society) and the Ioannes Marcus Marci Medal (Czechoslovak Spectroscopic Society). He has been granted the recognition of Fellow by the American Chemical Society, American Physical Society, Optical Society of America and American Association for the Advancement of Science. He presently serves as Editor-in-Chief of the Journal of Molecular Spectroscopy and for 22 years was Chair of the International Symposium on Molecular Spectroscopy which annually attracts approximately 500 conferees. He currently chairs the Advisory Committee for the International Free Radicals Symposium.



**Dr. Linda Kidder** was drawn to science because of her desire to understand how the world worked, and chose chemistry due to the influence of a nurturing and dedicated high school teacher. Graduating from Williams College with a B.A. in Chemistry, she chose to pursue physical chemistry, receiving her Ph.D. from the Johns Hopkins University where she was the recipient of the Sonneborn and Ernest

Marks Fellowships. During her post-doc, in the Laboratory of Chemical Physics at NIH, she developed a deep appreciation for molecular spectroscopy: developing, deploying, and characterizing Raman and Fourier transform infrared hyperspectral imaging systems. She gained extensive experience in applying these techniques to a variety of materials characterization, biological and biomedical research applications. In 1998, Dr. Kidder co-founded Spectral Dimensions with Neil Lewis, developing a deep, hands-on appreciation of all aspects of the analytical instrumentation business through the "crash-course" environment of a startup company. When this company was purchased by Malvern Instruments, she "retired" from the role of Vice President of Operations to become the Product Manager of Chemical Imaging within Malvern.

With a focus on the development and commercialization of novel analytical instrumentation, she developed project and product marketing skills that ultimately fueled her move to become Vice President of Market Development at BrightSpec, a startup focused on chemical identification of complex mixtures. The tug of vibrational spectroscopy was strong though, and she has returned to her roots, currently as Product Manager of Molecular Spectroscopy at Shimadzu Scientific.

She has given numerous presentations, co-authored articles and book chapters, taught short-courses, and is co-inventor on several patents. She is a long-standing member of the Society for Applied Spectroscopy, the Coblentz Society, and the American Chemical Society, and has contributed to ASTM on both E13.10 and E55 committees. She has had participated in the governance of professional societies, serving on the Board of Director for both SAS and the Coblentz Society, as well as in the corporate world, where she was Corporate Secretary and Treasurer at Spectral Dimensions, and Corporate Secretary of Malvern Biosciences, Inc. She has also worked on outreach for vibrational spectroscopy, at program coordinator for this topic at the FACSS (now Scix) and EAS meetings, as well as organizing the SAS Tour Speakers program in 2011 and upcoming in 2018.

In her "spare time" she and her husband are raising two active boys (11 and 9), and looking after a flock of pets including 2 Australian shepherds, 3 hamsters, a rabbit, a guinea pig and a parakeet.



## COBLENTZ SOCIETY'S CLARA CRAVER AWARD

The Craver Award honoring **Clara Craver** is presented annually to an outstanding young molecular spectroscopist whose efforts are in the area of applied analytical vibrational spectroscopy. Clara Craver was the editor of the Coblentz Desk reference and other subsequent libraries that later became databases of infrared spectra that is the foundation for the application of modern vibrational spectroscopy. Her efforts resulted in the creation of the endowment that supports the Coblentz Society and many of the awards that it gives out annually. The candidate must be under the age of 45 on January 1st of the year of the award. The work may include any aspect of infrared (NIR, MIR, or Far), and/or THz, and/or Raman spectroscopy in applied analytical vibrational spectroscopy. The nominees may come from an academic, government lab, or industrial backgrounds. Click here for information on the Coblentz Society Craver Award.



### **Martin Zanni**

University of Wisconsin - Madison

**Presentation: Tuesday, 8:30 am, Tahoe Ballroom**



**Martin T. Zanni** is the Meloche-Bascom Professor of Chemistry at the University of Wisconsin-Madison. He received his PhD from the University of California-Berkeley, working with Dan Neumark, and was an NIH Postdoctoral Fellow at the University of Pennsylvania with Robin Hochstrasser. He is one of the earliest innovators in 2D IR spectroscopy and has made many technological innovations in 2D IR, 2D Visible, and 2D SFG spectroscopy that has broadened the capabilities and scope of multidimensional spectroscopies. He utilizes these new spectroscopies to study topics in biophysics, chemical physics, photovoltaics, and surface science. He has received many national and international accolades for his research, including the Research Initiatives Award from the National Academy of Sciences for his work in optics, the Raymond and Beverly Sackler Prize from Tel Aviv University for his work in multidimensional spectroscopy, and the Early Career Scholar Award from the NIH/NIDDK for his work on Type 2 diabetes. He founded PhaseTech Spectroscopy Inc., which is the first company to commercialize 2D IR and 2D Visible spectroscopies.

## COBLENTZ SOCIETY'S WILLIAM G. FATELEY STUDENT AWARD

The William G. Fateley Student Award is given by the Coblentz Society annually to recognize outstanding contributions to vibrational spectroscopy during a current Ph.D. program. William G. (Bill) Fateley was among the first winners (1965) of the Coblentz award, and worked tirelessly to promote the Pittsburgh Conference and FACSS. Author of more than 350 publications and recipient of numerous other awards, he returned to his alma mater, Kansas State University, as chairman of his department in 1972 and served there until his retirement 1997 and beyond. He served as the Editor of *Applied Spectroscopy* for 20 years, and served as mentor to a generation of spectroscopists.



### **2017 Coblentz Society's William G. Fateley Student Awardee and Student Award – David Bryce**



**David A. Bryce** is currently a Ph.D. candidate at the University of Utah, working in the research lab of Joel M. Harris. David received a Bachelor of Science degree in Chemistry from Central Washington University in 2012. During his undergraduate studies, David did research with Prof. Dion Rivera, utilizing ATR-FTIR methods for investigating polyelectrolyte adsorption to oxide films. After graduation, David worked as a post bachelor's research assistant at Pacific Northwest National Lab, developing infrared spectroscopic methodology for in situ study of the partitioning of contaminants between water and supercritical CO<sub>2</sub>. Following this appointment, David enrolled in the Department of Chemistry at the University of Utah to pursue a Ph.D. in Analytical Chemistry. David is presently the National Student Representative to the Executive Committee of the Society for Applied Spectroscopy. David's research in the Harris group has focused on developing and utilizing confocal Raman microscopy methods for detection and analysis within individual chromatographic particles. David's work in the Harris group initially focused on the measurement and modeling of accumulation kinetics of polycyclic aromatic hydrocarbons in reversed-phase chromatographic silica. More recent work has focused on the preparation and characterization of supported phospholipid bilayers deposited throughout the pore-network of chromatographic silica particles. These pore-confined bilayers can be used for label-free confocal Raman microscopy experiments to detect membrane partitioning of small molecules, specific protein binding to membrane localized ligands, and detection of signaling peptide accumulation. This research provides both quantitative and structural information about molecular interactions with phospholipid membranes.

## COBLENTZ SOCIETY STUDENT AWARDS

*For many years, the Coblentz Society has encouraged young scientists to pursue studies on spectroscopy by seeking nominations of outstanding students for the Coblentz Student Awards. The awardees receive a copy of the Society's Deskbook, a certificate, and a year's membership in the Society. Their names, the names of their faculty advisors, their institute, and their anticipated graduation date appear in the Society's Fall Newsletter published in an issue of the journal, Applied Spectroscopy.*



**James Brooks** is a graduate student in Dr. Renee Frontiera's research group in the Department of Chemistry at the University of Minnesota. He received a B.A. in Chemistry and a Minor in Management from Gustavus Adolphus College. His current research investigates plasmon-driven photochemical reactions via ultrafast surface-enhanced Raman spectroscopy (SERS). More specifically, James is interested in probing the ultrafast dynamics that occur between an excited localized surface plasmon and a nearby molecular probe in hopes to elucidate the underlying charge transfer mechanism. Rather than directly studying the plasmonic material, ultrafast SERS provides a unique perspective as the plasmon-induced charge carriers interact with the molecular probe, resulting in a time-dependent evolution of the molecule's Raman signatures. His recent work has investigated the plasmon-driven hot electron transfer into methyl viologen, which acts as an electron acceptor on the surface of the plasmonic substrate. He has one first-author publication exploring the efficiencies and kinetics of a plasmon-induced dimerization reaction and was elected Chair for the 2018 Gordon Research Seminar for Noble Metal Nanoparticles.



**Christian Graefe** is a graduate student in Prof. Renee Frontiera's research group in the Department of Chemistry at the University of Minnesota. He received his B.A. in chemistry with a concentration in environmental studies from St. Olaf College in Northfield, MN. Following the completion of his undergraduate degree, Christian worked for Pace Analytical Services as a lab analyst on-site at 3M in Maplewood, MN before enrolling in the University of Minnesota's chemistry Ph.D. program. In Prof. Frontiera's group, he has contributed to the development of a new label-free sub-diffraction chemical imaging technique that combines stimulated Raman spectroscopy with ideas from stimulated emission depletion (STED) microscopy. He co-authored a paper demonstrating proof of concept results for this technique, including sub-diffraction resolution. His research interests include using super-

resolution Raman to observe supported lipid bilayer dynamics on the nanoscale in response to the presence of perturbants. His current work involves improving stimulated Raman resolution and adapting super-resolution Raman for use in biological materials and other soft matter samples.



**Ewelina Mistek** is a Ph.D. student in Chemistry at the University at Albany, State University of New York. After graduating high school in Poland, her home country, Ewelina went to college in Denmark and obtained an Academy Profession Degree in Chemical and Biotechnical Science from the Business Academy Aarhus, University of Applied Sciences. During the program, she pursued a one-year internship in a forensic science laboratory in the United States with the Lednev Research Group at the University at Albany. Her work involved the application of vibrational spectroscopy and statistical data analysis for the development of new forensic methods with a focus on the identification and characterization of body fluid traces. After returning to Europe, she continued her undergraduate program in Forensic and Analytical Science at the Robert Gordon University, Aberdeen in Scotland, earning her Bachelor of Science with Distinction. In 2016, she returned to the University at Albany to pursue her doctorate degree under the mentorship of Professor Igor Lednev.

So far, Ewelina has published two research articles as a first author in the top analytical chemistry journals and two other manuscripts are in preparation. The first study was focused on species identification based upon blood traces using infrared spectroscopy. The second publication reported on a new method for human race differentiation based on Raman spectroscopy of bloodstains. She has also utilized FT-IR spectroscopy for phenotype profiling based on human blood traces as well as for discriminating between menstrual and peripheral blood. During the first year of her graduate program, she presented her successful research projects at the 8th Annual Life Sciences Research Symposium, at the University at Albany, and the 2017 Green Mountain DNA Conference in Vermont.

## ELLIS R. LIPPINCOTT AWARD

*The Ellis R. Lippincott Award is awarded annually to recognize an individual that has made significant contributions to the field of vibrational spectroscopy. The award was jointly established in 1975 by The Optical Society of America, The Coblentz Society, and The Society for Applied Spectroscopy to honor the unique contributions of Professor Ellis R. Lippincott.*

**Roberto Merlin**  
University of Michigan

**Presentation: Monday, 8:30 am, Tahoe Ballroom**



**Roberto Merlin** is the Peter A. Franken Professor of Physics and a Professor in the EECS Department at the University of Michigan. He received the Licenciado en Ciencias Fisicas and the Dr. rer. nat. degrees from the University of Buenos Aires, Argentina (1973) and the University of Stuttgart, Germany (1978). Merlin is the recipient of 2006 APS Isakson Prize, a Fellow of AAAS, OSA, APS, and the von Humboldt, Guggenheim and Simons Foundation. Merlin's primary research specialty is experimental condensed matter physics. His areas of expertise include various continuous wave and ultrafast optical techniques and, in particular, spontaneous and impulsive (stimulated) Raman spectroscopy. His current interests focus on the generation of coherent vibrational and electronic fields using ultrafast laser and x-ray pulses and metamaterials. Merlin and collaborators pioneered work on folded acoustic and interface phonons in semiconductor heterostructures, and on Fibonacci superlattices, metasurfaces and squeezed phonons.

# Call for Award Nominations

## The Coblentz Society

[www.coblentz.org](http://www.coblentz.org)



- Coblentz Award
- Williams-Wright Award
- Ellis R. Lippincott Award
- Craver Award
- Coblentz and Fateley Student Awards
- Honorary Membership

**The Williams-Wright Award** is presented to an industrial spectroscopist who has made significant contributions to vibrational spectroscopy while working in industry. Government labs are not considered industry in this definition. The Awardee must still be working at the time the award is presented. Nominations will be accepted until **May 1<sup>st</sup>**.

**The Coblentz Award** is presented annually to an outstanding young molecular spectroscopist under the age of 40 (as of January 1 the year of the award). Nominations will be accepted **January 3<sup>rd</sup> – July 15<sup>th</sup>**.

**The Craver Award** recognizes young spectroscopists for efforts in applied analytical vibrational spectroscopy. Candidates must be under the age of 45 on January 1<sup>st</sup> of the year of the award. Nominations will be accepted until **August 30<sup>th</sup>**.

**The Lippincott Award** honors Dr. Ellis R. Lippincott's memory by the recognition of significant contributions and notable achievements in the field of vibrational spectroscopy. The medal is sponsored jointly by the Coblentz Society, the Optical Society of America, and the Society for Applied Spectroscopy. Nominations will be accepted until **October 1<sup>st</sup>**.

**Coblentz and William G. Fateley Student Awards** are awarded to graduate or undergraduate students who have shown excellence in vibrational spectroscopy research and/or coursework. The three leading graduate students selected by the award committee will also qualify for consideration for the William G. Fateley Student Award. Nominations will be accepted **November 1<sup>st</sup> – February 15<sup>th</sup>**.

**Honorary Membership:** The Coblentz Society awards honorary memberships in the Society to people who have made outstanding contributions to the field of vibrational spectroscopy or any other field related to the purposes of the Society. Nominations close on **February 1<sup>st</sup>**.

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**Additional information regarding nomination eligibility, requirements, and procedures can be found at <http://www.coblentz.org/awards>.**

## ACS DIVISION OF ANALYTICAL CHEMISTRY



### Call for Nominations ACS Division of Analytical Chemistry Awards 2018 Deadline: November 1, 2017

#### ELIGIBILITY

Eligibility is open to members and non-members of the Division of Analytical Chemistry. Nominees for the J. Calvin Giddings Award for Excellence in Education, however, must have demonstrated excellence in teaching through at least five years at the time the award is presented. Nominating and seconding letters may be submitted by persons who are not members of the Division.

#### DEADLINES

All nominations must be sent to the immediate past chairperson of the Division and must be received by November 1 of each year. The immediate past chairperson of the Division shall in turn transmit the nominations to the chairpersons of the appropriate juries. Nominations that are unsuccessful will be retained for jury consideration for the following three years.

For the 2018 Awards, nominations shall be sent by email or postal mail no later than November 1, 2017 to:

ACS Division of Analytical Chemistry  
Award Nominations  
2019 Galisteo St., Bldg I-1  
Santa Fe, NM 87505  
Phone: 505-820-0443; office@analyticalsciences.org

#### NOMINATIONS

Nominations shall consist of:

1. A letter of nomination.
2. Two seconding letters.
3. A biographical statement emphasizing the accomplishments of the nominee which pertain to the award.
4. The nominating documents shall be submitted in one package and shall not exceed 8 pages of text, including the nominating and seconding letters, biographical statement, and attachments to the nomination. **If the total pages for a nomination exceeds 8, then only the first 8 pages will be submitted to the jury for the award.**
5. Nominating and seconding letters may be submitted by persons who are not members of the Division.

Contributions by a candidate which have been recognized by a prior Divisional or ACS national award generally will not be considered by the jury for a Divisional award, especially if an award has been received within the past three years and within a similar area. The jury shall receive from its chairperson a list for each nominee of any such prior awards, their dates, and their citations. Any candidate previously nominated for an award who was not chosen as the awardee will be considered for up to three additional years without further action by the nominator being required. **More information is available at [www.analyticalsciences.org](http://www.analyticalsciences.org).**

## ANACHEM AWARD

*The ANACHEM Award is presented annually to an outstanding analytical chemist based on activities in teaching, research, administration or other activity, which has advanced the art and science of the field.*



**Jennifer Brodbelt**  
University of Texas at Austin

**Presentation: Thursday, 8:00 am; Tahoe Ballroom**

Dr. **Jennifer S. Brodbelt** is the Norman Hackerman Chaired Professor of Chemistry at the University of Texas at Austin. She earned her B.S. degree in chemistry at the University of Virginia and her doctorate in chemistry at Purdue University under the supervision of Prof. Graham Cooks. After a post-doctoral position at the University of California at Santa Barbara, she began her academic career at the University of Texas. Her research interests focus on the development and application of photodissociation mass spectrometry for characterization of the structures and modifications of biological molecules, including peptides, proteins, nucleic acids, oligosaccharides, and lipids. She

serves as an Associate Editor for the *Journal of the American Society for Mass Spectrometry* and recently served as President of the *American Society for Mass Spectrometry*.



## AES MID-CAREER AWARD

*This award is given for exceptional contributions to the field of electrophoresis, microfluidics, and related areas by an individual who is currently in the middle of their career.*



**R. Scott Martin**  
Saint Louis University

**Presentation: Thursday, 8:30 am; Tahoe Ballroom**

**R. Scott Martin** is Professor and Chair of Chemistry at Saint Louis University. He received his B.S. and M.S. degrees from Missouri State University and a Ph.D. in analytical chemistry from the University of Missouri-Columbia. He was then a NIH post-doctoral fellow in the Department of Pharmaceutical Chemistry at the University of Kansas. Dr. Martin started at Saint Louis University in 2003, where he was promoted to Associate Professor in 2008 and Full Professor in 2012. He served as the College of Arts and Sciences Endowed Chair in Chemistry from 2011-2015. He has also received other recognition including being named program chair of the 65th Midwestern Universities Analytical Chemistry Conference (MUACC 2011); the Graduate Mentor Award (Saint Louis University Graduate Student Association, 2011); member of the Board of Directors for the Association for LabAutomation (2009-2010); program chair for the LabAutomation conference (2009); and member of the editorial board for Electrophoresis (2005-2008). He has been actively involved with the journal Analytical Methods, which strives to publish early applications of new analytical methods with clear societal impact. This includes serving as an Associate Editor (2013-2017) and Editor-in-Chief (2017-present). His research interests involve the use of microchip devices for monitoring biological systems. This includes development of methods for analyzing cells on-chip through integration of multiple techniques such as cell culture, electrophoresis and electrochemistry.



## IRDG CHALMERS AND DENT STUDENT AWARD

*The Chalmers and Dent Student Travel Award has been established to recognise and support an outstanding PhD student through financial support to present their research to an international audience at the annual SciX meeting. The award is named after two previous chairs of the IRDG, John Chalmers and Geoff Dent, in recognition of their continuing support for the IRDG and in particular for their support of students and early career researchers. Throughout their careers, both John and Geoff have been highly active in the development and promotion of the vibrational spectroscopists of the future in both academia and industry through mentoring, encouragement and inspiration.*



**2017 IRDG Chalmers and Dent Student Award Recipient**  
**Rachael Cameron**, University of Strathclyde



**Rachael Cameron** obtained her B.Sc. Hons. degree in Biomedical Science at Edinburgh Napier University in 2006. Following this she embarked on a research career in a molecular biology lab within the Wellcome Trust Centre for Molecular Parasitology at the University of Glasgow from 2008-2014. Where she published her work on malaria vaccine candidates by disrupting the genome and tracking RNA and protein expression; in a book chapter, a methods paper and co-authored a Nature paper. In 2014 she joined the Centre for Molecular Nanometrology at the University of Strathclyde and the Edinburgh Cancer Research Centre at the University of Edinburgh, to begin her joint centre Ph.D. with integrated masters in Healthcare Innovation and Entrepreneurship within centre for doctoral training (CDT) programme of Optical Medical Imaging (OPTIMA). Her research involves using Raman spectroscopy to aid drug development and diagnostics for cancer.

Under the guidance of Prof Duncan Graham and Prof Margaret Frame, she has created a novel system to spectroscopically track the localisation and release of an unlabelled anti-cancer drug from nanoparticles in vitro in 3D using fixed and live cells, with plans to move in vivo. The focus of this work is on utilising the cellular silent region of the spectral fingerprint, where the alkyne vibrations reside. This is with a view to develop more informative pre-clinical study platforms to investigate why therapies fail; due the localisation, retention time, or metabolism, and can these be enhanced by nanodelivery of the drug. Rachael has presented her research at the Oxford Biomedical Imaging Summer School, RSC Early Careers Symposium and the IRDG and Martin and Willis Prize Meeting. Her recent successes include securing an early careers award to attend the Re-Thinking Cancer Workshop (London), where she contributed towards an editorial paper on translational cancer research, and she was awarded the best oral presentation at the TransMed Student Conference in 2016 (Edinburgh).



## ROYAL SOCIETY OF CHEMISTRY SIR GEORGE STOKES AWARD

The Sir George Stokes Award is given to a leading analytical scientist awarded for translating research in biomolecular engineering and nanotechnology into new analytical devices and reagents to improve human and animal health.



**Tony Cass**  
Imperial College London

**Presentation: Monday, 9:00 am; Tahoe Ballroom**



**Tony Cass** attended Sir Joseph Williamson's Mathematical School for Boys in Rochester Kent before graduating with a 1st Class Honours degree in Chemistry from the University of York. After working for a year as a laboratory technician he joined the group of Professor Allen Hill FRS in the Inorganic Chemistry Laboratory in Oxford and was a Hastings Senior Scholar at Queen's College Oxford. After a post-doctoral research assistantship with Allen Hill he was then awarded a BP Junior Research Fellowship at St Hugh's College, Oxford. During his time in Oxford his research with Allen Hill and colleagues led to the development of the first electronic blood glucose sensor an achievement recognised by the award of the Mullard Medal of the Royal Society (jointly with Allen and Dr Monika Green) and a Chemical Landmark Award of the RSC (with Allen and Dr Graham Davis). Tony then moved to Imperial College London as a lecturer in a newly established Centre for Biotechnology and was subsequently appointed to a chair in Chemical Biology in the Department of Biochemistry before becoming Deputy Director of the Institute of Biomedical Engineering at Imperial College London working closely with its founding director, Professor Chris Toumazou FRS FREng. During this time, he also founded Bionano Consulting Ltd. with Professor Gabriel Aeppli FRS. Tony then moved to the Chemistry Department where his research continues in collaboration with colleagues in the faculties of Natural Sciences, Medicine and Engineering. Tony is married, with 3 sons, to Dr Pam Ganju, a pharma industry executive.



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## PREVIOUS FACSS BOARD AND MEETING CHAIRS

1973			1984 - Philadelphia	
Jeannette Grasselli	Governing Board Chair		Theodore Rains	Governing Board Chair
1974 – Atlantic City			D. Bruce Chase	General
James White	Governing Board Chair		Patricia Rouse Coleman	Program
George Heinz	General		Fred Corcoran	Arrangements
James White	Program		Peter Keliher	Exhibit
Edward Ruffing	Exhibit		1985 - Philadelphia	
1975 - Indianapolis			Robert Barford	Governing Board Chair
James Holcombe	Governing Board Chair		Fred Corcoran	General
Gerald Wallace	General		Matthew Klee	Program
James Holcomb	Program		Marshall Fishman	Arrangements
Edward Ruffing	Exhibit		Peter Keliher	Exhibit
1976 - Philadelphia			1986 - St. Louis	
Edward Brame	Governing Board Chair		Ronald Schroeder	Governing Board Chair
Edward Brame	General		Marshall Fishman	General
Edward Dunlap	Program		Alexander Scheeline	Program
Douglas Robinson	Arrangements		Terry Hunter	Arrangements
Edward Ruffing	Exhibit		Edward Brame	Exhibit
1977 - Detroit			1987 - Detroit	
Edgar Peck	Governing Board Chair		Patricia Rouse Coleman	Governing Board Chair
Mitch Kapron and James Burns	General		David Coleman and L. Felix Schneider	General
Jeannette Grasselli	Program		John S. Beaty	Program
L. Felix Schneider	Arrangements		Edward Brame	Exhibit
Edward Ruffing	Exhibit		1988 - Boston	
1978 - Boston			James Cavanaugh	Governing Board Chair
James Williamson	Governing Board Chair		Frank Plankey and John S. Beaty	General
Paul Lublin	General		Roger Gilpin	Program
James Cosgrove	Program		Edward Brame	Exhibit
James Cornwell	Arrangements		1989 - Chicago	
Edward Ruffing	Exhibit		Alexander Scheeline	Governing Board Chair
1979 - Philadelphia			Paul Bourassa	General
Peter Keliher	Governing Board Chair		Robert G. Michel	Program
Douglas Robinson	General		Edward Brame	Exhibit
Philip LeFleur	Program		1990 - Cleveland	
Sydney Fleming	Arrangements		Nancy Miller-Ihli	Governing Board Chair
Edward Ruffing	Exhibit		Charles Belle	General
1980 - Philadelphia			Steven Hughes	Program
L. Felix Schneider	Governing Board Chair		Edward Brame	Exhibit
Sydney Fleming	General		1991 - Anaheim	
Theodore Rains	Program		David Coleman	Governing Board Chair
Robert Barford	Arrangements		Richard Deming and Constance Sobel	General
Edward Ruffing	Exhibit		James Holcombe	Program
1981 - Philadelphia			Edward Brame	Exhibit
Jack Katon	Governing Board Chair		1992 - Philadelphia	
Robert Barford	General		Karmie Galle	Governing Board Chair
Mary Kaiser	Program		Matthew Klee	General
James Cavanaugh	Arrangements		Barry Lavine	Program
Peter Keliher	Exhibit		Edward Brame	Exhibit
1982 – Philadelphia			1993 - Detroit	
Sydney Fleming	Governing Board Chair		Robert Watters	Governing Board Chair
James Cavanaugh	General		L. Felix Schneider and David Coleman	General
Andrew Zander	Program		Julian Tyson	Program
Matthew O'Brien	Arrangements		Mildred Barber	Exhibit
Peter Keliher	Exhibit		1994 - St. Louis	
1983 - Philadelphia			Paul Bourassa	Governing Board Chair
Mary Kaiser	Governing Board Chair		Terry Hunter	General
Matthew O'Brien	General		John Koropchak	Program
John Lephardt	Program		Mildred Barber	Exhibit
D. Bruce Chase	Arrangements			
Peter Keliher	Exhibit			

## PREVIOUS FACSS BOARD AND MEETING CHAIRS

1995 – Cincinnati		2006 – Orlando	
Jon W. Carnahan	Governing Board Chair	Diane Parry	Governing Board Chair
Joseph A. Caruso	General	Christine Wehlburg	General
Richard F. Browner and R. Kenneth Marcus	Program	S. Douglass Gilman	Program
Mildred Barber	Exhibit	Mike Carrabba	Exhibit
1996 – Kansas City		2007 – Memphis	
Rachael Barbour	Governing Board Chair	James Rydzak	Governing Board Chair
O. Karmie Galle	General	Paul Bourassa	General
William Fateley	Program	Ian R Lewis	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
1997 - Providence		2008 – Reno	
Mildred Barber	Governing Board Chair	Gary Brewer	Governing Board Chair
Chris Brown	General	John Hellgeth	General
John Olesik	Program	Greg Klunder	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
1998 - Austin		2009 – Louisville	
John Graham	Governing Board Chair	Becky Dittmar	Governing Board Chair
David Laude	General	Jessica Jarman	General
Isiah Warner and Linda McGown	Program	Curtis Marcott	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
1999 - Vancouver		2010 – Raleigh	
Robert G. Michel	Governing Board Chair	S. Douglass Gilman	Governing Board Chair
Michael Blades	General	David J. Butcher	General
Ronald Williams	Program	André J. Sommer	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
2000 - Nashville		2011 – Reno	
John Koropchak	Governing Board Chair	S. Douglass Gilman	Governing Board Chair
Arlene Garrison	General	Greg Klunder	General
Michael Carrabba	Program	Pavel Matousek	Program
Scott McGeorge	Exhibit	Mike Carrabba	Exhibit
2001 – Detroit		2012 – Kansas City	
David A. Laude	Governing Board Chair	Ian R. Lewis	Governing Board Chair
David Coleman and L. Felix Schneider	General Co-Chairs	Brandye Smith-Goettler	SciX General
David J. Butcher	Program	Steven Ray	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibits
2002 – Providence		2013 – Milwaukee, WI	
Michael Carrabba	Governing Board Chair	Ian R. Lewis	Governing Board Chair
Robert G. Michel	General Chair	Fred LaPlant	SciX General
Mark A. Hayes	Program Chair	Mike George	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit
2003 – Fort Lauderdale		2014 – Reno, NV	
Ronald Williams	Governing Board Chair	Greg Klunder	Governing Board Chair
Rina Dukor	General	Luisa T. M. Profeta	SciX General
James Rydzak	Program	José R. Almirall	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit
2004 – Portland		2015 – Providence, RI	
Michael Blades	Governing Board Chair	Greg Klunder	Governing Board Chair
David Trimble	General	Edita Botonjic-Sehic	SciX General
George Agnes	Program	Glen P. Jackson	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit
2005- Quebec City, Canada		2016 – Minneapolis, MN	
Mark Hayes	Governing Board Chair	Steven Ray	Governing Board Chair
Denis Boudreau	General	Mary Kate Donais	SciX General
Paul Farnsworth	Program	Alexandra Ros	SciX Program
Scott McGeorge	Exhibit	Mike Carrabba	SciX Exhibit

## SOCIETY AND COMMITTEE MEETINGS AND EVENTS

### FACSS/SciX ORGANIZATION

**Sunday, October 8, Room: Nevada 9, Spa Level**

1:00 – 3:00 pm     SciX Long Range Planning Meeting (Conference)  
 4:00 – 6:00 pm     FACSS Long Range Planning Meeting (Federation)  
 7:15 – 7:45 pm     Program Committee

**Monday, October 9, Room: Nevada 9, Spa Level**

12:15 – 1:15 pm     SciX 2018 Atlanta Meeting: Program

**Tuesday, October 10, Room: Nevada 9, Spa Level**

1:45 – 2:45 pm     SciX 2019 Palm Springs Meeting: Budget, Program and Planning

**Wednesday, October 11, Room: Nevada 9, Spa Level**

12:15 – 1:15 pm     SciX 2018 Atlanta Meeting: Budget and Planning  
 3:45 – 4:15 pm     Budget and Finance Committee

**Thursday, October 12**

Noon                Executive Committee Meeting (*for the Executive Committee only*), Room: Nevada 9  
 6:00 pm            Governing Board Meeting (light dinner will be provided), Room: Nevada 9  
 9:00 pm            Governing Board Chair Reception (delegates and invitees), Location TBA

### COBLENTZ SOCIETY

**Monday, October 9**

11:30 am – 1:00 pm     Coblentz and SAS Speed Mentoring Session, Room: Nevada 8, Spa Level. The Coblentz and SAS Societies are hosting a Speed Mentoring Event. Prospective mentors and mentees will interact in a fun, fast-paced one-on-one setting to meet other scientists, expand professional networks, and potentially form a mentoring relationship. Registration is free and lunch will be provided.

**Wednesday, October 11**

1:30 - 3:30 pm            Coblentz Board Meeting, Room: Nevada 9, Spa Level

**Thursday, October 12**

7:00 am                Coblentz Annual Members Meeting and Breakfast, Room: Nevada 11, Spa Level.

### SOCIETY FOR APPLIED SPECTROSCOPY

**Saturday, October 7**

1:00 – 9:00 pm        SAS Executive Committee, Room: Nevada 10, Spa Level

**Sunday, October 8**

12:00 – 4:00 pm        SAS Members Only Event, Room: Shasta, Grand Sierra Resort  
 7:15 pm                SAS Student Poster Session Room: Reno Ballroom

**Monday, October 9**

10:30 – 10:50 am        SAS PAT Technical Section Business Meeting Room: Nevada 6  
 12:00 – 2:00 pm        SAS Publications Committee Room: Nevada 10, Spa Level  
 8:00 – 11:00 pm        SAS Student Event, Sierra Bay Aqua Driving Range, GSR

**Tuesday, October 10**

12:00 – 2:00 pm        SAS Editorial Board Meeting Room: Nevada 10, Spa Level  
 4:00 – 7:00 pm        SAS Governing Board Meeting Room: Nevada 10, Spa Level  
 7:30 pm                SAS Wine and Cheese Awards Reception, Room: Tahoe Ballroom

**Wednesday, October 11**

9:00 – 11:00 am        SAS Membership/Publicity Committee Room: Nevada 10, Spa Level

### NASLIBS

**Monday, October 9**

5:00 – 7:00 pm        NASLIBS Board Meeting, Room: Nevada 9, Spa Level

## SciX EXHIBITORS and EXHIBIT HALL ACTIVITIES

The exhibit is one of the focal points of the SciX Conference. Exhibits are the realization of the research presented during the scientific symposia and include innovation instrumentation, software, and supplies. New technologies and products will be shown and you will find an interesting mix of sales, scientific, and engineering expertise among their representatives.

### Sunday, October 8

4:10 pm What's Hot Exhibitor Presentations, *Tahoe Ballroom*

### Monday, October 9

5:30 pm Exhibit Hall Opening Reception, *Exhibit Hall*

### Tuesday, October 10 and Wednesday, October 11

11:00 am – 12:00 pm Poster Session and Coffee Break in Exhibit Hall  
 11:40 am What's Hot Exhibitor Presentations in Exhibit Hall  
 12:00 noon Complimentary lunch for all attendees in Exhibit Hall  
 2:30 – 3:40 pm Drop off your raffle ticket for a chance to win a Samsung Tablet  
 (chance to win each day – see ticket for details)  
 3:10 – 3:50 pm Poster Viewing and Break

### Exhibit Hours:

Monday 5:30 pm – 7:30 pm  
 Tuesday 10:00 am – 4:30 pm  
 Wednesday 10:00 am – 4:00 pm

*Refer back inside cover for exhibit hall layout*

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art photonics GmbH .....	44	Necsel IP .....	55
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## EXHIBITOR INFORMATION

**ACS Division of Analytical Chemistry ..... Booth #70**  
 2019 Galisteo St., Bldg I-1  
 Santa Fe, NM 87505  
[www.analyticalsciences.org](http://www.analyticalsciences.org)

**AES Electrophoresis Society ..... Booth #96**  
 1202 Ann St  
 Madison, WI 53713  
[www.aesociety.org](http://www.aesociety.org)

**Agilent Technologies, Inc. .... Booth #61**  
 2850 Centerville Rd.  
 Wilmington, DE 19808  
[www.agilent.com](http://www.agilent.com)

**Alluxa, Inc. .... Booth #7**  
 3660 N Laughlin  
 Santa Rosa, CA 95403  
[www.alluxa.com](http://www.alluxa.com)

**Anasys Instruments ..... Booth #4**  
 325 Chapala St  
 Santa Barbara, CA 93101  
[www.anasysinstruments.com](http://www.anasysinstruments.com)

**Andor Technology ..... Booth #77**  
 300 Baker Avenue  
 Concord, CT 01742  
[www.andor.com](http://www.andor.com)

**Anton Paar USA ..... Booth #3**  
 10215 Timber Ridge Drive  
 Ashland, VA 23005  
[www.anton-paar.com](http://www.anton-paar.com)

**Applied Spectra, Inc. .... Booth #90**  
 46665 Fremont Blvd  
 Fremont, CA 94538  
[www.appliedspectra.com](http://www.appliedspectra.com)

**art photonics GmbH ..... Booth #44**  
 Rudower Chaussee 46  
 Berlin, Germany 12489  
[www.artphotonics.com](http://www.artphotonics.com)

**Avantes, Inc ..... Booth #80**  
 500 S. Aruther Ave, #500  
 Louisville, CO 80027  
[www.avantes.com](http://www.avantes.com)

**B&W Tek ..... Booth #42**  
 19 Shea Way, ste 301  
 Newark, DE 19713  
[www.bwtek.com](http://www.bwtek.com)

**Barnett Technical Services ..... Booth #26**  
 5050 Laguna Blvd., Suite 112-620  
 Elk Grove, CA 95758  
[www.Barnett-Technical.com](http://www.Barnett-Technical.com)

**BaySpec, Inc. .... Booth #28**  
 1101 McKay Drive  
 San Jose, CA 95131  
[www.bayspec.com](http://www.bayspec.com)

**Bio-Rad Laboratories, Informatics Division ... Booth #17**  
 2000 Market Street, Suite 1460  
 Informatics Div  
 Philadelphia, PA 19103  
[www.knowitall.com](http://www.knowitall.com)

**BioTools, Inc. .... Booth #57**  
 17546 Bee Line Highway  
 Jupiter, FL 33458  
[www.btools.com](http://www.btools.com)

**Bruker Corporation ..... Booth #18**  
 40 Manning Road  
 Billerica, MA 01821  
[www.bruker.com](http://www.bruker.com)

**CAMO Smart Software, Inc. .... Booth #48**  
 One Woodbridge Ctr, Suite 319  
 Woodbridge, NJ 07095  
[www.camo.com](http://www.camo.com)

**Catalina Scientific ..... Booth #45**  
 1870 West Prince Road, Ste 21  
 Tucson, AZ 85705  
[www.catalinasci.com](http://www.catalinasci.com)

**Cobalt Light Systems ..... Booth #30**  
 Suite 1319, 11951 Freedom Dr  
 Reston, VA 20190  
[www.cobaltlight.com](http://www.cobaltlight.com)

**Coblentz Society ..... Booth #81**  
 955 Drew Lane  
 Ashland, OR 97520  
[www.coblentz.org](http://www.coblentz.org)

**Cobolt AB ..... Booth #78**  
 Vretenvagen 13  
 Solna 17154,  
 Sweden  
[www.cobolt.se](http://www.cobolt.se)

**Continuum, Amplitude Laser Group ..... Booth #75**  
 140 Baytech Dr  
 San Jose, CA 95134  
[www.continuumlasers.com](http://www.continuumlasers.com)

**Czitek ..... Booth #63**  
 6 Finance Dr  
 Danbury, CT 06810  
[www.czitek.com](http://www.czitek.com)

**Daylight Solutions ..... Booth #46**  
 15378 Avenue of Science, Ste 200  
 San Diego, CA 92128  
[www.daylightsolutions.com](http://www.daylightsolutions.com)

**Eigenvector Research, Inc. .... Booth #67**  
 196 Hyacinth Rd  
 Manson, WA 98831  
<http://www.eigenvector.com>

**FACSS / SciX ..... Booth #TBA**  
 2019 Galisteo St., Bldg I-1  
 Santa Fe, NM 87505  
[www.facss.org/ SciXconference.org](http://www.facss.org/ SciXconference.org)

## EXHIBITOR INFORMATION

**FiberTech Optica, Inc. .... Booth #10**  
 330 Gage Avenue, Ste 1  
 Kitchener, ON, N2M 5C6  
 CANADA  
[www.fibertech-optica.com](http://www.fibertech-optica.com)

**Fiveash Data Management (FDM)..... Booth #27**  
 211 Vista Road  
 Madison, WI 53726  
[www.fdm-spectra.com](http://www.fdm-spectra.com)

**Flash Photonics, Inc. .... Booth #22**  
 PO Box 2197  
 Redmond, WA 98073  
[www.flashanalysis.com](http://www.flashanalysis.com)

**H2Optx Inc ..... Booth #12**  
 6830 Via Del Oro, Suite 200  
 San Jose, CA 95119  
[www.h2optx.com](http://www.h2optx.com)

**Hamamatsu Corporation..... Booth #41**  
 360 Foothill Rd.  
 Bridgewater, NJ 08807  
[www.hamamatsu.com](http://www.hamamatsu.com)

**Harrick Scientific ..... Booth #34**  
 141 Tompkins Ave  
 Box 277  
 Pleasantville, NY 10570  
[www.harricksci.com](http://www.harricksci.com)

**Hellma USA ..... Booth #66**  
 80 Skyline Drive  
 Plainview, NY 11704  
[www.hellmausa.com](http://www.hellmausa.com)

**Hindsight Imaging..... Booth #33**  
 1 Harvard St, Ste 302  
 Brookline, MA 02445  
[www.hindsight-imaging.com](http://www.hindsight-imaging.com)

**HORIBA Scientific..... Booth #100**  
 Attn: Raman Spectroscopy  
 3880 Park Avenue  
 Edison, NJ 08820  
[www.horiba.com/scientific](http://www.horiba.com/scientific)

**Ibsen Photonics..... Booth #92**  
 Ryttermarken 15-21  
 Farum,  
 Denmark DK-3520  
[www.ibsen.com](http://www.ibsen.com)

**ICP Information Newsletter, Inc..... Booth #20**  
 PO Box 666  
 Hadley, MA 01035-0666  
<http://icpinformation.org>

**Innovative Photonic Solutions..... Booth #114**  
 4250 U. S. Highway 1, Ste 1  
 Monmouth Junction, NJ 08852  
[www.innovativephotonics.com](http://www.innovativephotonics.com)

**Kaiser Optical Systems, Inc./Analytik Jena...Booth #106**  
 371 Parkland Plaza  
 Ann Arbor, MI 48103  
[www.kosi.com](http://www.kosi.com)

**LEONI Fiber Optics, Inc.....Booth #39**  
 PO Box 615  
 Lightfoot, VA 23090  
[www.leoni-fiber-optics.com](http://www.leoni-fiber-optics.com)

**LLA Instruments GmbH .....Booth #69**  
 Justus-von-Liebig-Str. 9/11  
 Berlin, 12489  
 Germany  
[www.lla.de](http://www.lla.de)

**Metrohm USA .....Booth #53**  
 6555 Pelican Creek Circle  
 Riverview, FL 33578  
[www.metrohmusa.com](http://www.metrohmusa.com)

**Molecular Vista .....Booth #47**  
 6840 Via Del Oro, Suite 110  
 San Jose, CA 95119  
[www.molecularvista.com](http://www.molecularvista.com)

**MONTFORT Laser GmbH.....Booth #62**  
 Im Holderlob 6A  
 Goetzix, VA 6840,  
 Austria  
[www.montfortlaser.com](http://www.montfortlaser.com)

**Necsel IP.....Booth #55**  
 30-B Pennington-Hopewell Rd  
 Pennington, NJ 08534  
[www.pd-ld.com](http://www.pd-ld.com)

**Ocean Optics, Inc. ....Booth #118**  
 830 Douglas Avenue  
 Dunedin, FL 34698  
[www.oceanoptics.com](http://www.oceanoptics.com)

**Ondax, Inc. ....Booth #51**  
 850 E. Duarte Rd.  
 Monrovia, CA 91016  
[www.ondax.com](http://www.ondax.com)

**Optigrate Corp ..... Booth #1**  
 562 S Econ Cir.  
 Oviedo, FL 32765  
[www.optigrate.com](http://www.optigrate.com)

**PerkinElmer .....Booth #98**  
 940 Winter St.  
 Waltham, MA 02461  
[www.perkinelmer.com](http://www.perkinelmer.com)

**Photometrics ..... Booth #6**  
 3440 E. Britannia Dr. #100  
 Tucson, AZ 85706  
[www.photometrics.com](http://www.photometrics.com)

## EXHIBITOR INFORMATION

**Photon Systems, Inc. .... Booth #13**  
 1512 W Industrial Park St  
 Covina, CA 91722  
[www.photonsystems.com](http://www.photonsystems.com)

**PIKE Technologies..... Booth #14**  
 6125 Cottonwood Drive  
 Madison, WI 53719  
[www.piketech.com](http://www.piketech.com)

**Princeton Infrared Technologies, Inc. .... Booth #21**  
 9 Deerpark Dr, Ste J5  
 Monmouth Junction, NJ 08852  
[www.princetonirtech.com](http://www.princetonirtech.com)

**Princeton Instruments, Inc. .... Booth #73**  
 3660 Quakerbridge Road  
 Trenton, NJ 01720  
[www.princetoninstruments.com](http://www.princetoninstruments.com)

**Quantel Laser ..... Booth #59**  
 49 Willow Peak Dr  
 Bozeman, MT 59718  
[www.quantel-laser.com](http://www.quantel-laser.com)

**Renishaw, Inc..... Booth #110**  
 5277 Trillium Blvd.  
 Hoffman Estates, IL 60192  
[www.renishaw.com](http://www.renishaw.com)

**Royal Society of Chemistry ..... Booth #97**  
 Thomas Graham House  
 Science Park, Milton Road  
 Cambridge, UK CB4 0WF  
[www.rsc.org](http://www.rsc.org)

**RPMC Lasers, Inc. .... Booth #72**  
 203 Joseph Street  
 Ofallon, MO 63366  
[www.rpmclasers.com](http://www.rpmclasers.com)

**SciAps, Inc. .... Booth #76**  
 2 Constitution Way  
 Woburn, MA 01801  
[www.sciaps.com](http://www.sciaps.com)

**Shimadzu Scientific Instruments, Inc. .... Booth #38**  
 7102 Riverwood Dr.  
 Columbia, MD 21046  
[www.ssi.shimadzu.com](http://www.ssi.shimadzu.com)

**Society for Applied Spectroscopy..... Booth #82**  
 168 West Main Street #300  
 New Market, MD 21774  
[www.s-a-s.org](http://www.s-a-s.org)

**Specac, Inc. .... Booth #68**  
 414 Commerce Dr, Suite 175  
 Fort Washington, PA 19034  
[www.specac.com](http://www.specac.com)

**Spectral Systems LLC..... Booth #19**  
 35 Corporate Park Drive  
 Hopewell Junction, NY 12533  
[www.spectral-systems.com](http://www.spectral-systems.com)

**SpectroClick, Inc. .... Booth #64**  
 60 Hazelwood Dr. Rm. 226A  
 Champaign, IL 61820  
[www.spectroclick.com](http://www.spectroclick.com)

**Spectroscopy Magazine / LCGC Magazine..... Booth #94**  
 485F US Highway 1 South, Ste 100  
 Iselin, NJ 8830  
[www.spectroscopyonline.com](http://www.spectroscopyonline.com)

**Technospex Pte Ltd..... Booth #79**  
 1092 Lower Delta Road #04-01  
 Singapore, 169203  
 Singapore  
[www.technospex.com](http://www.technospex.com)

**Thermo Fisher Scientific ..... Booth #35**  
 2 Radcliff Road  
 Tewksbury, MA 01876  
[www.thermoscientific.com/portableid](http://www.thermoscientific.com/portableid)

**Tornado Spectral Systems ..... Booth #99**  
 555 Richmond Street West, Ste 402  
 Toronto, ON M5V 3B1 Canada  
[www.tornado-spectral.com](http://www.tornado-spectral.com)

**Triclinic Labs Inc ..... Booth #65**  
 2660 Schuyler Ave, Suite A  
 Lafayette, IN 47905  
[www.tricliniclabs.com](http://www.tricliniclabs.com)

**TSI Inc. .... Booth #50**  
 500 Cardigan Road  
 St. Paul, MN 55126  
[www.tsi.com](http://www.tsi.com)

**Wasatch Photonics ..... Booth #8**  
 4022 Stirrup Creek Dr., Ste 311  
 Durham, NC 27703  
[www.wasatchphotonics.com](http://www.wasatchphotonics.com)

**WITec Instruments Corp. .... Booth #37**  
 130G Market Place Blvd  
 Knoxville, TN 37922  
[www.WITec-Instruments.com](http://www.WITec-Instruments.com)

## SHORT COURSES / WORKSHOPS

*Short Courses and Workshops are a valuable component of the SciX conference and are conducted by leading experts. There is an additional charge for most short courses and workshops. Complete descriptions can be found on the SciX website*

### SUNDAY

- 9:00 am **Intro to Vibrational Spectroscopy**  
Instructors: Peter Larkin, *Cytec Solvay Group*; John Wasylyk, Ravi Kalyanaraman, *Bristol Myers Squibb*  
Date/Time: October 8 / 9:00 am - 4:00 pm  
Rate: Conferee \$450; Student \$50; Non-Conferee \$550
- 9:00 am **Intro to Laser-Induced Breakdown Spectroscopy (LIBS)**  
Instructor: Jhanis Gonzalez, *Applied Spectra/ Lawrence Berkeley National Laboratory*  
Date/Time: October 8 / 9:00 am - Noon  
Rate: Conferee: \$225; Student: \$25; Non-Conferee: \$325

### TUESDAY

- 9:00 am **Chemometrics Without Equations: Advanced**  
Instructors: Barry Wise and Neal Gallagher, *Eigenvector Research*  
Date/Time: October 10 / 9:00 am - 12:00 pm  
Rate: Conferee: \$225; Student: \$25; Non-Conferee: \$325
- 9:00 am **Basics of Multivariate Modeling of Spectroscopic Data**  
Instructor: Heather Brooke, *CAMO*  
Date/Time: October 10 / 9:00 am - 4:00 pm  
Rate: Conferee \$450; Student \$50; Non-Conferee \$550
- 1:00 pm **Laser Fundamentals for Spectroscopy**  
Instructor: Robert Chimenti, *Innovative Photonics Solutions / Rowan University*  
Date/Time: October 10 / 1:00 - 4:00 pm  
Rate: Conferee: \$225; Student: \$25; Non-Conferee: \$325

### MONDAY

- 9:00 am **Chemometrics Without Equations: Introduction**  
Instructors: Barry Wise and Neal Gallagher, *Eigenvector Research*  
Date/Time: October 9 / 9:00 am - 4:00 pm  
Rate: Conferee \$450; Student \$50; Non-Conferee \$550
- 11:00 am **Lunch & Learn Workshop - AFM/Raman: Multi-technique Analysis at the Nanoscale**  
Instructors: Andrey Krayev, Maruda Shanmugasundaram and Marc Chaigneau, *HORIBA Scientific*  
Date/Time: October 9 / 11:00 am - 1:00pm  
Rate: Conferee: \$25; Student: \$15; Non-Conferee: \$35
- 1:00 pm **Intro to Bio-Spectroscopy**  
Instructor: Frederic Leblond, *Polytechnique Montreal*  
Date/Time: October 9 / 1:00 - 4:00 pm  
Rate: Conferee: \$225; Student: \$25; Non-Conferee: \$325
- 7:30 pm **Water to Wine Workshop: Aqualog® Phenolic Fluorescence Fingerprinting**  
Instructor: Adam M. Gilmore, *HORIBA Scientific*  
Date/Time: October 9 / 11:00 am - 1:00pm  
Rate: Conferee: \$25; Student: \$15; Non-Conferee: \$35

### THURSDAY

- 11:00 am **Lunch & Learn Workshop: How to Get Published**  
Instructors: Kristin MacDonald, *University of Vancouver/Society for Applied Spectroscopy*; Louisa Strain and Lucy Price, *SAGE Publishing*  
Date/Time: October 12 / 11:00 am - 1:00pm  
Rate: Conferee: \$25; Student: \$15; Non-Conferee: \$35



## PROGRAM OVERVIEW

### SUNDAY

- 4:20 pm **What's Hot Vendor Presentations,**  
*Tahoe Ballroom, page 39*
- 6:15 pm **KEYNOTE LECTURE.** The Analytical and Economic Challenges of Maintaining Food Safety in a Global Supply Chain, **Janie Dubois,** *Tahoe Ballroom, page 39*
- 7:15 pm **Welcome Mixer, SAS Sponsored Student Poster Session, Coblentz Student Awards, FACSS Student and Tomas Hirschfeld Scholar Awards,**  
*Tahoe Ballroom*

### MONDAY MORNING

- 7:50 am Opening Address  
**PLENARY LECTURES** *Tahoe Ballroom, page 40*  
17PLEN07: *Spectroscopy's* Emerging Leader in Molecular Spectroscopy Award  
17PLEN08: Ellis R. Lippincott Award  
17PLEN09: RSC Sir George Stokes Award
- 9:45 am **POSTER SESSION & BREAK,**  
*Reno Ballroom page 40*  
Chemometrics  
Forensics  
LIBS  
Process Analytical Technology  
Raman  
SPSJ
- 10:50 am **SYMPOSIA,** page 42  
17ATOM01: Glow Discharge Spectroscopy I, *Crystal 2*  
17AWD07: *Spectroscopy's* Emerging Leader in Molecular Spectroscopy Award Symposium, *Crystal 1*  
17BIM01: Spectral Analysis of Biofluids, *Nevada 7*  
17CHEM01: New Frontiers in Chemometrics, *Crystal 5*  
17IR02: Applications of Nanoscale IR Spectroscopy to Polymeric Materials, *Carson 1*  
17LIBS01: LIBS Industrial Applications, *Crystal 3*  
17NANO01: Recent Progress in Carbon Nanotubes and Graphene Research, *Nevada 5*  
17PAT01: SAS PAT Technical section: PAT in the Pharmaceutical Industries - Session I, *Nevada 6*  
17PMA01: Pharmaceutical Applications of Low Frequency Raman Spectroscopy, *Carson 2*  
17RAM04: Bioanalytical SERS I, *Carson 3*  
17RAM07: IRDG Raman, *Carson 4*  
17SPECIAL03: Stand-off Sensing, *Crystal 4*  
17SPSJ01: Frontiers of Deep- and Far- Ultraviolet Spectroscopy I, *Nevada 4*

### MONDAY AFTERNOON

- 1:30 pm **SYMPOSIA,** page 45  
17AES03: Electrokinetics for Cellular Analysis and Separations, *Crystal 4*  
17ATOM02: Glow Discharge Spectroscopy II, *Crystal 2*  
17AWD11: Coblentz Lippincott Award Symposium, *Crystal 1*  
17BIM02: Nanomaterial-Assisted Imaging, *Nevada 7*  
17CHEM02: Spectral Fingerprinting for Characterization of Complex Materials, *Crystal 5*  
17IR03: Nanoscale IR Applications in the Life Sciences, *Carson 1*  
17LIBS02: LIBS for Forensic and Homeland Security, *Crystal 3*  
17NANO02: Nanomaterials and Nanostructures for Energy-Related Applications, *Nevada 5*

- 17PAT07: Hand-Held and Portable Spectrometers, *Nevada 6*  
17PMA02: Counterfeit Pharmaceuticals, *Carson 2*  
17RAM01: Emerging Raman I, *Carson 4*  
17RAM05: Bioanalytical SERS II, *Carson 3*  
17SPSJ03: pMAIRS, *Nevada 4*

3:10 pm **POSTER SESSION & BREAK,** *Reno Ballroom*

3:50 pm **SYMPOSIA,** page 47

- 17AES02: Novel Electrokinetic Phenomena, *Crystal 4*  
17ATOM03: Recent Advances in Liquid Electrode Glow Discharge Plasmas, *Crystal 2*  
17BIM03: Analytical Sciences in Molecular Biology, *Nevada 7*  
17CHEM03: Chemometric Opportunities in the Forensic Sciences, *Crystal 5*  
17FORENS01: Nuclear Forensics, *Nevada 6*  
17IR04: Practical Implementation of Diffuse Reflectance Spectroscopy, *Carson 1*  
17LIBS03: NASLIBS: Molecular Signal in LIBS, *Crystal 3*  
17NANO03: Nanomaterials and Related Spectroscopy Methods for Energy Conversion, *Nevada 5*  
17PMA03: Identification of Counterfeit Medicines, *Carson 2*  
17RAM06: Bioanalytical SERS III, *Carson 3*  
17RAM11: Spatially Offset Raman Spectroscopy (SORS), *Carson 4*  
17RSC01: RSC Award session, *Crystal 1*  
17SPSJ02: Frontiers of Deep- and Far- Ultraviolet Spectroscopy II, *Nevada 4*

### TUESDAY MORNING

- 7:50 am Awards Presentations  
**PLENARY LECTURES** *Tahoe Ballroom, page 51*
- 8:00 am 17PLEN04: Charles Mann Award for Raman Spectroscopy
- 8:30 am 17PLEN05: Coblentz Society Craver Award
- 9:15 am **SYMPOSIA,** page 51  
17ATOM04: Laser Ablation-ICP-MS I, *Crystal 2*  
17AWD04: Charles Mann Award Symposium, *Crystal 1*  
17CTP01: Analytical Chemists Easing World Poverty, *Crystal 5*  
17IR05: Quantum Cascade Lasers – I, *Carson 1*  
17MASS01: Integrated Micro-Extraction Platforms for Improved Ambient Spectrometry, *Nevada 7*  
17PAT03: Industrial Applications of Vibrational Spectroscopy, *Nevada 6*  
17PMA04: Raman Characterization of Proteins and Biologics, *Carson 2*  
17RAM08: Biomedical Raman (Clirspec), *Carson 3*  
17RAM15: Nano-Raman, *Carson 4*  
17SPECIAL01: Chemistry in Art & Archeology, *Crystal 4*  
17SPR01: Multimetallic Plasmonic Nanoparticles, *Nevada 5*
- 11:00 am **POSTER SESSION & BREAK,** *Exhibit Hall, page 53*  
Electrophoresis  
Archaeology  
Biomedical and Bioanalytical  
LIBS
- 11:40 am **WHAT'S HOT EXHIBITOR PRESENTATIONS**  
*Exhibit Hall, page 55*

## PROGRAM OVERVIEW

TUESDAY AFTERNOON	
Noon	Free lunch in exhibit hall for all registered conferees, <i>Exhibit Hall</i> (ticket required)
1:30 pm	<b>SYMPOSIA</b> , page 55 17AES01: Micro-Scale Electroporation and Electrokinetic Study of Cells and Biomolecules, <i>Crystal 4</i> 17ATOM05: Excitation and Ionization Techniques for Atomic and Molecular Spectroscopy, <i>Crystal 2</i> 17AWD05: Coblentz Craver Award Symposium, <i>Crystal 1</i> 17CTP02: Diversity, Equity, and Inclusion in Analytical Chemistry, <i>Crystal 5</i> 17IR06: Quantum Cascade Lasers – II, <i>Carson 1</i> 17LIBS05: Elemental Mapping by LIBS, <i>Crystal 3</i> 17MASS02: Recent Development in Single Cell Mass Spectrometry Analysis, <i>Nevada 7</i> 17PAT04: Online Analysis of Industrial Processes and Reactions, <i>Nevada 6</i> 17PMA05: Recent Advances in the Mode of Action of Biopharmaceuticals, <i>Carson 2</i> 17RAM09: Transmission Raman Spectroscopy, <i>Carson 3</i> 17RAM18: Nano IR / Nano-Raman I, <i>Carson 4</i> 17SPR03: Next Generation Plasmonics, <i>Nevada 5</i>
3:10 pm	<b>POSTER SESSION &amp; BREAK</b> , <i>Exhibit Hall</i>
3:50 pm	<b>SYMPOSIA</b> , page 58 17AES04: Designer (nano)Structures and Molecules for Separations and Analysis, <i>Crystal 4</i> 17ATOM06: Laser Ablation-ICP-MS II, <i>Crystal 2</i> 17CTP03: Innovative Approaches to Teaching Analytical Chemistry, <i>Crystal 5</i> 17FORENS02: Food Forensics, <i>Nevada 6</i> 17IR01: NanoIR/Nano-Raman II, <i>Carson 4</i> 17MASS03: Novel Ambient Mass Spectrometry Techniques for Forensic Science Analysis, <i>Nevada 7</i> 17PMA06: PAT in Biopharmaceutical Manufacturing, <i>Carson 2</i> 17RAM19: General Raman, <i>Carson 3</i> 17RSC02: RSC Sensors for Cancer Diagnostics, <i>Carson 1</i> 17SPR02: Plasmonic Nanoparticles, <i>Nevada 5</i>

WEDNESDAY MORNING	
7:50 am	Awards Presentations <b>PLENARY LECTURES</b> <i>Tahoe Ballroom</i> , page 61
8:00 am	17PLEN01: Applied Spectroscopy William F. Meggers Award
8:30 am	17PLEN02: Lester W. Strock Award
9:15 am	<b>SYMPOSIA</b> , page 61 17ATOM08: ICP-MS for Biomedical Applications, <i>Crystal 2</i> 17AWD01: William F. Meggers Award Symposium, <i>Crystal 1</i> 17BIM04: Endoscopy, <i>Nevada 7</i> 17CTP04: Making the Leap: Pathways from Graduate School to a Permanent Position, <i>Crystal 5</i> 17IR09: Ultrafast Two-Dimensional Spectroscopy – I, <i>Carson 1</i> 17LIBS07: LIBS Data Analysis, <i>Crystal 3</i> 17PAT05: Advances in On-line Process Analysis, <i>Nevada 6</i> 17PMA07: Spectroscopic Applications in the World of Biopharmaceuticals, <i>Carson 2</i> 17SPR06: Plasmonic-Powered Processes, <i>Nevada 5</i>

	17SURFACE01: Application of Surface Spectroscopic Techniques to Analysis of Nanomaterials and Devices, <i>Crystal 4</i>
11:00 am	<b>POSTER SESSION &amp; BREAK</b> , <i>Exhibit Hall</i> , page 63 Atomic Spectroscopy Infrared Spectroscopy Diverse Topics
11:40 am	<b>WHAT'S HOT EXHIBITOR PRESENTATIONS</b> <i>Exhibit Hall</i> , page 65

WEDNESDAY AFTERNOON	
Noon	Free lunch in exhibit hall for all registered conferees, <i>Exhibit Hall</i> (ticket required)
1:30 pm	<b>SYMPOSIA</b> , page 65 17ATOM09: ICP-MS for the Analysis of Nanomaterials, <i>Crystal 2</i> 17AWD02: Lester Strock Award Symposium, <i>Crystal 1</i> 17BIM05: Big Data in Biomedical Analyses <i>Nevada 7</i> 17CTP05: Food Safety and Analysis, <i>Crystal 5</i> 17IR10: Ultrafast Two-Dimensional Spectroscopy – II, <i>Carson 1</i> 17LIBS08: Fundamentals of Laser-Induced Plasmas, <i>Crystal 3</i> 17PAT06: Process Monitoring Enabled Flow API and Continuous Product Manufacture, <i>Nevada 6</i> 17PMA08: Biologics Characterization from Early to Late Stage Development, <i>Carson 2</i> 17RAM12: Portable Raman, <i>Carson 4</i> 17RAM14: Industrial Raman Spectroscopy, <i>Carson 3</i> 17SPR05: Plasmon-Enhanced Techniques, <i>Nevada 5</i> 17SURFACE02: Microscopic Methods for Surface Science Problems, <i>Crystal 4</i>
3:10 pm	<b>POSTER SESSION &amp; BREAK</b> , <i>Exhibit Hall</i>
3:50 pm	<b>SYMPOSIA</b> , page 67 17ATOM10: Atmospheric-Pressure Plasmas for Optical Mass Spectrometries, <i>Crystal 2</i> 17AWD10: Bruce R. Kowalski Award in Chemometrics Symposium, <i>Crystal 1</i> 17BIM06: Spectral Analysis of Collagenous Tissues, <i>Nevada 7</i> 17FORENS03: Proteomics for Forensic Analysis, <i>Nevada 6</i> 17IR11: Ultrafast Two-Dimensional Spectroscopy-III, <i>Carson 1</i> 17LIBS09: New Methods and Advancements in LIBS, <i>Crystal 3</i> 17PMA09: Advances in Micro-Analysis of Biologics, <i>Carson 2</i> 17RAM13: Pharmaceutical and Biotechnology Industrial Applications of Raman Spectroscopy, <i>Carson 3</i> 17RAM20: Raman Optical Activity (ROA), <i>Carson 4</i> 17SPR04: Point-of-Care Plasmonics, <i>Nevada 5</i> 17SURFACE03: Surface Analysis of Environmental Interfaces and Systems, <i>Crystal 4</i>

## PROGRAM OVERVIEW

### THURSDAY MORNING

- 7:50 am Awards Presentations  
**PLENARY LECTURES** *Tahoe Ballroom, page 70*  
 8:00 am 17PLEN03: ANACHEM Award  
 8:30 am 17PLEN06: AES Electrophoresis Mid Career Award  
 9:15 am **SYMPOSIA**, page 70  
 17ACS01: Recent Developments in Atomic Mass Spectrometry, *Crystal 2*  
 17AWD03: ANACHEM Award Symposium, *Crystal 1*  
 17CHEM04: Multiblock Methods, *Crystal 5*  
 17IR07: Clinical Applications of Vibrational Spectroscopy, *Carson 1*  
 17LIBS04: LIBS for Pharmaceutical and Biological Analysis, *Crystal 3*  
 17MASS04: 'Omics Frontiers: Ion Mobility and Mass Spectrometry, *Nevada 7*  
 17NANO04: Nano-Facilitated Sensing, *Nevada 5*  
 17PAT02: SAS PAT Technical section, *Nevada 6*  
 17RAM10: Raman Microscopy, *Carson 3*  
 17RAM17: Raman Spectroscopy for Security and Forensics Purposes, *Carson 4*  
 17SPECIAL02: Modern Techniques in Microscopy, *Crystal 4*  
 11:00 am **POSTER SESSION & BREAK**, *Exhibit Hall, page 72*  
 Forensics & Security  
 Mass Spectrometry  
 Microscopy  
 Nanotechnology  
 Pharmaceutical Analysis  
 Raman

### THURSDAY AFTERNOON

- 1:30 pm **SYMPOSIA**, page 74  
 17AWD06: AES Electrophoresis Award Symposium, *Crystal 1*  
 17CHEM05: New Developments in Calibration Methods, *Crystal 5*  
 17FORENS04: Forensic Analysis in the Lab and at the Crime Scene, *Nevada 6*  
 17IR08: Towards Point-of-Care Testing with Raman Spectroscopy, *Carson 1*  
 17LIBS11: Field Application of LIBS, *Crystal 3*  
 17MASS05: Recent Advances in Oligosaccharide Analysis by Mass Spectrometry, *Nevada 7*  
 17NANO05: Imaging and Sensing Applications of Atomic Precision NanoClusters, *Nevada 5*  
 17RAM03: Raman Imaging & Microscopy II, *Carson 3*  
 17RAM16: Pharmaceutical Raman, *Carson 4*  
 17SPECIAL04: Celebrating the FACSS membership of the Austrian Society of Analytical Chemistry (ASAC), *Crystal 4*  
 3:10 pm **POSTER SESSION & BREAK**, *Grand Salon*  
 3:50 pm **PLENARY SESSION**, *Tahoe Ballroom, page 97*  
 FACSS Distinguished Service Award  
 17AWD08: FACSS Innovation Award Symposium

### FRIDAY MORNING SPECIAL PLENARY SESSION

*Tahoe Ballroom, Page 77*

- 7:50 am Announcement of Innovation Award Winners  
 8:00 am The New Vision of Analytical Science by the World  
 10:00 am SciX 2018 Preview



**The Society for Applied Spectroscopy  
 Cordially Invites All SAS Members  
 to Join Us at Our Annual  
 Wine and Cheese Awards Reception  
 Tuesday, October 10, 2017 7:30 p.m.  
 Grand Sierra Resort, Tahoe Ballroom**

This is a free member's only event with food and drinks.  
**Doors will open to non-members at 9pm with limited refreshments.**  
 If you would like to become a member, please go to [www.s-a-s.org](http://www.s-a-s.org),  
 visit SAS booth 82, or contact the SAS Office at (301) 694-8122 or  
[sasadmin@s-a-s.org](mailto:sasadmin@s-a-s.org)

## TECHNICAL PROGRAM OVERVIEW BY TOPIC

### ATOMIC SPECTROSCOPY, *Crystal 2*

#### **Monday (9:15 am session)**

17ATOM01: Glow Discharge Spectroscopy

#### **Monday (1:30 pm session)**

17ATOM02: Glow Discharge Spectroscopy II

#### **Monday (3:50 pm session)**

17ATOM03: Recent Advances in Liquid Electrode Glow Discharge Plasmas

#### **Tuesday (9:15 am session)**

17ATOM04: Laser Ablation-ICP-MS I

#### **Tuesday (1:30 pm session)**

17ATOM05: Excitation and Ionization Techniques for Atomic and Molecular Spectroscopy

#### **Tuesday (3:50 pm session)**

17ATOM06: Laser Ablation-ICP-MS II

#### **Wednesday (9:15 am session)**

17ATOM08: ICP-MS for Biomedical Applications

#### **Wednesday (1:30 pm session)**

17ATOM09: ICP-MS for the Analysis of Nanomaterials

#### **Wednesday (3:50 pm session)**

17ATOM10: Atmospheric-Pressure Plasmas for Optical Mass Spectrometries

### AWARD SYMPOSIA, *Crystal 1 (unless otherwise noted)*

#### **Monday (10:50 am session)**

17AWD07: *Spectroscopy's* Emerging Leader in Molecular Spectroscopy Award Honoring Russ Algar

#### **Monday (1:30 pm session)**

17AWD11: Coblenz Lippincott Award Honoring Roberto Merlin

#### **Tuesday (9:15 am session)**

17AWD04: Charles Mann Award Honoring Duncan Graham

#### **Tuesday (1:30 pm session)**

17AWD05: Coblenz Craver Award Honoring Martin Zanni

#### **Wednesday (9:15 am session)**

17AWD01: William F. Meggers Award Honoring Naoto Nagai

#### **Wednesday (1:30 pm session)**

17AWD02: Lester Strock Award Honoring Frank Vanhaecke

#### **Wednesday (3:50 pm session)**

17AWD10: Bruce R. Kowalski Award in Chemometrics Honoring Joseph Smith

#### **Thursday (9:15 am session)**

17AWD03: ANACHEM Award Honoring Jennifer Brodbelt

#### **Thursday (1:30 pm session)**

17AWD06: AES Electrophoresis Award Honoring Scott Martin

#### **Thursday (3:50 pm session)**

17AWD08: FACSS Innovation Award, *Tahoe Ballroom*

### BIOLOGICAL/BIOMEDICAL, *Nevada 7*

#### **Monday (10:50 am session)**

17BIM01: Spectral Analysis of Biofluids

#### **Monday (1:30 pm session)**

17BIM02: Nanomaterial-Assisted Imaging

#### **Monday (3:50 pm session)**

17BIM03: Analytical Sciences in Molecular Biology

#### **Wednesday (9:15 am session)**

17BIM04: Endoscopy

#### **Wednesday (1:30 pm session)**

17BIM05: Big Data in Biomedical Analyses

#### **Wednesday (3:50 pm session)**

17BIM06: Spectral Analysis of Collagenous Tissues

### CHEMOMETRICS, *Crystal 5*

#### **Monday (10:50 am session)**

17CHEM01: New Frontiers in Chemometrics

#### **Monday (1:30 pm session)**

17CHEM02: Spectral Fingerprinting for Characterization of Complex Materials

#### **Monday (3:50 pm session)**

17CHEM03: Chemometric Opportunities in the Forensic Sciences

#### **Thursday (9:15 am session)**

17CHEM04: Multiblock Methods: The Key to Measurement Fusion

#### **Thursday (1:30 pm session)**

17CHEM05: New Developments in Calibration Methods

### CONTEMPORARY ISSUES IN ANALYTICAL SCIENCE, *Crystal 5*

#### **Tuesday (9:15 am session)**

17CTP01: Analytical Chemists Easing World Poverty

#### **Tuesday (1:30 pm session)**

17CTP02: Diversity, Equity, and Inclusion in Analytical Chemistry

#### **Tuesday (3:50 pm session)**

17CTP03: Innovative Approaches to Teaching Analytical Chemistry

#### **Wednesday (9:15 am session)**

17CTP04: Making the Leap: Pathways from Graduate School to a Permanent Position (Panel Discussion)

#### **Wednesday (1:30 pm session)**

17CTP05: Food Safety and Analysis: Issues and Solutions in Implementation in the Developing World

### ELECTROPHORESIS AND MIROFLUIDICS, *Crystal 4*

#### **Monday (1:30 pm session)**

17AES03: Electrokinetics for Cellular Analysis and Separations

#### **Monday (3:50 pm session)**

17AES02: Novel Electrokinetic Phenomena: Fundamentals and Applications

#### **Tuesday (1:30 pm session)**

17AES01: Micro-Scale Electroporation and Electrokinetic Study of Cells and Biomolecules

#### **Tuesday (3:50 pm session)**

17AES04: Designer (nano)Structures and Molecules for Separations and Analysis

### FORENSICS AND SECURITY, *Nevada 6*

#### **Monday (3:50 pm session)**

17FORENS01: Nuclear Forensics

#### **Tuesday (3:50 pm session)**

17FORENS02: Food Forensics

#### **Wednesday (3:50 pm session)**

17FORENS03: Proteomics for Forensic Analysis

#### **Thursday (3:50 pm session)**

17FORENS04: Special Pittcon/FACSS Joint Session: Forensic Analysis in the Lab and at the Crime Scene



## TECHNICAL PROGRAM OVERVIEW BY TOPIC

### **LASER-INDUCED BREAKDOWN SPECTROSCOPY, Crystal 3**

#### **Monday (10:50 am session)**

17LIBS01: LIBS Industrial Applications

#### **Monday (1:30 pm session)**

17LIBS02: LIBS for Forensic and Homeland Security

#### **Monday (3:50 pm session)**

17LIBS03: NASLIBS: Molecular Signal in LIBS

#### **Tuesday (1:30 pm session)**

17LIBS05: Elemental Mapping by LIBS

#### **Wednesday (9:15 am session)**

17LIBS07: LIBS Data Analysis

#### **Wednesday (1:30 pm session)**

17LIBS08: Fundamentals of Laser-Induced Plasmas

#### **Wednesday (3:50 pm session)**

17LIBS09: New Methods and Advancements in LIBS

#### **Thursday (9:15 am session)**

17LIBS04: LIBS for Pharmaceutical and Biological Analysis

#### **Thursday (1:30 pm session)**

17LIBS11: Field Application of LIBS

### **MASS SPECTROMETRY, Nevada 7**

#### **Tuesday (9:15 am session)**

17MASS01: Integrated Micro-Extraction Platforms for Improved Ambient Spectrometry

#### **Tuesday (1:30 pm session)**

17MASS02: Recent Development in Single Cell Mass Spectrometry Analysis

#### **Tuesday (3:50 pm session)**

17MASS03: Novel Ambient Mass Spectrometry Techniques for Forensic Science Analysis

#### **Thursday (9:15 am session)**

17MASS04: 'Omics Frontiers: Ion Mobility and Mass Spectrometry

#### **Thursday (1:30 pm session)**

17MASS05: Recent Advances in Oligosaccharide Analysis by Mass Spectrometry

### **MOLECULAR (IR AND NEAR IR), Carson 1**

#### **Monday (10:50 am session)**

17IR02: Applications of Nanoscale IR Spectroscopy to Polymeric Materials

#### **Monday (1:30 pm session)**

17IR03: Nanoscale IR Applications in the Life Sciences

#### **Monday (3:50 pm session)**

17IR04: Practical Implementation of Diffuse Reflectance Spectroscopy

#### **Tuesday (9:15 am session)**

17IR05: Quantum Cascade Lasers – I

#### **Tuesday (1:30 pm session)**

17IR06: Quantum Cascade Lasers – II

#### **Tuesday (3:50 pm session)**

17IR01: NanoIR/Nano-Raman II

#### **Wednesday (9:15 am session)**

17IR09: Ultrafast Two-Dimensional Spectroscopy – I

#### **Wednesday (1:30 pm session)**

17IR10: Ultrafast Two-Dimensional Spectroscopy – II

#### **Wednesday (3:50 pm session)**

17IR11: Ultrafast Two-Dimensional Spectroscopy – III

#### **Thursday (9:15 am session)**

17IR07: Clinical Applications of Vibrational Spectroscopy

#### **Thursday (1:30 pm session)**

17IR08: Towards Point-of-Care Testing with Raman Spectroscopy

### **NANOTECHNOLOGY, Nevada 5**

#### **Monday (10:50 am session)**

17NANO01: Recent Progress in Carbon Nanotubes and Graphene Research

#### **Monday (1:30 pm session)**

17NANO02: Nanomaterials and Nanostructures for Energy-Related Applications

#### **Monday (3:50 pm session)**

17NANO03: Nanomaterials and Related Spectroscopy Methods for Energy Conversion

#### **Thursday (9:15 am session)**

17NANO04: Nano-Facilitated Sensing

#### **Thursday (1:30 pm session)**

17NANO05: Imaging and Sensing Applications of Atomic Precision NanoClusters

### **PHARMACEUTICAL ANALYSIS, Carson 2**

#### **Monday (10:50 am session)**

17PMA01: Pharmaceutical Applications of Low Frequency Raman Spectroscopy

#### **Monday (1:30 pm session)**

17PMA02: Counterfeit Pharmaceuticals

#### **Monday (3:50 pm session)**

17PMA03: Identification of Counterfeit Medicines

#### **Tuesday (9:15 am session)**

17PMA04: Raman Characterization of Proteins and Biologics

#### **Tuesday (1:30 pm session)**

17PMA05: Recent Advances in the Mode of Action of Biopharmaceuticals

#### **Tuesday (3:50 pm session)**

17PMA06: PAT in Biopharmaceutical Manufacturing

#### **Wednesday (9:15 am session)**

17PMA07: Spectroscopic Applications in the World of Biopharmaceuticals

#### **Wednesday (1:30 pm session)**

17PMA08: Biologics Characterization from Early to Late Stage Development

#### **Wednesday (3:50pm session)**

17PMA09: Advances in Micro-Analysis of Biologics

### **PROCESS ANALYTICAL TECHNOLOGY, Nevada 6**

#### **Monday (10:30 am)**

SAS PAT Technical Section Business Meeting

#### **Monday (10:50 am session)**

17PAT01: SAS PAT Technical section: PAT in the Pharmaceutical Industries - Session I

#### **Monday (1:30 pm session)**

17PAT07: Hand-Held and Portable Spectrometers: Applications and Instrumental Methods

#### **Tuesday (9:15 am session)**

17PAT03: Industrial Applications of Vibrational Spectroscopy

#### **Tuesday (1:30 pm session)**

17PAT04: Online Analysis of Industrial Processes and Reactions - Improvements and Best Practices

#### **Wednesday (9:15 am session)**

17PAT05: Advances in On-line Process Analysis

#### **Wednesday (1:30 pm session)**

17PAT06: Process Monitoring Enabled Flow API and Continuous Product Manufacture

#### **Thursday (9:15 am session)**

17PAT02: SAS PAT Technical section: PAT in the Biopharmaceutical Industries - Session II

## TECHNICAL PROGRAM OVERVIEW BY TOPIC

### RAMAN, *Carson 3 & Carson 4*

#### **Monday (10:50 am session)**

- 17RAM04: Bioanalytical SERS I, *Carson 3*
- 17RAM07: IRDG Raman, *Carson 4*

#### **Monday (1:30 pm session)**

- 17RAM05: Bioanalytical SERS II, *Carson 3*
- 17RAM01: Emerging Raman I, *Carson 4*

#### **Monday (3:50 pm session)**

- 17RAM06: Bioanalytical SERS III, *Carson 3*
- 17RAM11: Spatially Offset Raman Spectroscopy (SORS), *Carson 4*

#### **Tuesday (9:15 am session)**

- 17RAM08: Biomedical Raman (Clirspec), *Carson 3*
- 17RAM15: Nano-Raman, *Carson 4*

#### **Tuesday (1:30 pm session)**

- 17RAM09: Transmission Raman Spectroscopy, *Carson 3*
- 17RAM18: Nano IR / Nano-Raman I, *Carson 4*

#### **Tuesday (3:50 pm session)**

- 17RAM19: General Raman, *Carson 3*

#### **Wednesday (1:30 pm session)**

- 17RAM14: Industrial Raman Spectroscopy, *Carson 3*
- 17RAM12: Portable Raman, *Carson 4*

#### **Wednesday (3:50 pm session)**

- 17RAM13: Pharmaceutical and Biotechnology Industrial Applications of Raman Spectroscopy, *Carson 3*
- 17RAM20: Raman Optical Activity (ROA), *Carson 4*

#### **Thursday (9:15 am session)**

- 17RAM10: Raman Microscopy, *Carson 3*
- 17RAM17: Raman Spectroscopy for Security and Forensics Purposes, *Carson 4*

#### **Thursday (1:30 pm session)**

- 17RAM03: Raman Imaging & Microscopy II, *Carson 3*
- 17RAM16: Pharmaceutical Raman, *Carson 4*

### SPECIAL TOPICS, *Crystal 4 (unless otherwise noted)*

#### **Monday (10:50 am session)**

- 17SPECIAL03: Stand-off Sensing

#### **Tuesday (9:15 am session)**

- 17SPECIAL01: Chemistry in Art and Archeology

#### **Thursday (9:15 am session)**

- 17SPECIAL02: Modern Techniques in Microscopy

#### **Thursday (1:30 pm session)**

- 17SPECIAL04: Celebrating the FACSS membership of the Austrian Society of Analytical Chemistry (ASAC)

#### **Friday (8:00 am session)**

- 17SPECIAL05: Closing Session: The New Vision of Analytical Science by the World, *Tahoe Ballroom*

### SURFACE PLASMON RESONANCE, *Nevada 5*

#### **Tuesday (9:15 am session)**

- 17SPR01: Multimetallic Plasmonic Nanoparticles

#### **Tuesday (1:30 pm session)**

- 17SPR03: Next Generation Plasmonics

#### **Tuesday (3:50 pm session)**

- 17SPR02: Plasmonic Nanoparticles - Beyond Sphere

#### **Wednesday (9:15 am session)**

- 17SPR06: Plasmonic-Powered Processes: Sensing, Imaging, Catalysis, and Beyond

#### **Wednesday (1:30 pm session)**

- 17SPR05: Plasmon-Enhanced Techniques

#### **Wednesday (3:50 pm session)**

- 17SPR04: Point-of-Care Plasmonics

### SURFACE SCIENCE, *Crystal 4*

#### **Wednesday (9:15 am session)**

- 17SURFACE01: Application of Surface Spectroscopic Techniques to Analysis of Nanomaterials and Devices

#### **Wednesday (1:30 pm session)**

- 17SURFACE02: Microscopic Methods for Surface Science Problems

#### **Wednesday (3:50 pm session)**

- 17SURFACE03: Surface Analysis of Environmental Interfaces and Systems

## SCIX 2017 AND FACSS THANKS ITS MEMBER ORGANIZATIONS FOR THEIR SUPPORT TO THE SciX PROGRAM

ACS Division of Analytical Chemistry

AES Electrophoresis Society

American Society for Mass Spectrometry

ANACHEM

Austrian Society of Analytical Chemistry

The Coblenz Society

Council for Near Infrared Spectroscopy

The Infrared and Raman Discussion Group

International Society of Automation – Analysis Division

North American Society for Laser-Induced Breakdown Spectroscopy

Royal Society of Chemistry Analytical Division

Society for Applied Spectroscopy

The Spectroscopical Society of Japan

## PROGRAM HIGHLIGHTS

### SUNDAY

- 8:00 am SciX Bike Ride  
 9 am – 4 pm Workshops  
*Tahoe Ballroom*
- 4:20 pm What's Hot Vendor Presentations  
 6:15 pm **SciX 2017 Welcome.** Becky Dittmar  
**Keynote Lecture: Janie Dubois**, University of Maryland, JIFSAN
- 7:15 pm *Reno Ballroom*  
**Welcome Mixer and SAS Sponsored Student Poster Session.** SAS, Coblenz, and FACSS Student Award Presentations, *Reno Ballroom*

### MONDAY

- 7:30 am Wake up coffee, *Grand Salon*  
*Tahoe Ballroom*
- 7:45 am Opening Address, Matthieu Baudelet  
 8:00 am **Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award Plenary**, Russ Algar, *University of British Columbia*
- 8:30 am **Ellis R. Lippincott Award Plenary**, Roberto Merlin, *University of Michigan*
- 9:00 am **Sir George Stokes Award Plenary**, Tony Cass, *Imperial College London*
- 9:00 am – 4:00 pm Workshops  
 9:45 – 10:45 am Poster Session & Break, *Reno Ballroom*  
 10:50 am – 12:30 pm Oral Symposia  
 12:30 pm Lunch on own  
 1:30 am Coblenz Speed Mentoring, *Nevada 8*  
 1:30 – 3:10 pm Oral Symposia  
 3:10 – 3:50 pm Poster Session & Break, *Reno Ballroom*  
 3:50 – 5:30 pm Oral Symposia  
 5:30 pm Reception for Exhibit Opening (wine, beer, light hors d'ouvres) *Exhibit Hall*

### TUESDAY

- 7:30 am Wake up coffee, *Grand Salon*  
*Tahoe Ballroom*
- 7:50 am Awards Presentation  
 8:00 am **FACSS Charles Mann Award for Applied Raman Spectroscopy Plenary**, Duncan Graham, *University of Strathclyde*
- 8:30 am **Coblenz Society Craver Award**, Martin Zanni, *University of Wisconsin – Madison*
- 9:00 am – 4:00 pm Workshops  
 9:15 – 10:55 am Oral Symposia  
*Exhibit Hall*
- 10:00 am – 4:30 pm Exhibits Open  
 11:00 am – 12:00 pm Poster Session & Break  
 11:40 am – 1:10 pm What's Hot Vendor Presentations  
 12:00 pm Complimentary lunch in the Exhibit Hall. Attendee must be present. Ticket required.
- 1:30 – 3:10 pm Oral Symposia  
 2:30 pm Raffle Drawing, *Exhibit Hall*  
 3:10 – 3:50 pm Poster Session & Break, *Exhibit Hall*  
 3:50 – 5:30 pm Oral Symposia  
 6:00 pm Raman Reception Invitation Only. *Reno Ballroom*  
 7:30 pm Society for Applied Spectroscopy Wine and Cheese Awards Reception. *Tahoe Ballroom*

### WEDNESDAY

- 7:30 am Wake up coffee, *Grand Salon*  
*Tahoe Ballroom*
- 7:50 am Awards Presentation  
 8:00 am **Applied Spectroscopy William F. Meggers Award Plenary**, Naoto Nagai, *Industrial Research Institute of Niigata Prefecture*
- 8:30 am **Lester W. Strock Award Plenary**, Frank Vanhaecke, *Ghent University*
- 9:15 – 10:55 am Oral Symposia  
*Exhibit Hall*
- 10 am – 4:00 pm Exhibits Open  
 11:00 am – 12:00 pm Poster Session & Break  
 11:40 am – 1:10 pm What's Hot Vendor Presentations  
 12:00 pm Complimentary lunch in Exhibit Hall  
 Ticket required.
- 1:30 – 3:10 pm Oral Symposia  
 2:30 pm Raffle Drawing, *Exhibit Hall*  
 3:10 – 3:50 pm Poster Session & Break, *Exhibit Hall*  
 3:50 – 5:30 pm Oral Symposia  
 6:00 pm Wednesday Evening Event, Conference badge required. *Reno Ballroom*

### THURSDAY

- 7:30 am Wake up coffee, *Grand Salon*  
*Tahoe Ballroom*
- 7:50 am Awards Presentation  
 8:00 am **ANACHEM Award Plenary**, Jennifer Brodbelt, *University of Texas at Austin*
- 8:30 am **AES Mid-Career Award Plenary**, R. Scott Martin, *Saint Louis University*
- 9:15 – 10:55 am Oral Symposia  
 11:00 am – 12:00 pm Poster Session & Break, *Grand Salon*  
 12:00 pm Lunch on own  
 1:30 – 3:10 pm Oral Symposia  
 3:10 – 3:50 pm Poster Session & Break, *Grand Salon*
- 3:50 pm **Plenary Session**, *Tahoe Ballroom*  
 FACSS Distinguished Service Award  
 FACSS Innovation Award Session

### FRIDAY

- Tahoe Ballroom*
- 7:30 am Wake up coffee and pastries  
 8:00 am Announcement of Innovation Award Winner  
 8:30 am Closing Session: The New Vision of Analytical Science by the World  
 10:00 am Preview of 2018 Conference in Atlanta

## TECHNICAL PROGRAM AND EVENTS – SUNDAY

### **What's Hot Vendor Presentations.** Presider: Brian Dable, *Arete Associates, Tahoe Ballroom*

- 4:10 pm **Applied Spectra** Novel applications with Tandem LA-ICP-MS and LIBS
- 4:20 pm **HORIBA Scientific** GD-OES Advanced Features to Answer to New Needs
- 4:30 pm **Flash Analysis** Flash Photonics sensing Solutions from the MIR to the UV
- 4:40 pm **Andor**
- 4:50 pm **LLA Instruments** New Echelle Spectrographs and Hyperspectral Imaging Cameras Developed by LLA Instruments
- 5:00 pm **Czitek** The Power of Vision - Enhancing Material Identification by Combining IR Spectroscopy with Visible Imaging
- 5:10 pm **Molecular Vista**
- 5:20 pm **SciAps** Only Handheld on the Market measuring Low Grade Carbon
- 5:30 pm **Analytik Jena** PlasmaQuant® MS Elite – The New Perspective in ICP-MS
- 5:40 pm **Photometrics** Cameras with Horsepower: Designing a Breakthrough Product with an Imaging Engine
- 5:50 pm **Anasys Instruments**

- 6:15 pm **Keynote Lecture; Tahoe Ballroom**  
**(1) The Analytical and Economic Challenges of Maintaining Food Safety in a Global Supply Chain;** Janie Dubois; University of Maryland, JIFSAN

Janie Dubois is Chair of the Laboratory Capacity Working Group at the World Bank's Global Food Safety Partnership



- 7:15 pm **Welcome Mixer**  
**SAS Sponsored Student Poster Session • Coblenz Student Awards • FACSS Student and Tomas Hirschfeld Scholar Awards – Reno Ballroom**

## TECHNICAL PROGRAM – MONDAY

Welcome – 7:50 am; Plenary Lectures – 8:00 am; *Tahoe Ballroom*

Presider: Karen Esmonde-White



**8:00 am – Spectroscopy Magazine's Emerging Leader in Molecular Spectroscopy Award**  
**(2) The Small Matter of Bioanalysis: Adventures at Less Than 10 nm with Quantum Dots and/or FRET;** Russ Algar; <sup>1</sup>University of British Columbia



**8:30 am – Ellis R. Lippincott Award**  
**(3) Vibrational Engineering: From Superlattices to Coherent and Squeezed Phonons;** Roberto Merlin<sup>1</sup>;  
<sup>1</sup>University of Michigan



**9:00 am – Royal Society of Chemistry Sir George Stokes Award**  
**(4) Tackling Global Health Challenges with Biosensor Technologies;** Tony Cass; <sup>1</sup>Imperial College London

## Poster Sessions and Coffee Breaks

**9:45 – 10:45 am & 3:10 – 3:50 pm, Reno Ballroom**

All Monday posters should be put up between 7:30 – 9:30 am and removed by 5:00 pm

### 17MPCHEM: Monday Posters - Chemometrics

#### Poster Board #1

**(5) Fine Tuning Model Updating for Multivariate Calibration Maintenance;** Anit Gurung<sup>1</sup>, John H. Kalivas<sup>1</sup>, Erik Andries<sup>2,3</sup>; <sup>1</sup>Idaho State University; <sup>2</sup>Central New Mexico Community College; <sup>3</sup>University of New Mexico

#### Poster Board #2

**(6) Leveraging Multiple Linear Regression for Wavelength Selection;** Tony Lemos<sup>1</sup>, John Kalivas<sup>1</sup>; <sup>1</sup>Idaho State University

#### Poster Board #3

**(7) Robustness Across Instruments: A Case Study on Calibration Transfer of NIR-based Multivariate Calibration Models;** Hua Yu<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals

#### Poster Board #4

**(8) Comparing NIR, MIR and Raman Spectroscopy for Classification of Edible Oils and Prediction of Edible Oil Peroxide Values;** Joshua Ottaway<sup>1</sup>, J. Chance Carter<sup>1</sup>, Kristl Adams<sup>1</sup>, Karl Booksh<sup>2</sup>; <sup>1</sup>Lawrence Livermore National Lab; <sup>2</sup>University of Delaware

#### Poster Board #5

**(9) Robust Calibration Model Transfer Between Portable Near-Infrared Spectrometers to Predict API of Pharmaceutical Oral Dosage Form;** Suyang Wu<sup>1</sup>, Md Nayeem Hossain<sup>1</sup>, Shikhar Mohan<sup>1</sup>, Md Anik Alam<sup>1</sup>, Dr. James Drennen<sup>1</sup>, Dr. Carl Anderson<sup>1</sup>; <sup>1</sup>Duquesne University

### 17MPFORENS: Monday Posters – Forensics

#### Poster Board #6

**(10) Forensic IR Spectroscopy: A Look Back, at the Present and Ahead;** Edward Bartick<sup>1</sup>, Rohit Bhargava<sup>2</sup>; <sup>1</sup>The George Washington University; <sup>2</sup>University of Illinois, Champaign

#### Poster Board #7

**(11) Infrared Absorption Spectra of Gas Phase Uranium Oxides;** Batikan Koroglu<sup>1</sup>, Marco Mehl<sup>1</sup>, Michael Armstrong<sup>1</sup>, Jonathan Crowhurst<sup>1</sup>, David Weisz<sup>1</sup>, Joseph Zaug<sup>1</sup>, Harry Radousky<sup>1</sup>, Mark Cappelli<sup>2</sup>, Timothy Rose<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>Stanford University

#### Poster Board #8

**(12) Determination of Residual Organic Compounds in Uranium Ore Concentrates by GC/Q-TOF After Monolithic Material Sorptive Extraction: Application to Nuclear Forensic Investigations.;** Maxime Bridoux, Françoise Leprince<sup>1</sup>; <sup>1</sup>CEA, DAM, DIF, Arpajon, France

#### Poster Board #9

**(13) TNT Reduction in Clostridium acetobutylicum Affected by Oxidation State of Substrates;** Sanchao Liu<sup>1</sup>, Christian Sund<sup>1</sup>, Elliot Gerlach<sup>1</sup>, Matthew Servinsky<sup>1</sup>; <sup>1</sup>U. S. Army Research Laboratory

#### Poster Board #10

**(14) Optimization of Single Hair Proteomics for Human Identification;** Fanny Chu<sup>1,2</sup>, Katelyn Mason<sup>1</sup>, Deon Anex<sup>1</sup>, A. Daniel Jones<sup>2</sup>, Bradley Hart<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>Michigan State University

#### Poster Board #11

**(15) One-Class Classification Method for Pharmaceutical Product Authentication System using Spectroscopy;** Md Nayeem Hossain<sup>1</sup>, Carl Anderson<sup>1</sup>, James Drennen<sup>1</sup>; <sup>1</sup>Duquesne University

### 17MPLIBS: Monday Posters - NASLIBS

#### Poster Board #12

**(16) Using LIBS in Hardness Measurements for Samples of Different Matrices;** Ahmed Galmed<sup>1,2,3</sup>, Mohamed Abdel Harith<sup>2</sup>, Malik Maaza<sup>1,3</sup>; <sup>1</sup>iThemba LABS, South Africa; <sup>2</sup>NILES, Cairo University; <sup>3</sup>UNESCO-UNISA Africa Chair in Nanosciences/Nanotechnology

#### Poster Board #13

**(17) Time-Resolved Absorption Measurements in Transient Plasmas: Towards Single-Shot Optical Measurements of Uranium Isotope Ratios;** Jonathan Merten<sup>1</sup>, Bruce Johnson<sup>1</sup>; <sup>1</sup>Arkansas State University

#### Poster Board #14

**(18) Multivariate Analysis of Complex Samples Using Atomic and Molecular Emission Spectra from LIBS/SIBS;** Sofia Pozsonyiova<sup>1,2</sup>, Prasoon Diwakar<sup>1,3</sup>, Nathalie Manzano<sup>4</sup>, Theodore Caplow<sup>4</sup>; <sup>1</sup>Frost Science Museum, Miami, FL; <sup>2</sup>Macalester College, St. Paul, MN; <sup>3</sup>Purdue University, West Lafayette, IN; <sup>4</sup>Grayscale Partners, Miami, FL



**TECHNICAL PROGRAM – MONDAY**  
**Poster Sessions 9:45 – 10:45 am & 3:10 – 3:50 pm, Reno Ballroom**

**Poster Board #15**

(19) **Classification of Milk Vetch Root by its Geographical Origins Using Laser-Induced Breakdown Spectroscopy;** ChangHwan Eum<sup>1</sup> Hoecil Chung<sup>1</sup>; <sup>1</sup>Hanyang University

**Poster Board #16**

(20) **Laser-Induced Breakdown Spectroscopy for Analysis of Gold and Silver in Mineral Synthetic Samples;** Daniel Diaz<sup>1,2</sup>, David Hahn<sup>2</sup>, Alejandro Molina<sup>1</sup>; <sup>1</sup>Universidad Nacional de Colombia - Sede Medellin; <sup>2</sup>MAE, University of Florida

**Poster Board #17**

(21) **Detection of Impurities Leached from Sugarcane by LIBS After Liquid-to-Solid Matrix Conversion;** Fabiola Pereira<sup>1,2</sup>, Wesley Guedes<sup>1</sup>, Daniel Andrade<sup>2</sup>; <sup>1</sup>São Paulo State University (UNESP); <sup>2</sup>Federal University of São Carlos (UFSCar)

**Poster Board #18**

(22) **Uncertainty Assessments and Plasma Modeling for Quantitative LIBS Applications;** David Surmick<sup>1,2</sup>, Noureddine Melikechi<sup>2</sup>, Hacene Boukari, Jonathan Woodward<sup>1,3</sup>, Ashley Stowe<sup>3</sup>; <sup>1</sup>Delaware State University; <sup>2</sup>Univeristy of Massachusetts Lowell; <sup>3</sup>Y-12 National Security Complex

**Poster Board #19**

(23) **Challenges and Strategies for the Simultaneous Determination of Cd, Cr, Ni and Pb in Micronutrient Fertilizers by Laser-Induced Breakdown Spectroscopy;** Lidiane Cristina Nunes<sup>1</sup>, Francisco José Krug<sup>1</sup>; <sup>1</sup>Center for Nuclear Energy in Agriculture -CENA/USP

**Poster Board #20**

(24) **Spatio-Temporal Evolution of Metal Oxide Diatomic Molecules in Tailored Ultrafast Laser-Induced Plasmas;** Yonghoon Lee<sup>1,2</sup>, Xianglei Mao<sup>1</sup>, George Chan<sup>1</sup>, Jhanis Gonzalez<sup>1,3</sup>, Rick Russo<sup>1,3</sup>, Vassilia Zorba<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory; <sup>2</sup>Mokpo National University; <sup>3</sup>Applied Spectra, Inc.

**17MPAT: Monday Posters - Process Analytical Technology**

**Poster Board #21**

(25) **Water Content Determination for Bilayer Tablets Using Near Infrared Spectroscopy and Multivariate Statistical Analysis;** Zhenyu Lu<sup>1</sup>, Yanqiao Shawn Xiang<sup>1</sup>, Daniel Pohlman<sup>1</sup>, David Webster<sup>1</sup>, Pete Mustonen<sup>1</sup>, Mark D. Trone<sup>1</sup>, Michael Palmieri, Jr.<sup>1</sup>; <sup>1</sup>Alkermes

**Poster Board #22**

(26) **Considerations of Model Validation of NIR Based Quantitative Methods;** Dongsheng Bu<sup>1</sup>, Jim Pratt<sup>1</sup>, Gary McGeorge<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

**Poster Board #23**

(27) **Triboluminescence Analysis of Pharmaceutical Formulations;** Garth J. Simpson<sup>1</sup>, Casey J. Smith<sup>1</sup>, Scott R. Griffin<sup>1</sup>, Gregory Eakins<sup>1</sup>, Fengyuan Deng<sup>1</sup>, Atanu Sangupta<sup>2</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Dr. Reddy Lab

**Poster Board #24**

(28) **Real-Time Fundamental Calibrations of Process Instruments - Properties and Advantages;** Robert Lascola<sup>1</sup>, Patrick O'Rourke<sup>1</sup>; <sup>1</sup>Savannah River National Laboratory

**Poster Board #25**

(29) **Portable, Rapid Analysis of MEA-Triazine and Dithiazine via Raman Spectroscopy;** Samuel Kleinman<sup>1</sup>, Merwan Benhabib<sup>1</sup>, Natalya Zhrebneenko, Mark Peterman<sup>1</sup>; <sup>1</sup>OndaVia

**Poster Board #26**

(30) **In-Situ FT-IR Reaction Monitoring using Standard Detector;** Michael Kleimann<sup>1</sup>; <sup>1</sup>ABB Automation GmbH, Frankfurt Germany

**Poster Board #27**

(31) **Principal Component Correlation Based Variable Selection to Improve Glucose Concentration Prediction in Mammalian Cell Cultivations by Raman Spectroscopy;** Bence Kozma<sup>1,2</sup>, Szilveszter Gergely<sup>1</sup>, László Párta<sup>2</sup>, András Salgó<sup>1</sup>; <sup>1</sup>Budapest University of Technology and Economics; <sup>2</sup>Gedeon Richter Plc.

**Poster Board #28**

(32) **Graphene Analyzer for Rapid On-line or At-line Graphene Quality Monitoring;** Dawn Yang<sup>1</sup>, Kristen Frano<sup>1</sup>; <sup>1</sup>BWTEK

**Poster Board #29**

(33) **Feed-Forward Process Control in Enzymatic Protein Hydrolysis of Byproducts: A Spectroscopic Approach;** Sileshi Wubshet<sup>1</sup>, Jens Petter Wold<sup>1</sup>, Nils Kristian Afseth<sup>1</sup>, Ulrike Böcker<sup>1</sup>, Ingrid Måge<sup>1</sup>; <sup>1</sup>Nofima AS

**Poster Board #31**

(35) **Raman Spectroscopy in Polymer Applications from Laboratory Discoveries to Large-Scale Production;** Karen Esmonde-White<sup>1</sup>, Patrick Wiegand<sup>1</sup>, Ian Lewis<sup>1</sup>; <sup>1</sup>Kaiser Optical Systems, Inc.

**Poster Board #32**

(36) **Raman Spectroscopy Technologies Enabling in situ Real-Time Bioprocess Monitoring;** Karen Esmonde-White<sup>1</sup>, Maryann Cuellar<sup>1</sup>, Alexander Pitters<sup>2</sup>, Sean Gilliam<sup>1</sup>, David Strachan<sup>1</sup>, Herve Lucas<sup>2</sup>, Bruno Lenain<sup>2</sup>, Ian Lewis<sup>1</sup>; <sup>1</sup>Kaiser Optical Systems Inc.; <sup>2</sup>Kaiser Optical Systems, SARL

**17MPRAM: Monday Posters – Raman**

**Poster Board #33**

(37) **Photo Oxidative Stability Study of Active Layers in Bulk Heterojunction Organic Photovoltaics by micro-RAMAN Spectroscopy.;** Vasilis Gregoriou, Christos Chochos<sup>1</sup>, Michalis Spanos<sup>1</sup>; <sup>1</sup>National Hellenic Research Foundation (NHRF)

**Poster Board #34**

(38) **Maximizing Performance and Reducing Variability for a SERS Substrate Self-Assembled Hot Spot Array Developed by HP Based on Nanofingers;** Milo Overbay<sup>1</sup>, Michael Delos-Reyes<sup>1</sup>, Steven Barcelo<sup>1</sup>, Christopher N. Young<sup>1</sup>, Anita Rogacs<sup>1</sup>; <sup>1</sup>HP

**TECHNICAL PROGRAM – MONDAY**  
**Poster Sessions 9:45 – 10:45 am & 3:10 – 3:50 pm, Reno Ballroom**  
**Orals 10:50 am – 12:30 pm**

**Poster Board #35**

(39) **Time Domain Diffuse Raman Instrumentation based on a TCSPC Camera for Depth Analysis of Diffusive Media;** Sanathana Konugolu Venkata Sekar<sup>1</sup>, Sara Mosca<sup>1</sup>, Gianluca Valentini<sup>1,2</sup>, Werner Zuschratter<sup>3</sup>, Rainer Erdmann<sup>4</sup>, Antonio Pifferi<sup>1,2</sup>; <sup>1</sup>Dept. physics, Politecnico di milano, Milan, Italy; <sup>2</sup>Consiglio Nazionale delle Ricerche, Milan, Italy; <sup>3</sup>Leibniz Inst. for Neurobiology, Magdeburg, Germany; <sup>4</sup>PicoQuant GmbH, Berlin, Germany

**Poster Board #36**

(40) **Spectrochemical Detection of Chemical Analytes in Microfluidic Systems;** Nalin Andersen<sup>1</sup>, Kateryna Artyushkova<sup>1</sup>, Ivana Matanovic<sup>1</sup>, Plamen Atanasov<sup>1</sup>; <sup>1</sup>University of New Mexico

**Poster Board #37**

(41) **Through-Skin Analysis of Quality Parameters in Intact Fish Using Spatially Offset Raman Spectroscopy;** Ulrike Böcker<sup>1</sup>, Nils Kristian Afseth<sup>1</sup>, Jens Petter Wold<sup>1</sup>, Chris Welsby<sup>2</sup>, Pavel Matousek<sup>2,3</sup>; <sup>1</sup>Nofima; <sup>2</sup>Cobalt Light Systems; <sup>3</sup>Central Laser Facility, STFC Rutherford Appleton

**Poster Board #38**

(42) **Fabrication and Evaluation of Surface Enhanced Raman Scattering Substrates of Gold Nanoparticles Embedded in a Polymer Matrix;** Md Shah Alam, Mary Tecklenburg; <sup>1</sup>Central Michigan University

**Poster Board #39**

(43) **Raman Spectroscopy for Undergraduate Laboratories;** Alexander Osterbaan<sup>1</sup>, Justin Shorb<sup>2</sup>, Stacey Carrier<sup>2</sup>, Giora Proskurowski<sup>3</sup>; <sup>1</sup>Hope College; <sup>2</sup>Hellma USA; <sup>3</sup>MarqMetrix

**Poster Board #40**

(44) **Experimental Artifacts Influencing Polarization Sensitive Magneto-Raman Spectroscopy;** Komalavalli Thirunavukkuarasu<sup>1</sup>, Zhenguang Lu<sup>2</sup>, Liqin Su<sup>3</sup>, Yifei Yu<sup>4</sup>, Linyou Cao<sup>4</sup>, Mariana Ballotin<sup>2</sup>, Peter Christianen<sup>2</sup>, Yong Zhang<sup>3</sup>, Dmitry Smirnov<sup>2</sup>; <sup>1</sup>Florida A&M University; <sup>2</sup>National High Magnetic Field Laboratory; <sup>3</sup>University of North Carolina Charlotte; <sup>4</sup>North Carolina State University

**Poster Board #41**

(45) **SEHRS of Rhodamine Derivatives as a Probe of Two-Photon Properties;** Jake Olson<sup>1</sup>, Jon Camden<sup>1</sup>; <sup>1</sup>University of Notre Dame

**17MPSPSJ: Monday Posters – SPSJ**

**Poster Board #42**

(46) **Hydration Effect on Lysozyme in Gas Phase Studied by UV-Photodissociation Spectroscopy in Combination with Droplet-Beam IR Laser Ablation;** Norishi Kawauchi<sup>1</sup>, Hiroya Asami<sup>1</sup>, Jun-ya Kohno<sup>1</sup>; <sup>1</sup>Graduate School of Science, Gakushuin University

**Poster Board #43**

(47) **Study for Structure Analysis of Ions Deep Eutectic Solvent by ATR-Far UV;** Kazutaka Nishikido<sup>1</sup>, Yusuke Morisawa<sup>1</sup>; <sup>1</sup>Kindai University

**Poster Board #44**

(48) **Accessing the Secondary Structure of Monoclonal Antibody (mAb) Pharmaceuticals under Stresses by Deep-UV Resonance Raman (DUVRR) Spectroscopy;** Chen Qiu<sup>1</sup>, Sergey Arzhantsev<sup>1</sup>; <sup>1</sup>US Food and Drug Administration

**Monday Morning, Crystal 2**

**17ATOM01: GLOW DISCHARGE SPECTROSCOPY I**

Organizer: Chair: Jorge Pisonero; Presider: Nerea Bordel

10:50 AM (49) **The History of Glow Discharge Mass**

**Spectrometers – A Manufacturer's Viewpoint;** Peter Robinson<sup>1</sup>; <sup>1</sup>MassCare Ltd

11:10 AM (50) **Glow Discharge Mass Spectrometry: A**

**Superstar for Fast Depth Profiling;** Jorge Pisonero Castro<sup>1</sup>, Jonatan Fandino<sup>1</sup>, Nerea Bordel<sup>1</sup>; <sup>1</sup>Department of Physics, University of Oviedo

11:30 AM (51) **Unique Features and Recent Developments for GD-OES Open the Way to New Applications;**

Matthieu Chausseau<sup>1</sup>, Philippe Hunault<sup>1</sup>, Patrick Chapon<sup>2</sup>, Sofia Gaiaschi<sup>2</sup>, Kayvon Savadkouei<sup>1</sup>; <sup>1</sup>HORIBA Instruments; <sup>2</sup>HORIBA France

11:50 AM (52) **Diffusion Study of Multilayer Film Stack by Pulsed RF Glow-Discharge Optical Emission**

**Spectrometry (GD-OES);** Helia Jalili<sup>1</sup>, Qi Zhang<sup>1</sup>, Kayvon Savadkouei<sup>2</sup>, Matthieu Chausseau<sup>2</sup>; <sup>1</sup>H.C. Starck; <sup>2</sup>Horiba Scientific

12:10 PM (53) **Comparison of "Half" and "Full" Dielectric Barrier Discharges – LTP vs. DBDI;** Pascal Vogel<sup>1</sup>,

Felix David Klute<sup>1</sup>, Sebastian Brandt<sup>1</sup>, Antje Michels<sup>1</sup>, Charlotte Reininger<sup>2</sup>, Daniel Thurston<sup>2</sup>, Beatrix Biskup<sup>3</sup>, Paul Farnsworth<sup>2</sup>, Joachim Franzke<sup>1</sup>; <sup>1</sup>ISAS; <sup>2</sup>Department of Chemistry and Biochemistry, BYU; <sup>3</sup>Ruhr-Universität Bochum

**Monday Morning, Crystal 1**

**17AWD07: SPECTROSCOPY'S EMERGING LEADER IN MOLECULAR SPECTROSCOPY AWARD SYMPOSIUM HONORING RUSS ALGAR**

Organizer and Presider: Russ Algar

10:50 AM (54) **Investigations of Plasmon-Enhanced**

**Fluorescence and Förster Resonant Energy Transfer in Composite Multilayer Nanoparticles;** Denis Boudreau<sup>1</sup>, Jérémie Asselin<sup>1</sup>, Samuel Ouellet<sup>1</sup>, Josée Richard-Daniel<sup>1</sup>, Nicolas Fontaine<sup>1</sup>; <sup>1</sup>Université Laval

11:10 AM (55) **Engineering and Imaging Excitons for Brain Imaging of Modulatory Neurotransmitters;** Markita Landry<sup>1</sup>, Abraham Beyene<sup>1</sup>, Jackson Travis Del Bonis O'Donnell<sup>1</sup>, Ralph Henry Page<sup>1</sup>; <sup>1</sup>UC Berkeley

11:30 AM (56) **A Single Tb-to-Quantum Dot FRET Pair for Temporally Multiplexed Detection of Nucleic Acids;**

Xue QIU<sup>1</sup>, Jiajia GUO<sup>1</sup>, Zongwen JIN<sup>2</sup>, Igor L. Medintz<sup>3</sup>, Niko Hildebrandt<sup>1</sup>; <sup>1</sup>Université Paris-Sud; <sup>2</sup>Shenzhen Institute of Advanced Integration Technol; <sup>3</sup>Naval Research Laboratory

11:50 AM (57) **Fabrication of Enzyme-Powered 3D DNA Nanomachine for Rapid Detection of Nucleic Acids and Single Nucleotide Variants;** Feng Li<sup>1</sup>, Xiaolong Yang<sup>1</sup>, Sean Mason<sup>1</sup>, Zechen Yu<sup>1</sup>, Yanan Tang<sup>1</sup>;

<sup>1</sup>Brock University

12:10 PM (58) **Focusing Light Energy with DNA**

**Nanostructures;** Igor Medintz<sup>1</sup>; <sup>1</sup>US Naval Research Laboratory

# TECHNICAL PROGRAM – MONDAY

Orals 10:50 am – 12:30 pm

## Monday Morning, Nevada 7

### 17BIM01: SPECTRAL ANALYSIS OF BIOFLUIDS

Organizer and Presider: Matthew Baker

- 10:50 AM (59) **A Spectroscopic Serum Based Blood Test for Brain Tumours: Optimisation for High-Throughput Sampling and the Health Economic Impacts;** Holly Butler<sup>1</sup>, Matthew Baker<sup>1</sup>, Mark Hegarty<sup>2</sup>, David Palmer<sup>1</sup>, Ewan Gray<sup>3</sup>, Duncan Finlayson<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>ClinSpec Dx; <sup>3</sup>Healthcare Improvement Scotland
- 11:10 AM (60) **Raman Spectroscopy to Aid Diagnosis of Colorectal Cancer;** Cerys Jenkins<sup>1</sup>, Peter Dunstan<sup>2</sup>, Catherine Thornton<sup>1</sup>, Dean Harris<sup>3</sup>; <sup>1</sup>Swansea University Medical School; <sup>2</sup>Swansea University Physics Department; <sup>3</sup>Singleton Hospital, Dept of Colorectal Surgery
- 11:30 AM (61) **Cardiovascular Disease Related Micro-RNA Detection Using Paper Based Devices and Surface Enhanced Raman Scattering;** Samuel Mabbott<sup>1</sup>, Syrena Fernandes<sup>2</sup>, Karen Faulds<sup>1</sup>, Charles Mace<sup>2</sup>, Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>Tufts University
- 11:50 AM (62) **Point-of-Care Field Trials in Laos and Papua New Guinea of ATR Spectroscopy for Malaria Diagnosis and Blood;** Bayden Wood<sup>1</sup>, Phipp Heraud<sup>1</sup>, David Perez-Guiata<sup>1</sup>, Anja Rüether<sup>1</sup>, Moritoshi Iwagami<sup>2</sup>, Paul Brey<sup>2</sup>, Christian Doerig<sup>1</sup>; <sup>1</sup>Monash University; <sup>2</sup>Intitute Pasteur-Laos
- 12:10 PM (63) **Diffuse Resonance Raman Spectroscopic Study of Red Blood Cells Inside Polymer-bag;** Rekha Gautam<sup>1</sup>, Joo-Yeun Oh<sup>2</sup>, Rakesh Patel<sup>2</sup>, Richard Dluhy<sup>2</sup>; <sup>1</sup>Chemistry, University of Alabama at Birmingham; <sup>2</sup>Pathology, University of Alabama at Birmingham

## Monday Morning, Crystal 5

### 17CHEM01: NEW FRONTIERS IN CHEMOMETRICS

Organizer and Presider: Peter Harrington

- 10:50 AM (64) **Multivariate Methods for Analyzing Designed Data;** Federico Marini<sup>1</sup>; <sup>1</sup>University of Rome La Sapienza
- 11:10 AM (65) **Enhancing Hyperspectral Image Exploration via Preprocessing and Targeted Anomaly Detection;** Neal Gallagher<sup>1</sup>; <sup>1</sup>Eigenvector Research, Inc.
- 11:30 AM (66) **Exploring Hyperspectral Images with Topological Data Analysis;** Ludovic Duponchel<sup>1</sup>; <sup>1</sup>Lille University
- 11:50 AM (67) **Mass Informatics of Stable Isotope Assisted Metabolomics;** Xiang Zhang<sup>1</sup>; <sup>1</sup>University of Louisville
- 12:10 PM (68) **Multiple Versus Single Set Validation to Avoid Erroneous Conclusions;** Peter Harrington<sup>1</sup>; <sup>1</sup>Ohio University

## Monday Morning, Carson 1

### 17IR02: APPLICATIONS OF NANOSCALE IR SPECTROSCOPY TO POLYMERIC MATERIALS

Organizer and Presider: Mark Rickard

- 10:50 AM (69) **Structure and Morphology of Biosynthesized and Biodegradable Polymer Ultrathin Films and Single Crystals Using AFM-IR, XRD and Selected Area Electron Diffraction (SAED);** John Rabolt<sup>1</sup>, Changhao Liu<sup>1</sup>, Bruce Chase<sup>1</sup>, Isao Noda<sup>1,2</sup>; <sup>1</sup>University of Delaware; <sup>2</sup>Danimer Scientific
- 11:10 AM (70) **Investigation of Nanodomain Composition in Impact Copolymer Polypropylene by AFM-IR;** Peite

Bao<sup>2</sup>, Fuguang Tang<sup>1</sup>, Zhaohui Su<sup>1</sup>; <sup>1</sup>Changchun Institute of Applied Chemistry; <sup>2</sup>ExxonMobil Asia Pacific R&D., Ltd.

- 11:30 AM (71) **Nanophotonic AFM Transducers Transform Chemical Composition and Thermal Conductivity Measurements at the Nanoscale;** Andrea Centrone<sup>1</sup>, Georg Ramer<sup>1</sup>, Jungseok Chae<sup>1</sup>, Vladimir Aksyuk<sup>1</sup>; <sup>1</sup>National Institute of Standard and Technology
- 11:50 AM (72) **AFM-IR for the Examination of Coating Nanostructure and Environmental Damage;** Suzanne Morsch<sup>1</sup>, Stuart Lyon<sup>1</sup>, Simon Gibbon<sup>2</sup>; <sup>1</sup>University of Manchester; <sup>2</sup>AkzoNobel RD&I
- 12:10 PM (73) **Orientation and Disentanglement in Electrospun Fibers;** Christian Pellerin<sup>1</sup>, Marie Richard-Lacroix<sup>1</sup>, Elise Siurdyban<sup>1</sup>; <sup>1</sup>Univ of Montreal

## Monday Morning, Crystal 3

### 17LIBS01: NALIBS: LIBS INDUSTRIAL APPLICATIONS

Organizer and Presider: Lütffü Özcan

- 10:50 AM (74) **Determination of Rare Earth Elements in Geological Minerals by Laser-Induced Breakdown Spectroscopy;** Jinesh Jain<sup>1,2</sup>, Chet Bhatt<sup>1</sup>, Christian Goueguel<sup>1</sup>, Christina Lopano<sup>1</sup>, Dustin McIntyre<sup>1</sup>; <sup>1</sup>National Energy Technology Laboratory; <sup>2</sup>AECOM
- 11:10 AM (75) **The Versatility of LIBS - Industrial Applications;** Dominik Schiller<sup>1</sup>, Tino Seger<sup>1</sup>, Lars Jacobsen<sup>1</sup>; <sup>1</sup>LTB Lasertechnik Berlin GmbH
- 11:30 AM (76) **Commercial LIBS Instrument that Combines Surface Preparation and Elemental Analysis for Metal Industries;** Lutfu Ozcan<sup>1</sup>, François Doucet<sup>1</sup>, Altan Muftuoglu<sup>1</sup>; <sup>1</sup>ELEMISSION INC.
- 11:50 AM (77) **Analysis of Gold in Rock Samples Using Laser-Induced Breakdown Spectroscopy: Matrix and Heterogeneity Effects;** Kheireddine Rifai<sup>1,2</sup>, Marcel Laflamme<sup>2</sup>, Marc Constantin<sup>2</sup>, Mohamad Sabsabi<sup>1</sup>, Alain Blouin<sup>1</sup>, François Vidal<sup>3</sup>, Paul Bouchard<sup>1</sup>, Konstantinos Fytas<sup>2</sup>; <sup>1</sup>NRC; <sup>2</sup>UlaVal; <sup>3</sup>INRS-EMT
- 12:10 PM (78) **Versatile Applications of Laser-Induced Breakdown Spectroscopy (LIBS): From Nanocatalysts and Semiconducting Materials Characterizations to Biomedical Applications.;** Ali Davari<sup>1</sup>, Dibendu Mukherjee<sup>1</sup>; <sup>1</sup>Univ of Tennessee

## Monday Morning, Nevada 5

### 17NANO01: RECENT PROGRESS IN CARBON NANOTUBES AND GRAPHENE RESEARCH

Organizer and Presider: Wei Zhao

- 10:50 AM (79) **Recent Advances in Analyzing Single-Walled Carbon Nanotube Samples by Optical Spectroscopy;** R. Bruce Weisman<sup>1</sup>; <sup>1</sup>Rice University
- 11:10 AM (80) **Differentiating Left- and Right-handed Carbon Nanotubes by DNA;** Ming Zheng<sup>1</sup>; <sup>1</sup>NIST
- 11:30 AM (81) **Quantum Defects of Carbon Nanotubes: Room Temperature, 1.5  $\mu$ m Single Photon Emitters for Quantum Information Technology;** Han Htoon<sup>1</sup>; <sup>1</sup>Center for Integrated Nanotechnologies, Materials
- 11:50 AM (82) **2D Nanomaterials for Membrane-Based Water Purification;** Baoxia Mi<sup>1</sup>, Sunxiang Zheng<sup>1</sup>, Casey Finnerty<sup>1</sup>, Zhongying Wang<sup>1</sup>; <sup>1</sup>UC Berkeley
- 12:10 PM (83) **Tunable Single-Photon Emission at Telecom Wavelengths from Carbon Nanotube Quantum Defects;** Xiaowei He<sup>1</sup>, Nicolai F. Hartmann<sup>1</sup>, Xuedan Ma<sup>1</sup>, Jeffrey L. Blackburn<sup>2</sup>, Weilu Gao<sup>3</sup>, Junichiro Kono<sup>3</sup>, Han Htoon<sup>1</sup>, Stephen K. Doorn<sup>1</sup>; <sup>1</sup>Los Alamos National Lab, MPA-CINT; <sup>2</sup>National Renewable Energy Lab; <sup>3</sup>Rice University



## TECHNICAL PROGRAM – MONDAY

Orals 10:50 am – 12:30 pm

### Monday Morning, Nevada 6

#### 17PAT01: SAS PAT TECHNICAL SECTION: PAT IN THE PHARMACEUTICAL INDUSTRIES - SESSION I

Organizer and Presider: Brandye Smith-Goettler

- 10:50 AM (84) **Development, Validation & Implementation of a Real Time Release Test for Dissolution**; Sarah Nielsen<sup>1</sup>, Yleana Colon<sup>1</sup>, Stan Altan<sup>1</sup>, Olav Lyngberg<sup>1</sup>; <sup>1</sup>Janssen Pharmaceuticals
- 11:10 AM (85) **Criticality of Attribute Measurement in the Feed-Frame for Low Dose Compounds – A Low Dose Formulation Example**; Benoit Igne<sup>1</sup>; <sup>1</sup>GlaxoSmithKline
- 11:30 AM (86) **Building Robustness into Chemometric Models for Supporting Continuous Manufacturing**; Caitlin Schram<sup>1</sup>, Justin Pritchard<sup>1</sup>, Kelly Swinney<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals
- 11:50 AM (87) **Improving On-line Monitoring of Tablet Coating Process with Terahertz Based Near-Infrared Coating Thickness Models**; Shikhar Mohan<sup>1</sup>, Noritaka Odani<sup>1</sup>, Hanzhou Feng<sup>1</sup>, James Drennen, III<sup>1</sup>, Carl Anderson<sup>1</sup>; <sup>1</sup>Duquesne University
- 12:10 PM (88) **1st Principles, Statistical, and Chemometric Modeling to Understand, Develop, Control, and Continuously Verify Drug Product Manufacturing**; Brandye Smith-Goettler<sup>1</sup>; <sup>1</sup>Merck & Co., Inc.

### Monday Morning, Carson 2

#### 17PMA01: PHARMACEUTICAL APPLICATIONS OF LOW FREQUENCY RAMAN SPECTROSCOPY

Organizer and Presider: Anjan Roy

- 10:50 AM (89) **Applying Low Frequency Raman to QbD in Pharmaceutical Development**; John Wasylyk<sup>1</sup>, Robert Wethman<sup>1</sup>, Ming Huang<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Co.
- 11:10 AM (90) **Two-Dimensional Low Frequency Raman Correlation Spectroscopy Study of Bioplastics**; Isao Noda<sup>1,2</sup>, Anjan Roy<sup>3</sup>, James Carriere<sup>3</sup>, Brian Sobieski<sup>1</sup>, <sup>4</sup>Bruce Chase<sup>1</sup>, John Rabolt<sup>1</sup>; <sup>1</sup>University of Delaware; <sup>2</sup>Danimer Scientific; <sup>3</sup>Ondax; <sup>4</sup>FXI
- 11:30 AM (91) **Using Low Frequency Raman and THz Absorption Spectroscopy to Understand Order in Metal-Organic Frameworks and Solar Cell Polymers**; Keith Gordon<sup>1</sup>; <sup>1</sup>University of Otago
- 11:50 AM (92) **Discriminative and Quantitative Analysis of Pharmaceutical Polytypes Using Low-Frequency Raman Spectroscopy**; Kentaro Iwata<sup>1</sup>, Masatoshi Karashima<sup>1</sup>, Yukihiro Ikeda<sup>1</sup>, Motoki Inoue<sup>2</sup>, Toshiro Fukami<sup>2</sup>; <sup>1</sup>Takeda Pharmaceutical Company Limited; <sup>2</sup>Meiji Pharmaceutical University
- 12:10 PM (93) **Solid-State Analysis of Amorphous and Crystalline Forms Using THz Raman Spectrometry**; Alison Nordon<sup>1</sup>, Joanna Lothian<sup>1</sup>, Pol Macfhionnghaile<sup>1</sup>, Paul Dallin<sup>2</sup>, John Andrews<sup>2</sup>, James Carriere<sup>3</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>Clairat Scientific; <sup>3</sup>Ondax Inc.

### Monday Morning, Carson 3

#### 17RAM04: BIOANALYTICAL SERS I

Organizers: Roy Goodacre, Duncan Graham, Colin Campbell  
Presider: Kirsten Gracie

- 10:50 AM (94) **Dynamic SERS Nanosensor for Neurotransmitters Sensing Near Neurons**; Jean-Francois Masson<sup>1</sup>, Felix Lussier<sup>1</sup>, Thibault Brulé<sup>1</sup>, Marie-Josée Bourque<sup>1</sup>, Louis-Éric Trudeau<sup>1</sup>; <sup>1</sup>Université de Montréal

- 11:10 AM (95) **Ultrasensitive Detection of Thyrotropin-Releasing Hormone Based on Azo Coupling and Surface-Enhanced Resonance Raman Spectroscopy**; Yukihiro Ozaki<sup>1,2</sup>; <sup>1</sup>Kwansei Gakuin University; <sup>2</sup>Jilin University

- 11:30 AM (96) **Combat Forensics: Identification of Bad Actors with the Aid of Microfluidic SERS**; Augustus Fountain<sup>1</sup>, Neal Kline<sup>1</sup>, Ashish Tripathi<sup>1</sup>, Rustin Mirsafavi<sup>2</sup>, Martin Moskovits<sup>2</sup>, Carl Meinhardt<sup>2</sup>, Jason Guicheteau<sup>1</sup>, Jason Guicheteau<sup>1</sup>; <sup>1</sup>Edgewood Chemical Biological Center; <sup>2</sup>UC Santa Barbara

- 11:50 AM (97) **Application of SERS in Bioanalytical Detection Schemes**; Dana Cialla-May<sup>1,2,3</sup>, Karina Weber<sup>1,2,3</sup>, Juergen Popp<sup>1,2,3</sup>; <sup>1</sup>Leibniz Institute of Photonic Technology (IPHT); <sup>2</sup>Friedrich Schiller University Jena; <sup>3</sup>InfectoGnostics Research Campus Jena

- 12:10 PM (98) **A New Laboratory Instrument for Raman Detection of Thin Films on Planar Surfaces – Surface Plasmon Enhanced Surface Raman Spectroscopy (SPESRS)**; Stephen Weibel<sup>1</sup>, Emily Smith<sup>2</sup>, Charles Kofi Adarkwa Nyamekye<sup>2</sup>, Jonathon Bobbitt<sup>2</sup>; <sup>1</sup>Surface Photonics Inc.; <sup>2</sup>Iowa State Univ. Ames Lab., U.S. Dept. of Energy

### Monday Morning, Carson 4

#### 17RAM07: IRDG RAMAN

Organizer and Presider: Karen Faulds

- 10:50 AM (99) **Neurological Disease Diagnosis with Surface-Enhanced Raman Spectroscopy**; Bhavya Sharma<sup>1</sup>; <sup>1</sup>University of Tennessee
- 11:10 AM (100) **The development of Stable Isotope Probing with Raman Spectroscopy for Studying Single Cell Bacterial Metabolism**; Roy Goodacre<sup>1</sup>, Howbeer Muhamadali, Malama Chisanga; <sup>1</sup>University of Manchester
- 11:30 AM (101) **Raman Spectroscopy as a Tool for Studying the Role of Lipids in Prostate Cancer**; Lauren Jamieson<sup>1</sup>, Mark Salji<sup>2</sup>, Rachana Patel<sup>2</sup>, Hing Leung<sup>2</sup>, Karen Faulds<sup>1</sup>, Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>The Beatson Institute for Cancer Research
- 11:50 AM (102) **Life, Death and Spectroscopy**; Colin Campbell, Hannah Johnstone<sup>1</sup>, Lauren Jamieson<sup>1</sup>, David Harrison<sup>2</sup>, Tim Morley<sup>3</sup>; <sup>1</sup>University of Edinburgh; <sup>2</sup>University of St Andrews; <sup>3</sup>Smith and Nephew
- 12:10 PM (103) **Multi-Modal Imaging of Erlotinib-Nanoparticle Conjugates in Lung Cancer Cells**; Rachael Cameron<sup>1</sup>; <sup>1</sup>Bionano, University of Strathclyde; <sup>2</sup>Cancer Research Centre, University of Edinburgh

### Monday Morning, Crystal 4

#### 17SPECIAL03: STAND-OFF SENSING

Organizer and Presider: Shermineh Rostami

- 10:50 AM (104) **High Recognition Specificity Remote Sensing of Trace Gases Using IR/THz Double Resonance Spectroscopy**; Henry Everitt<sup>1</sup>, Dane Phillips<sup>2</sup>, Elizabeth Tanner<sup>3</sup>, Frank De Lucia<sup>4</sup>; <sup>1</sup>Army Aviation & Missile RD&E Center; <sup>2</sup>IERUS Technologies; <sup>3</sup>IERUS Technologies; <sup>4</sup>Ohio State University
- 11:10 AM (105) **Open-Path Dual Comb Spectroscopy for Atmospheric Measurements**; Nathan Newbury, Kevin Cossel<sup>1</sup>, Eleanor Waxman<sup>1</sup>, Gabriel Ycas<sup>1</sup>, Fabrizio Giorgetta<sup>1</sup>, Esther Baumann<sup>1</sup>, Sean Coburn<sup>2</sup>, Ian Coddington<sup>1</sup>, Daniel Herman<sup>1</sup>, Gregory Rieker<sup>2</sup>; <sup>1</sup>NIST; <sup>2</sup>University of Colorado

# TECHNICAL PROGRAM – MONDAY

## Orals 10:50 am – 12:30 pm & 1:30 – 3:10 pm

11:30 AM (106) **Polarization-Controlled White Light LIDAR;** Matthieu Baudeler<sup>1,2,3</sup>, Shermineh Rostami<sup>3</sup>, Martin Richardson<sup>3</sup>; <sup>1</sup>UCF - NCFS; <sup>2</sup>UCF - Chemistry; <sup>3</sup>UCF - CREOL

11:50 AM (107) **Projecting High Power Density at Long Distance for Standoff Spectroscopy;** Jean-Claude Diels<sup>1</sup>; <sup>1</sup>CHTM-UNM

12:10 PM (108) **Development and Characterization of a Short-Wave Infrared Conformal Filter Hyperspectral Imager for Real-Time Standoff Detection of Materials;** Shawna Tazik<sup>1</sup>, Matthew Nelson<sup>1</sup>, Patrick Treado<sup>1</sup>, Srinivasa Narasimhan<sup>2</sup>, Bernardo Pires<sup>2</sup>, Martial Hebert<sup>2</sup>; <sup>1</sup>ChemImage Sensor Systems; <sup>2</sup>Carnegie Mellon Robotics Institute

### Monday Morning, Nevada 4

#### 17SPSJ01: FRONTIERS OF DEEP- AND FAR-ULTRAVIOLET SPECTROSCOPY I

Organizers: Yukihiro Ozaki, Satoshi Kawata, Yuika Saito, Yusuke Morisawa; President: Yukihiro Ozaki

10:50 AM (109) **Tip-Enhanced Raman Microscopy in Deep UV;** Atsushi Taguchi<sup>1</sup>, Satoshi Kawata<sup>1</sup>; <sup>1</sup>Osaka University

11:10 AM (110) **Monomeric Polyglutamine Structures that Evolve into Fibrils;** Sanford Asher<sup>1</sup>, David Punihaole<sup>2</sup>, Ryan Jakubek<sup>1</sup>, Riley Workman<sup>4</sup>, Lauren Marbella<sup>3</sup>, Patricia Campbell<sup>2</sup>, Jeffry Madura<sup>4</sup>; <sup>1</sup>University of Pittsburgh; <sup>2</sup>University of Minnesota; <sup>3</sup>University of Cambridge; <sup>4</sup>Duquesne University; <sup>5</sup>University of Pittsburgh, School of Medicine

11:30 AM (111) **Hydrogen Sulfide Inhibits lysozyme Fibrillation: DUV Raman Spectroscopic Study;** Igor Lednev<sup>1</sup>, Tatiana Quiñones-Ruiz<sup>1</sup>, Manuel Rosario-Alomar<sup>1</sup>, Juan López-Garriga<sup>2</sup>; <sup>1</sup>University at Albany, SUNY; <sup>2</sup>University of Puerto Rico at Mayaguez

11:50 AM (112) **Sample Photodegradation and Protection in Deep-UV Resonance Raman Spectroscopy;** Yasuaki Kumamoto<sup>1</sup>; <sup>1</sup>Kyoto Pref. Univ. of Medicine

12:10 PM (113) **Deep Ultraviolet Resonance Raman (DUVRR) Spectroscopy of Protein Therapeutics;** Sergey Arzhantsev<sup>1</sup>, Chen Qiu<sup>1</sup>; <sup>1</sup>US Food and Drug Administration

### Monday Afternoon, Crystal 4

#### 17AES03: ELECTROKINETICS FOR CELLULAR ANALYSIS AND SEPARATIONS

Organizer: Darwin Reyes;  
Presiders Zachary Gagnon, Christopher Harrison

1:30 PM (114) **Multi-Channel Detection for Electrophoretic Analysis of Individual Organelles;** Edgar Arriaga<sup>1</sup>, Erik Tyrrell<sup>1</sup>, Katherine Muratore<sup>1</sup>, Heather Brown<sup>1</sup>; <sup>1</sup>University of Minnesota

1:50 PM (115) **Enhancing the Information Content of Single Cell Analysis on Microfluidic Devices Using Optical Fiber Bridges;** Christopher Culbertson<sup>1</sup>, Damith Padabadge<sup>1</sup>, Jalal Sadeghi<sup>1</sup>, Jay Sibbitts<sup>1</sup>; <sup>1</sup>Kansas State University

2:10 PM (116) **Physical Properties of Bioparticles and High Resolution Separations with Dielectrophoresis;** Mark Hayes<sup>1</sup>, Shannon Hilton<sup>1</sup>, Claire Crowther<sup>1</sup>; <sup>1</sup>Arizona State University

2:30 PM (117) **Multi-Spectroscopic NVU-on-a-Chip System for Developing Efficient Nanoparticle Strategies for Increased Drug Efficacy;** Sagnik Basuray<sup>1</sup>, Bhuvana Mohanlal<sup>1</sup>, Victoria Harbour<sup>1</sup>, Samuel Roy<sup>1</sup>, Tarun Masimukku<sup>1</sup>, Jocelyn Davis<sup>1</sup>; <sup>1</sup>New Jersey Institute of Technology

2:50 PM (118) **Improving the Separation Resolution of Insulator-based Dielectrophoresis;** Claire Crowther<sup>1</sup>, Mark Hayes<sup>1</sup>; <sup>1</sup>Arizona State University

### Monday Afternoon, Crystal 2

#### 17ATOM02: GLOW DISCHARGE SPECTROSCOPY II

Organizer and Presider: Jorge Pisonero Castro

1:30 PM (119) **Glow Discharge Time of Flight Mass Spectrometry for Fast Multidimensional Analysis of VOCs;** Nerea Bordel<sup>1</sup>, Jonatan Fandiño<sup>1</sup>, Marcos Bouza<sup>1</sup>, Jorge Pisonero<sup>1</sup>, Alfredo Sanz-Medel<sup>1</sup>; <sup>1</sup>University of Oviedo

1:50 PM (120) **Recent Advances in Elemental Mapping through Glow Discharge Optical Emission Spectroscopy;** Gerardo Gamez<sup>1</sup>; <sup>1</sup>Texas Tech University Dept. Chemistry&Biochemistry

2:10 PM (121) **Comparison of VUV and NIR wavelengths for O and H in GD-OES Compositional Depth Profiling;** Arne Bengtson<sup>1</sup>; <sup>1</sup>Swerea KIMAB AB

2:30 PM (122) **Compositional Depth Profile Analysis by Radio Frequency Glow Discharge Utilizing a Solid-State Spectrometer;** Kim Marshall<sup>1</sup>; <sup>1</sup>Leco Corporation

2:50 PM (123) **On the Roles of Metastable and Quasi-Metastable Species in Atmospheric Noble Gas Dielectric Barrier Discharges;** Felix David Klute<sup>1</sup>, Sebastian Burhenn<sup>1</sup>, Pascal Vogel<sup>1</sup>, Antje Michels<sup>1</sup>, Charlotte Lewis<sup>2</sup>, Daniel Thurston<sup>2</sup>, Beatrix Biskup<sup>3</sup>, Paul Farnsworth<sup>2</sup>, Joachim Franzke<sup>3</sup>; <sup>1</sup>ISAS; <sup>2</sup>Dept of Chemistry - BYU; <sup>3</sup>Experimental Physics II –RUB

### Monday Afternoon, Crystal 1

#### 17AWD11: COBLENTZ LIPPINCOTT AWARD SYMPOSIUM HONORING ROBERTO MERLIN

Organizer and Presider: Jim Rydzak

1:30 PM (124) **Time-Domain Inelastic X-Ray Scattering from Short-Wavelength Phonons;** David A. Reis; <sup>1</sup>Stanford PULSE Institute

1:50 PM (125) **Multidimensional Spectroscopic Probes of Vibrational and Vibronic Coherence in Photosynthetic Systems;** Jennifer Ogilvie<sup>1</sup>; <sup>1</sup>University of Michigan

2:10 PM (126) **Monolayer Magnets;** Xiaodong Xu<sup>1</sup>; <sup>1</sup>University of Washington

2:30 PM (127) **Ultrafast Reversal of the Ferroelectric Polarization;** Roman Mankowsky<sup>1,2</sup>, Alexander von Hoegen<sup>1</sup>, Michael Först<sup>1</sup>, Andrea Cavalleri<sup>1,2</sup>; <sup>1</sup>Max Planck Institute for the Structure and Dynamics; <sup>2</sup>University of Hamburg

2:50 PM (128) **Raman Spectroscopy of Collective Excitations in Correlated Electron Systems;** Girsh Blumberg<sup>1</sup>; <sup>1</sup>Rutgers University

### Monday Afternoon, Nevada 7

#### 17BIM02: NANOMATERIAL-ASSISTED IMAGING

Organizer and Presider: Steven Asiala

1:30 PM (129) **Using Novel Deep Raman Approaches to Measure Multiple Characteristics of Biomaterials at Depth in Scattering Media / Mammalian Tissues;** Nick Stone<sup>1</sup>, Ben Gardner<sup>1</sup>, Pavel Matousek<sup>2</sup>; <sup>1</sup>University of Exeter; <sup>2</sup>STFC Rutherford Appleton Lab

1:50 PM (130) **Dynamic SERS Imaging of Intracellular Environment;** Kazuki Bando<sup>1</sup>, Jun Ando<sup>1</sup>, Nicholas Smith<sup>1</sup>, Katsumasa Fujita<sup>1</sup>, Satoshi Kawata<sup>1</sup>; <sup>1</sup>Osaka University



# TECHNICAL PROGRAM – MONDAY

Orals 1:30 – 3:10 pm

2:10 PM (131) **Surface Enhanced Raman Spectroscopy (SERS) Optofluidics for Whole Cell Analysis;** Marjorie Willner<sup>1</sup>, Kay McMillan<sup>2</sup>, Rachael Cameron<sup>2</sup>, Duncan Graham<sup>2</sup>, Peter Vikesland<sup>1</sup>, Michele Zagnoni<sup>2</sup>; <sup>1</sup>Virginia Tech; <sup>2</sup>University of Strathclyde

2:30 PM (132) **Engineering Non-Cadmium I-III-VI Quantum Dots for Bioimaging and Sensing;** Xiaoshan Zhu<sup>1</sup>; <sup>1</sup>University of Nevada Reno

2:50 PM (133) **Biosensors for Cellular Nucleic Acids Detection Using SERS;** Pietro Strobbia<sup>1</sup>, Bridget Crawford<sup>1</sup>, Hsin-Neng Wang<sup>1</sup>, Tuan Vo-Dinh<sup>1</sup>; <sup>1</sup>Duke University

## Monday Afternoon, Crystal 5

### 17CHEM02: SPECTRAL FINGERPRINTING FOR CHARACTERIZATION OF COMPLEX MATERIALS

Organizers: Mengliang Zhang, Pei Chen;

Presider: Mengliang Zhang

1:30 PM (134) **Development of a Comprehensive Flavonoid Analysis Computational Tool for Ultra High-Performance Liquid Chromatography-Diode Array Detection-High Resolution Accurate Mass-Mass Spectrometry Data;** Mengliang Zhang<sup>1</sup>, Jianghao Sun<sup>1</sup>, Pei Chen<sup>1</sup>; <sup>1</sup>United States Department of Agriculture

1:50 PM (135) **Fingerprinting Food Ingredients for Authentication By Portable Vibrational Spectroscopy Technologies;** Luis Rodriguez-Saona<sup>1</sup>; <sup>1</sup>The Ohio State University

2:10 PM (136) **Rapid Prediction of Milk Powder Adulteration Based on Portable Vibrational Spectroscopic Devices;** Betsy Jean Yakes<sup>1</sup>, Sanjeewa R. Karunathilaka<sup>1</sup>, Keqin He<sup>2</sup>, Lea Brückner<sup>1</sup>, Magdi Mossoba<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration; <sup>2</sup>University of Maryland

2:30 PM (137) **Greater than the Sum of its Parts—Exploiting Ambient Ionization Mass Spectrometry-Derived Chemical Fingerprints for Complex Matrix Identification;** Rabi Ann Musah, Justine E Giffen, Kristen L Fowble, Meghan G Fogerty; <sup>1</sup>State University of New York at Albany; <sup>2</sup>State University of New York at Albany; <sup>3</sup>State University of New York at Albany; <sup>4</sup>State University of New York at Albany

2:50 PM (138) **Detection of Nitrogen-Containing Pollutants with a Chip-Based Sensor;** Peng Zheng<sup>1</sup>, Nianqiang Wu<sup>1</sup>; <sup>1</sup>West Virginia University

## Monday Afternoon, Carson 1

### 17IR03: NANOSCALE IR APPLICATIONS IN THE LIFE SCIENCES

Organizer and Presider: Bayden Wood

1:30 PM (139) **Correlating Biophysical Properties of Amyloid Aggregates in vitro and in vivo by AFM-based Infrared Nanospectroscopy;** Francesco Simone Ruggeri<sup>1</sup>, Chris Dobson<sup>1</sup>, Michele Vendruscolo<sup>1</sup>, Thomas Knowles<sup>1</sup>; <sup>1</sup>University of Cambridge

1:50 PM (140) **Advanced IR Nanospectroscopy to Study Lipids Bodies in Micro-Organisms: Toward a Better Understanding of Metabolic Pathways at Stake.;** Ariane Deniset-Besseau<sup>1,2</sup>, Rolando Rebois<sup>1,2</sup>, Alexandre Dazzi<sup>1,2</sup>; <sup>1</sup>Laboratoire de Chimie-Physique; <sup>2</sup>Université Paris-sud

2:10 PM (141) **AFM-IR Explores a Chromatin Role in Formation of Chromosomal Aberrations;** Ewelina Lipiec; <sup>1</sup>Institute of Nuclear Physics, PAN

2:30 PM (142) **In vivo AFM-IR Nano-Spectroscopic Investigation of the Bacterial Cell Wall;** Philip

Heraud<sup>1</sup>, Kamila Kochan<sup>1</sup>, David Perez-Guaita<sup>1</sup>, Julia Pissang<sup>1</sup>, Jhih-Hang Jiang<sup>1</sup>, Anton Peleg<sup>1</sup>, Bayden Wood<sup>1</sup>; <sup>1</sup>Monash University

2:50 PM (143) **Nanoinfrared Spectroscopy of Cell Membranes and Extracellular Vesicles;** Leonetta Baldassarre<sup>1,2</sup>, Valeria Giliberti<sup>1,2</sup>, Alessandro Nucara<sup>1</sup>, Paolo Calvani<sup>1</sup>, Alessandro Rosa<sup>1,2</sup>, Valeria De Turris<sup>2</sup>, Mattia Musto<sup>3</sup>, Loredana Casalis<sup>3</sup>, Eglof Ritter<sup>4</sup>, Michele Ortolani<sup>1,2</sup>; <sup>1</sup>Sapienza University of Rome; <sup>2</sup>Istituto Italiano di Tecnologia; <sup>3</sup>ELETTRA Sincrotrone Trieste; <sup>4</sup>Humboldt University Berlin

## Monday Afternoon, Crystal 3

### 17LIBS02: NALIBS: LIBS FOR FORENSIC AND HOMELAND SECURITY

Organizer and Presider: Mauro Martinez

1:30 PM (144) **Biological Sex Determination via Elemental Analysis by LIBS;** Mauro Martinez<sup>1</sup>, Abigail Woltering<sup>1</sup>, Maria Andreoli<sup>1</sup>, Lana Williams<sup>1</sup>, Tosha Dupras<sup>1</sup>, Matthieu Baudelet<sup>1</sup>; <sup>1</sup>University of Central Florida

2:10 PM (145) **Elemental Analysis of Packaging Tapes by LA-ICP-MS and LIBS;** Claudia Martinez Lopez<sup>1</sup>, Masataka Sakayanagi<sup>2,3</sup>, Jose R. Almirall<sup>1</sup>; <sup>1</sup>Florida International University; <sup>2</sup>Scientific Crime Laboratory; <sup>3</sup>National Research Institute of Police Science

2:30 PM (146) **Gunshot Residues Analysis Using LIBS for the Estimation of Firing Distance.;** César Alvarez-Llamas<sup>1</sup>, María López-López<sup>2</sup>, Carmen García-Ruiz<sup>2</sup>, Jorge Pisonero<sup>1</sup>, Bordel Nerea<sup>1</sup>; <sup>1</sup>University of Oviedo; <sup>2</sup>University of Alcalá

2:50 PM (147) **Nanosecond-Pulsed Laser Ablation for Explosives Characterization: Emission and Shock Wave Measurements;** Jennifer Gottfried<sup>1</sup>; <sup>1</sup>US Army Research Laboratory

## Monday Afternoon, Nevada 5

### 17NANO02: NANOMATERIALS AND NANOSTRUCTURES FOR ENERGY-RELATED APPLICATIONS

Organizer and Presider: Wei Zhao

1:30 PM (148) **Nanomaterials in Energy Generation and Storage Devices;** Meyya Meyyappan<sup>1</sup>; <sup>1</sup>NASA Ames Research Center

2:10 PM (149) **Hydrogen Evolution Reaction Catalyzed by Ruthenium Ion-Complexed Graphitic-like Carbon Nitride Nanosheets;** Shaowei Chen<sup>1</sup>; <sup>1</sup>University of California Santa Cruz

2:30 PM (150) **Plasmonic Enhanced Catalysis Based on Rh Nanostructures;** Jie Liu<sup>1</sup>, Xiao Zhang<sup>1</sup>, Xueqian Li<sup>1</sup>, Henry Everitt<sup>1</sup>; <sup>1</sup>Duke University

2:50 PM (151) **A Graded Nanoscale Catalytic MoSx/TiO2 Interface for Hydrogen Evolution;** Jing Gu<sup>1</sup>; <sup>1</sup>San Diego State University

## Monday Afternoon, Nevada 6

### 17PAT07: HAND-HELD AND PORTABLE SPECTROMETERS: APPLICATIONS AND INSTRUMENTAL METHODS

Organizer and Presider: David Schiering

1:30 PM (152) **Portable Standoff Detection of Materials Using Monolithic QCL Arrays;** Mark Witinski<sup>1</sup>, Romain Blanchard<sup>1</sup>, Kalyani Krishnamurthy<sup>1</sup>; <sup>1</sup>Pendar Technologies

1:50 PM (153) **Handheld and Portable FTIR: After a Decade, What Have We Learned?;** Norman Wright<sup>1</sup>; <sup>1</sup>Agilent Technologies

## TECHNICAL PROGRAM – MONDAY

**Orals 1:30 – 3:10 pm & 3:50 – 5:30 pm**

- 2:10 PM (154) **The Use of Spatially-Offset Raman Spectroscopy (SORS) to Identify Unknown Threats through Opaque Containers;** Eric Roy<sup>1</sup>; <sup>1</sup>Cobalt Light Systems
- 2:30 PM (155) **Development and Implementation of a Pass/Fail Field-Friendly Method for Detecting Sildenafil in Suspect Pharmaceutical Tablets Using a Handheld Raman Spectrometer and Silver Colloids;** Adam Lanzarotta<sup>1</sup>, Lisa Lorenz<sup>1</sup>, JaCinta Batson<sup>1</sup>, Cheryl Flurer<sup>1</sup>; <sup>1</sup>FDA Forensic Chemistry Center
- 2:50 PM (156) **MicroNIR PAT – Spectroscopic Sensor for Industrial Process Monitoring;** Peng Zou<sup>1</sup>; <sup>1</sup>Viavi Solutions

### Monday Afternoon, Carson 2 17PMA02: COUNTERFEIT PHARMACEUTICALS

Organizer: Anna Luczak; President: Ravi Kalyanaraman

- 1:30 PM (157) **Laboratory Investigation of Suspected Materials at Celgene;** Ming Wang<sup>1</sup>, Dong Xiang<sup>1</sup>, Xiaoxuan (Jason) Shen<sup>1</sup>; <sup>1</sup>Celgene Corporation
- 1:50 PM (158) **The Use of X-Ray Powder Diffraction (XRD) and Vibrational Spectroscopic Techniques in the Analysis of Pharmaceutical Forensic Samples;** Mark Witkowski<sup>1</sup>, Kelsey DeWitt<sup>1</sup>; <sup>1</sup>US FDA Forensic Chemistry Center
- 2:10 PM (159) **Multispectral Approach for Identifying Counterfeit Lifestyle and Medicinal Products of Different Formulations;** Sulaf Assi<sup>1</sup>; <sup>1</sup>Bournemouth University
- 2:30 PM (160) **Key Indicators of Falsified Medicines;** Susan Macha<sup>1</sup>; <sup>1</sup>Takeda Pharmaceuticals
- 2:50 PM (161) **Screening Technologies for the Detection of Substandard and Falsified Medicines: Public Standards for Quality;** Daniel Bempong<sup>1</sup>, Lukas Roth<sup>1</sup>; <sup>1</sup>U.S. Pharmacopeia

### Monday Afternoon, Carson 4 17RAM01: EMERGING RAMAN I

Organizers and Presidents: Ian Lewis, Duncan Graham, Pavel Matousek

- 1:30 PM (162) **Coupling and Stacking Order of ReS2 Atomic Layers Revealed by Ultralow-Frequency Raman Spectroscopy;** Chun Hung Lui<sup>1</sup>; <sup>1</sup>University of California Riverside
- 1:50 PM (163) **Raman Hyperspectroscopy of a Biological Stain for Forensic Phenotype Profiling;** Igor Lednev<sup>1</sup>; <sup>1</sup>University at Albany, SUNY
- 2:10 PM (164) **Transmission Raman Measurements Using a Spatial Heterodyne Raman Spectrometer;** K. Alicia Strange<sup>1</sup>, Kelly C. Paul<sup>2</sup>, S. Michael Angel<sup>2</sup>; <sup>1</sup>Savannah River National Lab; <sup>2</sup>University of South Carolina
- 2:30 PM (165) **TERS with Angstrom Resolution;** Richard Van Duyne<sup>1</sup>; <sup>1</sup>Northwestern University

### Monday Afternoon, Carson 3 17RAM05: BIOANALYTICAL SERS II

Organizers and Presidents: Roy Goodacre, Duncan Graham, Colin Campbell

- 1:30 PM (166) **Accurate, High Speed Immunodiagnosics using SERS;** Marc Porter<sup>1</sup>, Jennifer Granger<sup>1</sup>, China Lim<sup>1</sup>, Aleksander Skuratovskiy<sup>1</sup>, Courtney Scaife<sup>1</sup>, Jill Shea<sup>1</sup>; <sup>1</sup>University of Utah
- 1:50 PM (167) **SERS for Rapid Detection of Bacterial Infection;** Steven Bell<sup>1</sup>, Jessica Kelly<sup>1</sup>, Virginia Blaque<sup>1</sup>, Miguel Valvano<sup>1</sup>, Sheila Patrick<sup>1</sup>; <sup>1</sup>Queen's University Belfast

- 2:10 PM (168) **An Innovative SERS Approach for in situ and Real Time Study of Pesticide Behaviors in Live Plants;** Lili He<sup>1</sup>, Tianxi Yang<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst
- 2:30 PM (169) **Surface Enhanced Raman Spectroscopy for Rapid Selenium Monitoring in Flue Gas Desulfurization Water;** Merwan Benhabib, Mark Charles Peterman, Samuel Kleinman; <sup>1</sup>OndaVia, Inc
- 2:50 PM (170) **Detection of CVD Biomarkers Using Functionalised Nanoparticles and SERS;** Kirsten Gracie<sup>1</sup>, Samuel Mabbott<sup>1</sup>, Steven Asiala<sup>1</sup>, Jonathan Noonan<sup>2</sup>, Neil MacRitchie<sup>2</sup>, Gianluca Grassia<sup>2</sup>, Pasquale Maffia<sup>2</sup>, Karen Faulds<sup>1</sup>, Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>University of Glasgow

### Monday Afternoon, Nevada 4 17SPSJ03: PMAIRS: A CUTTING-EDGE ANALYTICAL TECHNIQUE OF MOLECULAR ORIENTATION IN A THIN FILM HAVING SURFACE ROUGHNESS

Organizer and President: Takeshi Hasegawa

- 1:30 PM (171) **Quantitative Molecular Orientation Analysis in Organic Semiconductor Thin Films Having a Rough Surface by pMAIRS;** Takafumi Shimoaka<sup>1</sup>, Nobutaka Shioya<sup>1</sup>, Miyako Hada<sup>1</sup>, Takeshi Hasegawa<sup>1</sup>; <sup>1</sup>Institute for Chemical Research, Kyoto University
- 1:50 PM (172) **Analysis of Carbon Nanotube Films on Silicon by p-Polarized Multiple Angle Incidence Resolution Spectrometry (pMAIRS);** Steve Lowry<sup>1</sup>, David Drapcho<sup>1</sup>, Amir Mashal<sup>1</sup>, Matthew Meyer<sup>1</sup>, Nathaniel Saffron<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific
- 2:10 PM (173) **Recent Progress of MAIRS;** Takeshi Hasegawa<sup>1</sup>; <sup>1</sup>ICR, Kyoto University
- 2:30 PM (174) **Interfacial Molecular Structure and Proton Transport Characteristics of Polymer Thin Films for Fuel Cells;** Yuki Nagao<sup>1</sup>; <sup>1</sup>Japan Advanced Institute of Science and Technology
- 2:50 PM (175) **Impact of pMAIRS on Metal Oxide Nanowires;** Takeshi Yanagida<sup>1</sup>; <sup>1</sup>Kyushu University

### 3:10 PM Poster Session and Coffee Break, Reno Ballroom

### Monday Afternoon, Crystal 4 17AES02: NOVEL ELECTROKINETIC PHENOMENA: FUNDAMENTALS AND APPLICATIONS

Organizer and President: Jeffery Moran

- 3:50 PM (176) **Influence of Polarization and Ion Crowding Effects on Nonlinear Electrophoresis;** Bruno Figliuzzi<sup>1</sup>, Jeffrey Moran<sup>2</sup>; <sup>1</sup>Mines ParisTech - PSL Research University; <sup>2</sup>MIT; <sup>3</sup>Stanford University
- 4:10 PM (177) **Electrokinetic Fingering: A Problem in Vector Laplacian Growth;** Mohammad Mirzadeh<sup>1</sup>, Martin Bazant<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology
- 4:30 PM (178) **Using Dielectrophoresis to Separate Protists Present in Termite Hindguts;** Claire Crowther<sup>1</sup>, Katalina Freeman<sup>1</sup>, Mark Hayes<sup>1</sup>, Gillian Gile<sup>1</sup>; <sup>1</sup>Arizona State University
- 4:50 PM (179) **Mechanism of Sequence-Based Separation of Single-Stranded DNA in Capillary Zone Electrophoresis;** Jia Zhao, Steve Cramer<sup>1</sup>, Linda McGown<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute
- 5:10 PM (180) **Initial Evaluation of a Commercially Available MicroFluidic Capillary Electrophoresis Mass Spectrometric Interface;** Joseph Snodgrass<sup>1</sup>, Alexander Langston<sup>2</sup>, Eric Chan<sup>1</sup>, Shuojia Bai<sup>1</sup>, Eduard Luss<sup>1</sup>, Ricardo Borjas<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals, Inc; <sup>2</sup>Northeastern University

## TECHNICAL PROGRAM – MONDAY

**Orals 3:50 – 5:30 pm**

### Monday Afternoon, *Crystal 2* 17ATOM03: RECENT ADVANCES IN LIQUID ELECTRODE GLOW DISCHARGE PLASMAS

Organizers and Presiders: Jaime Orejas, Andrew Schwartz

- 3:50 PM (181) **Optimization And Characterization of the Solution Electrode Interface for Improved Performance of the Solution Cathode Glow Discharge**; Stuart Schroeder<sup>1</sup>; <sup>1</sup>InnoTech Alberta
- 4:10 PM (182) **Industrial SCGD – A Technique for Inline Analysis of Metals in Liquids**; David Malmström<sup>1</sup>, Arne Bengtson<sup>1</sup>; <sup>1</sup>Swerea KIMAB
- 4:30 PM (183) **Enhanced Performance of the Liquid Sampling-Atmospheric Pressure Glow Discharge Ion Source for Elemental Isotope Ratio Mass Spectrometry**; Edward Hoegg<sup>1,2</sup>, Garret Hart<sup>2</sup>, David Koppenaal<sup>2</sup>, George Hager<sup>2</sup>, R. Kenneth Marcus<sup>1</sup>; <sup>1</sup>Clemson University; <sup>2</sup>Pacific Northwest National Lab
- 4:50 PM (184) **Analysis of Solid and Aqueous Samples for Atomic and Molecular Species with Solution-Cathode Glow Discharge Mass Spectrometry (SCGD-MS)**; Jacob Shelley<sup>1</sup>, Andrew Schwartz<sup>2</sup>, Courtney Walton<sup>1</sup>, Garrett MacLean<sup>1</sup>, Judy Wu<sup>1</sup>, Gary Hieftje<sup>3</sup>; <sup>1</sup>Rensselaer Polytechnic Institute; <sup>2</sup>State University of New York at Buffalo; <sup>3</sup>Indiana University
- 5:10 PM (185) **Pushing the Limits: Exploration of Pulsed Solution Cathode Glow Discharge**; Jaime Orejas Ibanez<sup>1</sup>, Andrew J. Schwartz<sup>1</sup>, Steven J. Ray<sup>1</sup>; <sup>1</sup>SUNY at Buffalo

### Monday Afternoon, *Nevada 7* 17BIM03: ANALYTICAL SCIENCES IN MOLECULAR BIOLOGY

Organizer and Presider: Zachary Schultz

- 3:50 PM (186) **Fluorescence Microscopy for Biomedical Applications: Imaging Nanoparticle-Cell Interactions**; Christine Payne<sup>1</sup>; <sup>1</sup>Georgia Tech
- 4:10 PM (187) **SERS Optophysiology of Small Organic Metabolites in Biosensing Applications**; Jean-Francois Masson<sup>1</sup>, Felix Lussier<sup>1</sup>, Benjamin Charron<sup>1</sup>, Dimitris Missirlis, Joachim Spatz, Thibault Brulé; <sup>1</sup>Universite de Montreal
- 4:30 PM (188) **Resonance Raman and Fluorescence Studies of Membrane Proteins**; Judy Kim<sup>1</sup>; <sup>1</sup>UC San Diego
- 4:50 PM (189) **Imaging Lipid Turnover Rates in Mouse Brains with Desorption Electrospray Ionization Mass Spectrometry**; Paul Farnsworth<sup>1</sup>, Richard Carson<sup>1</sup>, Charlotte Lewis<sup>1</sup>, Mercedes Erickson<sup>1</sup>, Anna Zagieboylo<sup>1</sup>, Bradley Naylor<sup>1</sup>, Kelvin Lee<sup>1</sup>, John Price<sup>1</sup>; <sup>1</sup>Brigham Young University
- 5:10 PM (190) **Investigating Photophysical Properties Associated with Bumble Bee Venom Antimicrobial Peptide-Membrane Interactions**; Matthew Roberson<sup>1</sup>, Devin Smith<sup>1</sup>, Simon White<sup>1</sup>, Ian Wallace<sup>1</sup>, Matthew Tucker<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### Monday Afternoon, *Crystal 5* 17CHEM03: CHEMOMETRIC OPPORTUNITIES IN THE FORENSIC SCIENCES

Organizer and Presider: Steve Morgan

- 3:50 PM (191) **Non-Destructive Recovery of Defaced Serial Numbers Using Infrared Thermal Imaging**; John Kalivas<sup>1</sup>, Ikwulono Unobe<sup>1</sup>, Lisa Lau<sup>1</sup>, Andrew Sorensen<sup>1</sup>, Rene Rodriguez<sup>1</sup>; <sup>1</sup>Idaho State University

- 4:10 PM (192) **The Use of LA-ICP-MS Databases to Estimate Likelihood Ratios for the Forensic Evaluation of Glass Evidence**; Jose Almirall<sup>1</sup>, Daniel Ramos<sup>2</sup>, Ruthie Corzo<sup>1</sup>; <sup>1</sup>Florida International University; <sup>2</sup>Universidad Autonoma de Madrid
- 4:30 PM (193) **Modeling, Inference, and Predictive Calibrations for Forensic Spectroscopic Data**; Stephen Morgan<sup>1</sup>, Michael Myrick<sup>1</sup>, Edsel Pena<sup>1</sup>; <sup>1</sup>University of South Carolina
- 4:50 PM (194) **Building Forensic Science on a ROC**; Michael Sigman<sup>1</sup>, Mary Williams<sup>1</sup>; <sup>1</sup>University of Central Florida
- 5:10 PM (195) **Modeling and Performance Evaluation of Real-Time Standoff Hazardous Materials Detection**; Arjun Bangalore<sup>1</sup>, Mathew Nelson<sup>1</sup>, Shawna Tazik<sup>1</sup>, Robert Schweitzer<sup>1</sup>, Patrick Treado<sup>1</sup>; <sup>1</sup>ChemImage Corp.

### Monday Afternoon, *Nevada 6* 17FORENS01: NUCLEAR FORENSICS

Organizers: Andrew Duffin, Dallas Reilly; Presider: Dallas Reilly

- 3:50 PM (196) **Sample Preparation Approaches for Laser Ablation Inductively Coupled Plasma Mass Spectrometry**; Jhanis J. Gonzalez<sup>1,2</sup>; <sup>1</sup>Lawrence Berkeley National Lab.; <sup>2</sup>Applied Spectra, Inc.
- 4:10 PM (197) **Initial Attempts Into Characterizing Surrogate Nuclear Fireballs**; John Auxier II, Eric Francis<sup>1</sup>, Lajos Majcos<sup>1</sup>, Howard Hall<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville
- 4:30 PM (198) **Uranium Isotope Ratios by Laser Absorption Spectroscopy**; Alonso Castro<sup>1</sup>, Joshua Bartlett<sup>1</sup>, Vyacheslav Lebedev<sup>1</sup>; <sup>1</sup>Los Alamos National Laboratory
- 4:50 PM (199) **Cat Litter, Nitric Acid, Plutonium, and \$2.4 Billion Dollars: The Microscopic Investigation into the 2014 Contamination at WIPP**; Jon Schwantes<sup>1</sup>, David Atkinson<sup>1</sup>, Edgar Buck<sup>1</sup>, Carlos Fraga<sup>1</sup>, Larry Greenwood<sup>1</sup>, Bruce McNamara<sup>1</sup>, Michael Minnette<sup>1</sup>, Randal Scheele<sup>1</sup>, Luke Sweet<sup>1</sup>, Jon Wahl<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

### Monday Afternoon, *Carson 1* 17IR04: PRACTICAL IMPLEMENTATION OF DIFFUSE REFLECTANCE SPECTROSCOPY

Organizer and Presider: Benoit Inge

- 3:50 PM (200) **Near-IR Quality Control of a Drug to Treat a Rare Tropical Disease**; Robert Lodder<sup>1</sup>, Mayte Hernandez-Murtillo<sup>1</sup>; <sup>1</sup>University of Kentucky
- 4:10 PM (201) **Determination of the Volume of Interrogation of Powder for NIR Monitoring of a Continuous Powder Flow**; Carl Anderson<sup>1</sup>, Anik Alam<sup>1</sup>, Zhenqi Shi<sup>2</sup>, James Drennen<sup>1</sup>; <sup>1</sup>Duquesne University; <sup>2</sup>Lilly Research Laboratories
- 4:30 PM (202) **Multivariate Curve Resolution (MCR) and PARAFAC Analysis of Infrared Specular Reflection Spectra of Quartz Particles: Strategies for Optimal Surface Sensing**; Thomas Blake<sup>1</sup>, Paul Gassman<sup>1</sup>, Neal Gallagher<sup>2</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Eigenvector Research, Inc.
- 4:50 PM (203) **Possible Application of Near Infrared Reflectance Spectroscopy to Quantify a Parasite (*Perkinsus marinus*) in Oyster Tissues (*Crassostrea virginica*)**; Eric Guevelou<sup>1</sup>, Jessica M. Small<sup>1</sup>, Standish K. Allen Jr.<sup>1</sup>; <sup>1</sup>Virginia Institute of Marine Science
- 5:10 PM (204) **Using Near Infrared Spectroscopy Monitoring Heavy Crude Oil of Production**; Toni Miao<sup>1</sup>, Ajit Pradhan<sup>1</sup>, Michael Moir<sup>1</sup>, Eddy Lee<sup>1</sup>; <sup>1</sup>Chevron

*Future SciX Meeting: October 21 – 26, 2018, Atlanta, GA*



# TECHNICAL PROGRAM – MONDAY

Orals 3:50 – 5:30 pm

## Monday Afternoon, *Crystal 3*

### 17LIBS03: NASLIBS: MOLECULAR SIGNAL IN LIBS

Organizer and Presider: George Chan

- 3:50 PM (205) **Molecular Laser-Induced Breakdown Spectroscopy**; Christian Parigger<sup>1</sup>; <sup>1</sup>University of Tennessee Space Institute
- 4:10 PM (206) **Predicting Molecules in Laser-Induced Plasma Based on Equilibrium Plasma Model**; Igor Gornushkin<sup>1</sup>, Sergei Shabanov<sup>1,2</sup>, Ulrich Panne<sup>1,3</sup>; <sup>1</sup>BAM Federal Institute for Materials Research; <sup>2</sup>University of Florida; <sup>3</sup>Humboldt University, Berlin
- 4:30 PM (207) **Overcoming Spectral Interference in LAMIS with Robust Statistical Spectral Fitting**; George Chan<sup>1</sup>, Xianglei Mao<sup>1</sup>, Vassilia Zorba<sup>1</sup>, Richard Russo<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory
- 4:50 PM (208) **Partial Least Squares Calibration Modeling Towards the Multivariate Limit of Detection for Enriched Isotopic Mixtures via Laser Ablation Molecular Isotopic Spectroscopy**; Candace Harris<sup>1</sup>, Luisa T.M. Profeta<sup>2</sup>, Codjo Akpovo<sup>1</sup>, Ashley C. Stowe<sup>3</sup>, Lewis E. Johnson<sup>1</sup>; <sup>1</sup>Florida Agriculture & Mechanic University - CePaST; <sup>2</sup>Alakai Defense Systems Inc.; <sup>3</sup>Y-12 National Security Complex
- 5:10 PM (209) **Chemical Imaging of Thin Films with High Spatial Resolution by Femtosecond Laser-Induced Breakdown Spectroscopy**; Johannes D. Pedarnig<sup>1</sup>, Christoph M. Ahamer<sup>1</sup>, Kevin M. Riepl<sup>1</sup>, Norbert Huber<sup>1</sup>; <sup>1</sup>Johannes Kepler University Linz / Applied Physics

## Monday Afternoon, *Nevada 5*

### 17NANO03: NANOMATERIALS AND RELATED SPECTROSCOPY METHODS FOR ENERGY CONVERSION

Organizer and Presider: Jing Gu

- 3:50 PM (210) **High Photoelectrochemical Water Splitting Efficiencies: Materials Development and Measurement Challenges**; John Turner<sup>1</sup>, Todd Deutsch<sup>1</sup>, James Young<sup>1</sup>, Henning Döscher<sup>2</sup>, Myles Steiner<sup>1</sup>; <sup>1</sup>National Renewable Energy Lab; <sup>2</sup>Philipps-Universität Marburg
- 4:10 PM (211) **Nanoscale Infrared, Mechanical, and Electrical Characterization of Surface Defects in Perovskite Crystals via Peak Force Tapping Based Characterization Techniques**; Xiaoji Xu<sup>1</sup>; <sup>1</sup>Lehigh University
- 4:30 PM (212) **Understanding Rechargeable Batteries by Synchrotron X-ray Spectroscopy at Multiple Length Scales**; Feng Lin<sup>1</sup>; <sup>1</sup>Virginia Tech
- 4:50 PM (213) **Infrared Spectroscopy and Confocal Raman Microscopy Measurements in the Study of Materials for Energy Conversion**; Carol Korzeniewski<sup>1</sup>, Ying Liang<sup>1</sup>; <sup>1</sup>Texas Tech University
- 5:10 PM (214) **Developing Quantum Dot Solids for Next-Generation Photovoltaics**; Matt Law<sup>1</sup>; <sup>1</sup>UC, Irvine

## Monday Afternoon, *Carson 2*

### 17PMA03: IDENTIFICATION OF COUNTERFEIT MEDICINES

Organizer and Presider: Sulaf Assi

- 3:50 PM (215) **Rapid Identification of Biotherapeutics with Label-Free Raman Spectroscopy**; Ishan Barman<sup>1</sup>; <sup>1</sup>Johns Hopkins University
- 4:10 PM (216) **Screening Technologies and the Fight Against Substandard and Falsified Medicines**; Lukas Roth<sup>1</sup>; <sup>1</sup>U.S. Pharmacopeia

4:30 PM (217) **CSI: GAT - Finding the “DNA” of Counterfeit Drugs Using Raman Spectroscopy**; Jeremy Peters<sup>1</sup>, Eugene Park<sup>1</sup>, Ravi Kalyanaraman<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

4:50 PM (218) **Raman Technology for Bio and Pharmaceutical Counterfeits**; Anna Luczak<sup>1</sup>, Ravi Kalyanaraman<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

5:10 PM (219) **Going Digital: A Landscape View of Digital Technologies to Combat the Fake Medicines Trade**; Tim Mackey<sup>1,2</sup>; <sup>1</sup>UC San Diego - School of Medicine; <sup>2</sup>Global Health Policy Institute

## Monday Afternoon, *Carson 3*

### 17RAM06: BIOANALYTICAL SERS III

Organizer and Presider: Roy Goodacre, Duncan Graham, Colin Campbell

- 3:50 PM (220) **Development of SERS-Based Microfluidic Technology for Biomedical Diagnosis**; Jacbum Choo<sup>1</sup>; <sup>1</sup>Hanyang University
- 4:10 PM (221) **SERS-Based Bioassay for Detection of Biomolecules**; Young Mee Jung<sup>1</sup>; <sup>1</sup>Kangwon National University
- 4:30 PM (222) **Sensing Biomolecules Using SERS Platforms for Medical Point of Care Applications**; Gerard Cote<sup>1</sup>, Haley Marks<sup>2</sup>, Monika Schechinger<sup>1</sup>, Javier Garza<sup>1</sup>, Brian Walton<sup>1</sup>, Andrea Locke<sup>1</sup>, Dandan Tu<sup>1</sup>, Po-Jung Huang<sup>1</sup>, Jun Kameoka<sup>1</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Wellman Center, Mass General Hospital
- 4:50 PM (223) **Quantitative SERS by “Hot Spot” Normalization**; Haoran Wei<sup>1</sup>, Weinan Leng<sup>1</sup>, Junyeob Song<sup>1</sup>, Marjorie Willner<sup>1</sup>, Linsey Marr<sup>1</sup>, Wei Zhou<sup>1</sup>, Peter Vikesland<sup>1</sup>; <sup>1</sup>Virginia Tech
- 5:10 PM (224) **Surface Enhanced Raman Spectroscopy of Aerosol Particles**; Vasanthy Sivaprakasam<sup>1</sup>, Matthew Hart<sup>1</sup>, Paul Lane<sup>1</sup>, Gary Kushto<sup>1</sup>, Jay Eversole<sup>1</sup>; <sup>1</sup>Naval Reserach Laboratory

## Monday Afternoon, *Carson 4*

### 17RAM11: SPATIALLY OFFSET RAMAN SPECTROSCOPY (SORS)

Organizer and Presider: Pavel Matousek

- 3:50 PM (225) **Longitudinal Monitoring of Murine Bone Quality Using Transcutaneous Raman Spectroscopy**; Andrew Berger<sup>1</sup>, Jason Maher<sup>1</sup>, Marien Ochoa Mendoza<sup>1</sup>, Guanping Feng<sup>1</sup>, Hani Awad<sup>1</sup>; <sup>1</sup>University of Rochester
- 4:10 PM (226) **Frequency Offset Raman Spectroscopy (FORS) for Subsurface Probing of Scattering Media**; Antonio Pifferi<sup>1,2</sup>, Sanathana Konugolu Venkata Sekar<sup>1</sup>, Sara Mosca<sup>1</sup>, Andrea Farina<sup>2</sup>, Fabrizio Martelli<sup>3</sup>, Paola Taroni<sup>1,2</sup>, Gianluca Valentini<sup>1,2</sup>, Rinaldo Cubeddu<sup>1</sup>; <sup>1</sup>Politecnico di Milano; <sup>2</sup>Istituto Fotonica e Nanotecnologie, CNR; <sup>3</sup>Università degli Studi di Firenze
- 4:30 PM (227) **Tracking of Reporter Functionalised Nanoparticles in Tissue Using Handheld Surface Enhanced Spatially Offset Raman Spectroscopy**; Fay Nicolson<sup>1</sup>, Neil Shand<sup>2</sup>, Duncan Graham<sup>1</sup>, Karen Faulds<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>DSTL
- 4:50 PM (228) **Surface Enhanced Spatially Offset Raman Spectroscopy Detection of Neurochemicals Through the Skull**; Bhavva Sharma<sup>1</sup>; <sup>1</sup>University of Tennessee
- 5:10 PM (229) **Deep Raman Spectroscopy: A Novel Platform to Non-Invasively Measure Physical Properties Deep Within Turbid Samples**; Ben Gardner, Nick Stone<sup>1</sup>, Pavel Matousek<sup>2</sup>; <sup>1</sup>University of Exeter; <sup>2</sup>Rutherford Appleton laboratory (STFC)

# TECHNICAL PROGRAM – MONDAY

Orals 3:50 – 5:30 pm

**Monday Afternoon, *Crystal 1***  
**17RSC01: RSC AWARD SESSION**  
 Organizers: Maria Southall, Duncan Graham;  
 Presider: Duncan Graham

- 3:50 PM (230) **Microelectrode Collector-Generator Systems for Biomedical Applications: New Insights from Theory;** Danny O'Hare<sup>1</sup>, C.G. Bell<sup>1</sup>, P. Seelanan<sup>1</sup>; <sup>1</sup>Imperial College London
- 4:10 PM (231) **Construction of DNA-Protein Hybrid Molecules for Bioanalyses;** Eiry Kobatake<sup>1</sup>; <sup>1</sup>Tokyo Institute of Technology
- 4:30 PM (232) **Producing New Sensing Molecules with Gene Technology – An Ascendant Topic;** Xian-En Zhang; <sup>1</sup>National Laboratory of Biomacromolecules & CAS Center for Excellence for Biomacromolecules, Institute of Biophysics, Chinese Academy of Sciences
- 4:50 PM (233) **Metabolic Enzymes as Sensors for Arsenic;** Joanne Santini<sup>1</sup>, Thomas Osborne<sup>1</sup>, Cameron Watson<sup>1</sup>, Thomas Warelow<sup>1,4</sup>, Dimitri Niks<sup>2</sup>, Russ Hille<sup>2</sup>, Graham George<sup>3</sup>, Tony Cass<sup>4</sup>; <sup>1</sup>UCL; <sup>2</sup>UC Riverside; <sup>3</sup>University of Saskatchewan; <sup>4</sup>Imperial College London
- 5:10 PM (234) **Cytochrome P450 Electrodes for Drug Metabolism Screening and Metabolite Biocatalysis;** Gianfranco Gilardi<sup>1</sup>; <sup>1</sup>University of Torino, Italy

**Monday Afternoon, *Nevada 4***  
**17SPSJ02: FRONTIERS OF DEEP- AND FAR-ULTRAVIOLET SPECTROSCOPY II**  
 Organizers: Yukihiro Ozaki, Satoshi Kawata, Yuika Saito, Yusuke Morisawa; Presider: Yukihiro Ozaki

- 3:50 PM (235) **Conformer-Selective Spectroscopy of Flexible Molecules: When IR/UV Double Resonance Techniques Reveal Peptide Conformation;** Michel Mons<sup>1</sup>; <sup>1</sup>Commissariat à l'Energie Atomique, Saclay
- 4:10 PM (236) **Following Electronic and Structural Dynamics with VUV Photoelectron Spectroscopy of Liquids.;** Christopher Arrell<sup>1</sup>, Jose Ojeda<sup>1</sup>, Luca Longetti<sup>1</sup>, Majed Chergui<sup>1</sup>; <sup>1</sup>EPFL
- 4:30 PM (237) **ATR FUV-DUV Spectra of Graphene Polymer Nanocomposites;** Yukihiro Ozaki<sup>1</sup>, Yusuke Morisawa<sup>2</sup>, Krzysztof Beć<sup>1</sup>, Justyna Grabska<sup>1</sup>, Ichiro Tanabe<sup>3</sup>, Harumi Sato<sup>4</sup>; <sup>1</sup>Kwansei Gakuin University; <sup>2</sup>Kinki University; <sup>3</sup>Osaka University; <sup>4</sup>Kobe University
- 4:50 PM (238) **Changes in Electronic States of Organic Solids Observed by Attenuated Total Reflectance Spectroscopy in the Far Ultraviolet region.;** Yusuke Morisawa<sup>1</sup>; <sup>1</sup>Kindai University
- 5:10 PM (239) **Surface Plasmon Resonance Sensors in Far- and Deep-Ultraviolet Regions Using Al Thin Films;** Ichiro Tanabe<sup>1</sup>, Yoshito Tanaka<sup>2</sup>, Koji Watari<sup>3</sup>, Taras Hanulia<sup>4</sup>, Takeyoshi Goto<sup>3</sup>, Wataru Inami<sup>4</sup>, Yoshimasa Kawata<sup>4</sup>, Yukihiro Ozaki<sup>3</sup>; <sup>1</sup>Osaka University; <sup>2</sup>the University of Tokyo; <sup>3</sup>Kwansei Gakuin University; <sup>4</sup>Shizuoka University



**TECHNICAL PROGRAM – TUESDAY**  
**Awards Presentations - 7:50 am; Plenary Lectures - 8:00 am; Tahoe Ballroom**  
**Presider: Karen Esmonde-White**



**8:00 am – Charles Mann Award for Applied Raman Spectroscopy**  
**(250) Mann up, SERS Can Be Useful!; Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde**



**8:30 am – Coblentz Society Craver Award**  
**(251) The Technology Behind Coherent 2D IR Spectroscopy and its Application to Amyloid Diseases; Martin Zanni<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison**

**Orals 9:15 – 10:55 am**

**Tuesday Morning, Crystal 2**

**17ATOM04: LASER ABLATION-ICP-MS I**

Organizers: Alexander Gundlach-Graham, Marcel Burger;  
 Presider: Alexander Gundlach-Graham

- 9:15 AM (252) **Advances in 3D and High-Resolution LA-ICP-MS Bioimaging**; Stijn J. M. Van Malderen<sup>1</sup>, Brecht Laforce<sup>1</sup>, Thibaut Van Acker<sup>1</sup>, Olga Borovinskaya<sup>2</sup>, Laszlo Vincze<sup>1</sup>, Frank Vanhaecke<sup>1</sup>; <sup>1</sup>Ghent University; <sup>2</sup>TOFWERK AG
- 9:35 AM (253) **High Repetition Rate Femtosecond Laser Ablation Inductively Coupled Plasma Time-of-Flight Mass Spectrometry**; Jhanis J. Gonzalez<sup>1,2</sup>; <sup>1</sup>Lawrence Berkeley National Lab.; <sup>2</sup>Applied Spectra, Inc
- 9:55 AM (254) **High-Resolution LA-ICP-TOFMS Imaging: Advances in Instrumentation and Data Analysis**; Alexander Gundlach-Graham<sup>1</sup>, Marcel Burger<sup>1</sup>, Gunnar Schwarz<sup>1</sup>, Jovana Teofilovic<sup>1</sup>, Paulo Garafalo<sup>2</sup>, Bodo Hattendorf<sup>1</sup>, Detlef Günther<sup>1</sup>; <sup>1</sup>ETH Zurich; <sup>2</sup>University of Bologna
- 10:15 AM (255) **ION Dynamics and Ablation Mechanisms of Femtosecond and Nanosecond Laser Produced Plasmas**; Prasoon Diwakar<sup>1</sup>, Ahmed Elseid<sup>1</sup>, Ahmed Hassanein<sup>1</sup>; <sup>1</sup>CMUXE, Purdue University
- 10:35 AM (256) **Atmospheric-Pressure Plasma Assisted Reaction Chemical Ionization: A New Ion Sampling Interface for ICP-MS**; Kaveh Jorabchi<sup>1</sup>, Joseph Lesniewski<sup>1</sup>, William McMahon<sup>1</sup>, Hamid Badiei<sup>2</sup>; <sup>1</sup>Georgetown University; <sup>2</sup>PerkinElmer Inc.

**Tuesday Morning, Crystal 1**

**17AWD04: CHARLES MANN AWARD SYMPOSIUM HONORING DUNCAN GRAHAM**

Organizer and Presider: Duncan Graham

- 9:15 AM (257) **Mann in Shorts - The Future of Pocket Sized Raman**; Neil Shand<sup>1</sup>, Clare Nixon<sup>1</sup>, Terry Clark<sup>1</sup>; <sup>1</sup>Dstl, Porton Down, Salisbury, Wiltshire
- 9:35 AM (258) **3D SERS Imaging**; Yukihiro Ozaki<sup>1</sup>, Sanpon Vantasin<sup>1</sup>; <sup>1</sup>Kwansei Gakuin University
- 9:55 AM (259) **What is that Mann wearing?**; Karen Faulds<sup>1</sup>, Kirsten Gracie<sup>1</sup>, Hayleigh Kearns<sup>1</sup>, Sian Sloan-Dennison<sup>1</sup>, Duncan Graham<sup>1</sup>, Roy Goodacre<sup>2</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>University of Manchester
- 10:15 AM (260) **The Taming of the SERS**; Katsumasa Fujita<sup>1</sup>; <sup>1</sup>Osaka University
- 10:35 AM (261) **The Great Rock and Roll Swindle**; Roy Goodacre<sup>1</sup>, Howbeer Muhamadali, Malama Chisanga; <sup>1</sup>University of Manchester

**Tuesday Morning, Crystal 5**

**17CTP01: ANALYTICAL CHEMISTS EASING WORLD POVERTY**

Organizer and Presider: Rebecca Airmet

- 9:15 AM (262) **3D Patterned Paper Immunoassay Coupled with SERS for the Sensitive Detection of Malaria Biomarkers**; Laura Frame, Karen Faulds<sup>1</sup>, Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde

- 9:35 AM (263) **Mechanical Recycling of Waste Plastic Streams in Zhejiang Province, China**; Peter Summers<sup>1</sup>, Zheng Wang<sup>1</sup>, Fu Gu<sup>1</sup>, Bin Wang<sup>1</sup>, Michael George<sup>1</sup>, Philip Hall<sup>1</sup>; <sup>1</sup>The University of Nottingham Ningbo China
- 9:55 AM (264) **New Strategies for Low-Cost Energy Storage for the Grid: A Size - Exclusion Approach Using Polymer Colloids**; Joaquin Rodriguez-Lopez<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign
- 10:15 AM (265) **InSciEd India: Using K-12 Education to Renew Connectedness to Nature**; Seth Thompson<sup>1</sup>, Christopher Pierret<sup>2</sup>; <sup>1</sup>University of Minnesota; <sup>2</sup>Mayo Clinic
- 10:35 AM (266) **A Compelling Homecoming- Zebrafish as a Tool for High-Quality, Low-Cost Science and Education in India**; Chris Pierret<sup>1</sup>; <sup>1</sup>Mayo Clinic

**Tuesday Morning, Carson 1**

**17IR05: QUANTUM CASCADE LASERS – I**

Organizer: Bernhard Lendl;

Presiders: Bernhard Lendl, Gerard Wysocki

- 9:15 AM (267) **Open-Path, Quantum Cascade Laser Spectroscopy for Atmospheric Measurements in Power-Constrained Platforms**; Mark Zondlo, Levi Golston, Dana Caulton, Da Pan, Kang Sun, David Miller, Lei Tao; <sup>1</sup>Princeton University
- 9:35 AM (268) **Mid-Infrared Process and Emission Monitoring**; Peter Geiser<sup>1</sup>; <sup>1</sup>NEO Monitors AS
- 9:55 AM (269) **Novel Improvements and Applications Using Tunable Infrared Laser Direct Absorption Spectroscopy**; Scott Herndon, Mark Zahniser, David Nelson, Barry McManus, Joanne Shorter, Rob Roscioli, Tara Yacovitch, Christoph Dyroff, Conner Daube; <sup>1</sup>Aerodyne Research, Inc.
- 10:15 AM (270) **Broadband Multi-Heterodyne Spectroscopic Chemical Sensing in the mid-IR and THz with Quantum and Interband Cascade Laser Frequency Combs**; Gerard Wysocki, Jonas Westberg<sup>1</sup>, Lukasz Sterczewski<sup>1</sup>, Link Patrick<sup>1</sup>; <sup>1</sup>Princeton University
- 10:35 AM (271) **Infrared Spectroscopic Method for Uranium Isotopic Analysis in UF<sub>6</sub> Gas**; K. Alicia Strange<sup>1</sup>, Patrick O'Rourke<sup>1</sup>, William Spencer<sup>1</sup>, Nicholas Deroller<sup>1</sup>, Steven Serkiz<sup>1</sup>, Leigh Martin<sup>2</sup>, Darrell Simmons<sup>2</sup>; <sup>1</sup>Savannah River National Laboratory; <sup>2</sup>Oak Ridge National Laboratory

**Tuesday Morning, Nevada 7**

**17MASS01: INTEGRATED MICRO-EXTRACTION PLATFORMS FOR IMPROVED AMBIENT SPECTROMETRY**

Organizer: Yu Xia; Presider: Abraham Badu-Tawiah

- 9:15 AM (272) **Direct Coupling of SPME to Mass Spectrometry**; Janusz Pawliszyn<sup>1,2,3,4</sup>, German Augusto Gomez Rios<sup>1,2,4</sup>; <sup>1</sup>University of Waterloo; <sup>2</sup>Department of Chemistry; <sup>3</sup>Waterloo; <sup>4</sup>Ontario, Canada

## TECHNICAL PROGRAM – TUESDAY

**Orals 9:15 – 10:55 am**

- 9:55 AM (273) **Single-Use Cartridges for Protein and Drug Detection**; Nicholas Manicke<sup>1</sup>, Chengsen Zhang<sup>1</sup>, Brandon Bills<sup>1</sup>, Greta Ren<sup>1</sup>, Trevor Glaros<sup>2</sup>; <sup>1</sup>Indiana University-Purdue University Indianapolis; <sup>2</sup>Edgewood Chemical Biological Center
- 10:15 AM (274) **Improvement in Ambient Mass Spectrometry Sensitivity via Computational Fluid Dynamics**; Jin Young Song<sup>1</sup>, Allen R. White<sup>1</sup>, Brian T. Molnar<sup>3</sup>, Jacob T. Shelley<sup>3</sup>, Gary M. Hieftje<sup>2</sup>; <sup>1</sup>Rose-Hulman Institute of Technology; <sup>2</sup>Indiana University; <sup>3</sup>Rensselaer Polytechnic Institute Chemistry
- 10:35 AM (275) **Direct Extraction and Detection of Analytes from Biofluids Using Functionalized Paper Substrates**; Abraham Badu-Tawiah<sup>1</sup>, Deidre Damon<sup>1</sup>, Tatiana Velez<sup>1</sup>; <sup>1</sup>The Ohio State University

### Tuesday Morning, Nevada 6

#### 17PAT03: INDUSTRIAL APPLICATIONS OF VIBRATIONAL SPECTROSCOPY

Organizers: Xiaoyun (Shawn) Chen, Mark Rickard;  
 Presider: Xiaoyun (Shawn) Chen

- 9:15 AM (276) **TBA**; Mark Kemper, H2Optx, Inc.
- 9:35 AM (277) **Photo-Oxidation Studies of Polyester Coatings**; Allison Pymer<sup>1</sup>, Rebekah Scott<sup>1</sup>, Pam White<sup>1</sup>; <sup>1</sup>The Eastman Chemical Company
- 9:55 AM (278) **Development of Process Analytical Solutions for Real-time Monitoring of Continuous Flow Reactors**; Brian Marquardt<sup>1</sup>, Natasha Hippler<sup>1</sup>, Michael Roberto<sup>2</sup>, Patrick Witham<sup>3</sup>, Kendra Cochran<sup>3</sup>; <sup>1</sup>MarqMetrix Inc.; <sup>2</sup>Infometrix; <sup>3</sup>Applied Physics Lab, UW
- 10:15 AM (279) **Online Analysis of the De-hydration of Glycol Using a Novel Solid State FTIR Spectrometer**; Dan Wood<sup>1</sup>, Jonathon Speed<sup>1</sup>; <sup>1</sup>Keit Spectrometers
- 10:35 AM (280) **Molecular Modeling in In Situ Monitoring Spectra Analysis**; Xianghuai Wang<sup>1</sup>, Ronen Weingarten<sup>1</sup>, Xiaoyun Chen<sup>1</sup>; <sup>1</sup>The Dow Chemical Company

### Tuesday Morning, Carson 2

#### 17PMA04: RAMAN CHARACTERIZATION OF PROTEINS AND BIOLOGICS

Organizer: Anna Luczak; Presider: Ravi Kalyanaraman

- 9:15 AM (281) **Chemometric Modeling and Classification of IgG Monoclonal Antibodies Utilizing Drop Coat Deposition Raman**; Eric Reichard<sup>1</sup>, Cara Fowler<sup>1</sup>, Jeff Denault<sup>1</sup>; <sup>1</sup>Eli Lilly and Company
- 9:35 AM (282) **Monitoring Protein Structural Changes Using Raman Spectroscopy**; Marinella Sandros<sup>1</sup>; <sup>1</sup>HORIBA Scientific; <sup>2</sup>University of Tokyo
- 9:55 AM (283) **Probing the Conformation and Orientation of Disulfide Groups in Proteins and Protein Aggregates by Means of Normal and Polarized Raman Spectroscopy**; Igor Lednev<sup>1</sup>; <sup>1</sup>University at Albany, SUNY
- 10:15 AM (284) **Drop Coat Deposition (DCD) Confocal Raman Spectroscopy: Waking Sleeping Beauty with Coffee Ring for Protein Characterization**; Ravi Kalyanaraman<sup>1</sup>, Jeremy Peters<sup>1</sup>, Anna Luczak<sup>1</sup>, Varsha Ganesh<sup>1</sup>, Eugene Park<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb
- 10:35 AM (285) **Vibrational Sensing of Albumin Glycation: A Route to Facile Detection of Proteins and Biologics**; Ishan Barman<sup>1</sup>; <sup>1</sup>Johns Hopkins University

### Tuesday Morning, Carson 3

#### 17RAM08: BIOMEDICAL RAMAN (CLIRSPEC)

Organizer and Presider: Nick Stone

- 9:15 AM (286) **Rapid In Vivo Raman Spectroscopy for Endoscopic Lung Cancer Detection**; Haishan Zeng<sup>1</sup>; <sup>1</sup>BC Cancer Agency Research Centre
- 9:35 AM (287) **Forward-Adjoint Monte Carlo Modeling of SORS Sampling Depth in Bone and Soft Tissue**; Andrew Berger<sup>1</sup>, Guanping Feng<sup>1</sup>; <sup>1</sup>University of Rochester
- 9:55 AM (288) **Raman Microspectroscopic Analysis of Pancreatic Endocrine Precursor Cells Derived from Human Embryonic Stem Cells**; Michael Blades, H. Georg Schulze<sup>1</sup>, Stanislav O. Konorov<sup>1</sup>, Ali Asadi<sup>1</sup>, Timothy J. Kieffer<sup>1</sup>, James M. Piret<sup>1</sup>, Robin F. B. Turner<sup>1</sup>; <sup>1</sup>University of British Columbia
- 10:15 AM (289) **In vivo Interstitial Raman and Diffuse Optical Spectroscopy to Improve the Safety and Accuracy of Brain Biopsy Procedures**; Frederic Leblond<sup>1,2</sup>, Joannie Desroches<sup>1,2</sup>, Fabien Picot<sup>1,2</sup>, Michael Jermyn<sup>1,3</sup>, Michael Pinto<sup>1</sup>, Sami Obaid<sup>2</sup>, Marie-Christine Guiot<sup>3</sup>, Kevin Petrecca<sup>3</sup>, Brian Wilson<sup>4</sup>; <sup>1</sup>Polytechnique Montreal; <sup>2</sup>Centre Hospitalier de l'Université de Montréal; <sup>3</sup>Montreal Neurological Institute and Hospital; <sup>4</sup>University Health Network/university of Toronto
- 10:35 AM (290) **A SERS-Based Strategy for Multiplexed Detection of Cardiovascular Disease Biomarkers in vitro, ex vivo, and in vivo**; Steven Asiala<sup>1</sup>, Jonathan Noonan<sup>2</sup>, Kirsten Gracie<sup>1</sup>, Gianluca Grassia<sup>2</sup>, Neil MacRitchie<sup>2</sup>, Pasquale Maffia<sup>2</sup>, Paul Garside<sup>2</sup>, Iain McInnes<sup>2</sup>, Karen Faulds<sup>1</sup>, Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>University of Glasgow

### Tuesday Morning, Carson 4

#### 17RAM15: NANO-RAMAN

Organizer and Presider: Andrew Whitley

- 9:15 AM (291) **Stress Measurement Through Tip Enhanced Raman Spectroscopy**; Razvigor Ossikovski<sup>1</sup>, Marc Chaigneau<sup>2</sup>; <sup>1</sup>Ecole Polytechnique - PICM; <sup>2</sup>HORIBA Scientific
- 9:35 AM (292) **Tip-Enhanced Raman Scattering Beyond Chemical Nanoscopy**; Patrick El-Khoury<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory
- 9:55 AM (293) **TERS as an Analytical Probe of Local Physicochemical Properties**; Erin Wood<sup>2,3</sup>, Maruda Shanmugasundaram<sup>1</sup>, Angela Hight Walker<sup>3</sup>, Katherine Tyner<sup>2</sup>; <sup>1</sup>Horiba Scientific; <sup>2</sup>FDA; <sup>3</sup>NIST
- 10:15 AM (294) **TMDCs on Metals: Importance of Nanoscale Heterogeneity for Thin Film Optoelectronic Devices**; Deep Jariwala, Michelle Sherrott<sup>1,2</sup>, Andrey Krayev<sup>3</sup>, Harry Atwater<sup>1,2</sup>; <sup>1</sup>California Institute of Technology; <sup>2</sup>Resnick Sustainability Institute, CalTech; <sup>3</sup>AIST-NT Inc
- 10:35 AM (295) **Tip-Enhanced Nano-Imaging of 2D Materials with Improved Resolution**; Dmitri Voronine<sup>1</sup>; <sup>1</sup>University of South Florida

### Tuesday Morning, Crystal 4

#### 17SPECIAL01: CHEMISTRY IN ART AND ARCHEOLOGY

Organizer and Presider: Mary Kate Donais

- 9:15 AM (296) **Non-Invasive Spectroscopy for the Analysis of Cultural Materials in the Field**; Christian Fischer<sup>1</sup>; <sup>1</sup>University of California Los Angeles

## TECHNICAL PROGRAM – TUESDAY

Orals 9:15 – 10:55 am

Poster Sessions and Coffee Breaks

11:00 am – 12:00 pm & 3:10 – 3:50 pm, *SciX Exhibit Hall*

9:55 AM (297) **The Kenya Red Ochre Chemistry (KROC)**  
**Database: Integrating Geochemistry and Ethnography for a New Approach to Archaeometric Provenience Studies;** Andrew Zipkin<sup>1</sup>, Craig Lundstrom<sup>1</sup>, Stanley Ambrose<sup>1</sup>, Gideon Bartov<sup>1</sup>, Alyssa Dwyer<sup>1</sup>, Alex Taylor<sup>1</sup>, Mercy Gakii<sup>2</sup>;  
<sup>1</sup>University of Illinois at Urbana-Champaign; <sup>2</sup>National Museums of Kenya

10:15 AM (298) **Identification of Historic Carbonaceous Media on Drawings Using Raman Microscopy and Macroscopic X-Ray Fluorescence Scanning;** Nathan Daly<sup>1</sup>, Michelle Sullivan<sup>2</sup>, Lynn Lee<sup>1</sup>, Karen Trentelman<sup>1</sup>; <sup>1</sup>Getty Conservation Institute; <sup>2</sup>J. Paul Getty Museum

10:35 AM (299) **Effects of Sample Preparation on XRF Measurements of Ancient Mortars;** Mary Kate Donais<sup>1</sup>, Mina Alrais<sup>1</sup>, David B. George<sup>2</sup>, Eric Smith<sup>3</sup>;  
<sup>1</sup>Saint Anselm College, Dept of Chemistry; <sup>2</sup>Saint Anselm College, Dept of Classics; <sup>3</sup>SPEX SamplePrep

### Tuesday Morning, Nevada 5 17SPR01: MULTIMETALLIC PLASMONIC NANOPARTICLES

Organizer: Emilie Ringe; Presider: Amanda Haes

9:15 AM (300) **Tuning Chiral and Mechanical Properties in Assemblies of Plasmonic Nanocrystals;** Vivian Ferry<sup>1</sup>; <sup>1</sup>University of Minnesota - Twin Cities

9:35 AM (301) **Optical Devices Based on Plasmonic Nanoparticles;** Mahmoud Mahmoud; <sup>1</sup>University of Texas at San Antonio

9:55 AM (302) **Bimetallic Nanostructures: Decoration and Alloying Effects on Plasmonic Properties;** Emilie Ringe<sup>1,2</sup>, Josee Daniel<sup>3</sup>, Dayne Swearer<sup>1</sup>, Lauren McCarthy<sup>1</sup>, Anjali Kumar<sup>1</sup>, Sadegh Yazdi<sup>1</sup>, Denis Boudreau<sup>3</sup>; <sup>1</sup>Rice University; <sup>2</sup>Cambridge University; <sup>3</sup>Universite Laval

10:15 AM (303) **Plasmonic Nanoparticles: Synthesis and Catalytic Application;** Supriya Atta<sup>1</sup>, Laura Fabris<sup>1</sup>, Ashley Pennington<sup>1</sup>, Fuat E. Celik<sup>1</sup>; <sup>1</sup>Rutgers University, New Brunswick

10:35 AM (304) **Synthesis of Bimetallic Hollow AgM Nanoparticles, Structure and Composition Analysis;** Josee R. Daniel<sup>1</sup>, Sadegh Yazdi<sup>2</sup>, Lauren McCarthy<sup>2</sup>, Emilie Ringe<sup>2</sup>, Denis Boudreau<sup>1</sup>; <sup>1</sup>Université Laval; <sup>2</sup>Rice University

**All Tuesday posters should be put up between 9:00 – 10:45 am and removed by 4:30 pm**

### 17TPAES: Tuesday Posters - Electrophoresis

#### Poster Board #1

(305) **Capillary Electrophoresis-Based Enzyme Assay of Acetyl Coenzyme A Carboxylase;** Thu Nguyen<sup>1</sup>, Alexandra Evans<sup>1</sup>, Grover Waldrop<sup>1</sup>, Samuel Douglass Gilman<sup>1</sup>; <sup>1</sup>Louisiana State University

#### Poster Board #2

(306) **Sequence Based Separation of DNA Using Microfluidic Chip Electrophoresis;** Wyatt Stevens<sup>1</sup>, Jia Zhao<sup>1</sup>, Linda McGown<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute

#### Poster Board #3

(307) **Capillary Electrophoresis of Intact Erythrocytes for Anti-Doping Analysis;** Christopher Harrison<sup>1</sup>, Jessica Torres<sup>1</sup>, Thirada Kingphua<sup>1</sup>, Shane

Alexis Apostol<sup>1</sup>, Sangho Yun<sup>1</sup>; <sup>1</sup>San Diego State University

#### Poster Board #4

(308) **Assessing Hydrophobicity of Antibody-Drug Conjugate Payload Molecules Utilizing Lipid-Surfactant Mixtures;** Suvi-Katriina Ruokonen<sup>1</sup>, Marina Redon<sup>1</sup>, Emilio Gonzalez-Jalonen<sup>1</sup>, Filip Ekholm<sup>1</sup>, Susanne Kristina Wiedmer; <sup>1</sup>University of Helsinki, Department of Chemistry

#### Poster Board #5

(309) **Capillary Electrophoresis for Quantitative Determination of Ionic Liquids and their Degradation Products;** Susanne Wiedmer<sup>1</sup>, Joanna Witos<sup>1</sup>, Antti Rantamäki<sup>1</sup>, Jesper Långbacka<sup>1</sup>; <sup>1</sup>Department of Chemistry, University of Helsinki

#### Poster Board #6

(310) **A Method for Fabricating a Through-Microhole by Using a Near Ultra Violet Femtosecond Laser;** Shoichi Kubodera, Masahiko Shiraishi, Kazuhiro Watanabe; <sup>1</sup>Soka University

#### Poster Board #7

(311) **A Deterministic Ratchet for Sub-Micrometer Particle Separation;** Dai Hyun Kim<sup>1</sup>, Jinghui Luo<sup>1</sup>, Edgar Arriaga<sup>2</sup>, Alexandra Ros<sup>1</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>University of Minnesota

#### Poster Board #8

(312) **Neural Stem and Progenitor Cells Separation Based on Insulator-Based Direct Current Dielectrophoresis;** Yameng Liu<sup>1</sup>, Mark Hayes<sup>1</sup>; <sup>1</sup>Arizona State University

### 17TPARCH: Tuesday Posters - Archaeology

#### Poster Board #9

(313) **Spectroscopic Analysis of the Maya Blue Pigment;** Jeremiah Lopez<sup>1</sup>, Jorge Lopez<sup>1</sup>, Carlos Diaz-Moreno<sup>1</sup>; <sup>1</sup>University of Texas at El Paso

#### Poster Board #10

(314) **FTIR Microscopic Analysis of Plant and Animal Tissue Residues on Stone Tools;** Bing Luo<sup>1</sup>, Gilliane Monnier<sup>1</sup>, Ellery Frahm<sup>1,2</sup>, Kele Missal<sup>1</sup>; <sup>1</sup>University of Minnesota; <sup>2</sup>Yale University

### 17TPBIM: Tuesday Posters - Biomedical and Bioanalytical Sciences

#### Poster Board #11

(315) **Potential G-Quadruplex Forming Aptamers Using a Genome-Inspired Reverse Selection Approach;** Kathleen Morrissey<sup>1</sup>, Linda McGown<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute

#### Poster Board #12

(316) **Biophysical Characterization of Antibiotic Resistance;** Shannon Huey Hilton<sup>1</sup>, Mark A. Hayes<sup>1</sup>; <sup>1</sup>Arizona State University

#### Poster Board #13

(317) **Optimization of Cold Atmospheric Plasma and Electroporation for Cancer Cells;** Prasoon Diwakar<sup>1</sup>, Arianna Avellan<sup>1,2</sup>, Liesl Krause<sup>1,3</sup>, Rohil Jain<sup>4</sup>, Cagri Savran<sup>4</sup>, Tatyana Sizyuk<sup>1</sup>, Ahmed Hassanein<sup>1</sup>; <sup>1</sup>CMUXE, Nuclear Engineering, Purdue University; <sup>2</sup>University of Maryland, College Park; <sup>3</sup>Biomedical Engineering, Purdue University; <sup>4</sup>Birck Nanotechnology Center, Purdue University



## TECHNICAL PROGRAM – TUESDAY

**Poster Sessions 11:00 am – 12:00 pm & 3:10 – 3:50 pm, SciX Exhibit Hall**

### Poster Board #14

(318) **31P Magnetic Resonance Spectroscopy for In Vivo Illness Analysis;** Liesl Krause<sup>1</sup>, Frederick Damen<sup>1</sup>, Craig Goergen<sup>1</sup>, Joseph Rispoli<sup>1,2</sup>, <sup>1</sup>Weldon School of Biomedical Engineering, Purdue; <sup>2</sup>School of Electrical & Computer Engineering, Purdue

### Poster Board #15

(319) **Correlation Between Ionic Liquid Cytotoxicity and Ionic Liquid-Liposome Interactions;** Suvi-Katriina Ruokonen<sup>1</sup>, Alexandra Robciuc<sup>2</sup>, Joanna Witos<sup>2</sup>, Alistair King<sup>1</sup>, Sami Hietala<sup>1</sup>, Susanne Wiedmer<sup>1</sup>; <sup>1</sup>University of Helsinki, Department of Chemistry; <sup>2</sup>Helsinki University Hospital, Ophthalmology

### Poster Board #16

(320) **A Temporal Study of Cell Death Signaling Responses to Cold Atmospheric Plasma and Electroporation in Human Cancer Cells;** Danielle Krug<sup>1</sup>, Prasoon Diwakar<sup>1</sup>, Ahmed Hassanein<sup>1</sup>; <sup>1</sup>CMUXE, Nuclear Engineering, Purdue University

### Poster Board #17

(321) **Investigating Cytotoxicity of Ionic Liquids Using Mammalian and Bacterial Cells;** Antti Rantamäki<sup>1</sup>, Suvi-Katriina Ruokonen<sup>1</sup>, Alexandra Robciuc<sup>1</sup>, Corinna Sanwald<sup>2</sup>, Susanne Wiedmer<sup>1</sup>; <sup>1</sup>University of Helsinki; <sup>2</sup>University of Tübingen

### Poster Board #18

(322) **Drug Monitoring and Toxicology: Quantification of Antifungal Drug Voriconazole in Human Plasma and Serum by High-Performance Liquid Chromatography with Fluorescence Detection;** Peter Tang<sup>1,2</sup>; <sup>1</sup>Cincinnati Children; <sup>2</sup>University of Cincinnati College of Medicine

### Poster Board #19

(323) **A Tale of Two Local Sites: Simultaneous Probing of Two Locations in MLCK Upon Binding;** Natalie Fetto<sup>1</sup>, Ian Wallace<sup>1</sup>, Matthew Tucker<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### Poster Board #20

(324) **Confocal Raman Microscopy of Silica- and Cyano-Supported Phospholipid Bilayers within Porous Chromatographic Supports;** David Bryce<sup>1</sup>, Jay Kitt<sup>1</sup>, Joel Harris<sup>1</sup>; <sup>1</sup>University of Utah

### Poster Board #21

(325) **Investigating the Competence Stimulating Peptide-Induced Quorum Sensing Circuit in Streptococcus mutans;** Chowdhury Raihan Bikash<sup>1</sup>, Sally R. Hamry<sup>1</sup>, Yftah Tal-Gan<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### Poster Board #22

(326) **Genome Inspired Approach to Aptamer Discovery Using Genome-Wide-High-Resolution ChIP Techniques;** Casey Fong, Linda McGown<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute

### Poster Board #23

(327) **Analyzing the Effect of Simulated Heart Attacks on the Protein Profile and Structure of a Mouse Heart's Left Ventricle Through the Use of Matrix Assisted Laser Desorption/Ionization Mass Spectrometry Imaging;** Emma Chowdhury<sup>1</sup>; <sup>1</sup>Bruker Daltonics

### Poster Board #24

(328) **Developing a Non-Invasive Spectroscopic Technique for Detecting Liver Damage;** Katherine Ember<sup>1,4</sup>, Gabriel Onsicu<sup>2</sup>, Fiona Hunt<sup>2</sup>, Hannah

Johnston<sup>1</sup>, George Georges<sup>3</sup>, John Hallett<sup>1,2</sup>, Karen Faulds<sup>4</sup>, Stuart Forbes<sup>1</sup>, Colin Campbell<sup>1</sup>, Lauren Jamieson<sup>4</sup>; <sup>1</sup>University of Edinburgh; <sup>2</sup>Royal Infirmary of Edinburgh; <sup>3</sup>Princeton University; <sup>4</sup>University of Strathclyde

### Poster Board #25

(329) **Magnetic Resonance Spectroscopy: A Tool for Assessing Concussion Injuries;** Nicole Vike<sup>1</sup>, Jonathan Tang<sup>1</sup>, Thomas Talavage<sup>1</sup>, Riyi Shi<sup>1</sup>, Joseph Rispoli<sup>1</sup>; <sup>1</sup>Purdue University

### Poster Board #26

(330) **Investigating the Potential of Silver Hydroxyapatite as an Implant Coating for Preventing Prosthetic Joint Infection;** Luke DeHart<sup>1</sup>, Austin Dinkins<sup>1</sup>, Mary Tecklenburg<sup>1</sup>; <sup>1</sup>Central Michigan University

### Poster Board #27

(331) **Structure-Activity Relationship Studies of the Competence Stimulating Peptide (CSP) Signal Utilized by Streptococci Species;** Sally Hamry<sup>1</sup>, Chowdhury Raihan Bikash<sup>1</sup>, Yifang Yang<sup>1</sup>, Bimal Koirala<sup>1</sup>, Lucia Sanchez<sup>1</sup>, Naiya Phillips<sup>1</sup>, Yftah Tal-Gan<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### Poster Board #28

(332) **Bacterial Identification in ex vivo Human Fetal Membrane Biofilms Using Raman Microspectroscopy;** Oscar Ayala<sup>1,2</sup>, Ryan Doster<sup>3</sup>, David Aronoff<sup>3</sup>, Jennifer Gaddy<sup>3,4</sup>, Anita Mahadevan-Jansen<sup>1,2</sup>; <sup>1</sup>Vanderbilt Biophotonics Center; <sup>2</sup>Vanderbilt University; <sup>3</sup>Vanderbilt University Medical Center; <sup>4</sup>Tennessee Valley Healthcare Systems

### Poster Board #29

(333) **Spectroscopic Investigation of Early Tissue Pathology in Combat-Wounded Patients Diagnosed with Heterotopic Ossification;** Krystine Hill<sup>1,2</sup>, Katherine E. Cilwa<sup>1</sup>; <sup>1</sup>Naval Medical Research Center; <sup>2</sup>Stevenson University

### Poster Board #30

(334) **Dried Blood Spot and Microwave-Induced Combustion: The Perfect Combination for Iodine Determination in Human Blood;** Fabio Duarte, Samuel Waechter<sup>1,2</sup>, Paula Dalla Vecchia<sup>1,2</sup>, Karine Reinke<sup>1,2</sup>, Erico Flores<sup>1,2</sup>; <sup>1</sup>Universidade Federal de Santa Maria; <sup>2</sup>Chemistry Department

### Poster Board #31

(335) **Using Attenuated Total Reflectance Infrared Spectroscopy to Monitor Changes in Protein-Substrate Binding of Human Liver Pyruvate Kinase;** Reid Brenner<sup>1</sup>, Charles Wurrey<sup>1</sup>, Aron Fenton<sup>2</sup>; <sup>1</sup>University of Missouri-Kansas City; <sup>2</sup>The University of Kansas Medical Center

### Poster Board #32

(336) **Raman Spectroscopy for Monitoring Cervical Remodeling in Pregnant Women in vivo;** Christine M. O'Brien<sup>1,2</sup>, Elizabeth Vargis<sup>1</sup>, Amy Rudin<sup>1</sup>, James C. Slaughter<sup>3</sup>, Kelly A. Bennett<sup>3</sup>, Jeff Reese<sup>3</sup>, Anita Mahadevan-Jansen<sup>1,2</sup>; <sup>1</sup>Vanderbilt University; <sup>2</sup>Biophotonics Center, Vanderbilt University; <sup>3</sup>Vanderbilt University Medical Center

### Poster Board #33

(337) **Selectively Trapping Residual Vancomycin with Peptide Analogs to Prevent Colonic Bacterial Stress;** Brittany Russ<sup>1</sup>, Ryan Mull<sup>1</sup>, Yftah Tal-Gan<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

## TECHNICAL PROGRAM – TUESDAY

Poster Sessions 11:00 am – 12:00 pm & 3:10 – 3:50 pm, *SciX Exhibit Hall*

What's Hot Vendor Presentations ♦ Orals 1:30 – 3:10 pm

### Poster Board #34

(338) **Chemical Trapping of Vancomycin: A Method to Attenuate the Selection of Vancomycin Resistance in Enterococcus**; Ryan Mull<sup>1</sup>, Brittany Russ<sup>1</sup>, Yftah Tal-Gan<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### Poster Board #35

(339) **Investigate Photo-Induced Skin Damages and Skin Protection Provided by Different UV Filters Using FTIR Spectroscopy Analysis**; Samuel Gourion-Arsiquaud<sup>1</sup>, Arianna Cozzi<sup>1</sup>; <sup>1</sup>TRI Princeton

### Poster Board #36

(340) **Raman Spectroscopy and Neural Network to Detect the Glucose Level**; Jorge Castro-Ramos<sup>1</sup>, Naara González-Viveros<sup>1</sup>, Pilar Gómez-Gil<sup>1</sup>, Fabián Villa-Manríquez<sup>1</sup>, Francisco Gutiérrez-Delgado<sup>2</sup>; <sup>1</sup>Instituto Nacional de Astrofísica Óptica y Electro; <sup>2</sup>CEPREC, Centro para la prevención del cáncer, AC

### Poster Board #37

(341) **A Systematic Investigation of the Structure-Activity Relationships between GBAP and the fsr Quorum Sensing Circuit in Enterococcus Faecalis**; Brooke Gantman<sup>1</sup>, Dominic McBrayer<sup>1</sup>, Crissey Cameron<sup>1</sup>, Yftah Tal-Gan<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### 17TPLIBS: Tuesday Posters - NASLIBS

### Poster Board #38

(342) **Handheld Laser-Induced Breakdown Spectroscopy (LIBS) for Field Archaeology**; Luke DOuglass<sup>1</sup>, Mary Kate Donais<sup>1</sup>, David George<sup>1</sup>; <sup>1</sup>Saint Anselm College

### Poster Board #39

(343) **Detection of Anti-Toxin Heavy-Metal Tagged Antibodies Using Laser-Induced Breakdown Spectroscopy (LIBS)**; Carmen Gondhalekar, Eva Biela<sup>1</sup>, Bartek Rajwa<sup>1</sup>, Euiwon Bae<sup>1</sup>, Valery Patsekina<sup>1</sup>, Jennifer Sturgis<sup>1</sup>, Huisung Kim<sup>1</sup>, Iyil-Joon Doh<sup>1</sup>, Larry Stanker<sup>1,2</sup>, Paul Robinson<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>USDA-ARS, California

### Poster Board #40

(344) **Bacterial Mounting and Concentration Techniques to Translate Laser-Induced Breakdown Spectroscopy into a Clinical Setting**; Alexandra Paulick<sup>1</sup>, Naila Rahman<sup>1</sup>, Steven Rehse<sup>1</sup>; <sup>1</sup>University of Windsor

### Poster Board #41

(345) **Laser-Induced Breakdown Spectroscopy for Elemental Analysis of the Thyroid**; Condon Lau<sup>1</sup>, Irfan Ahmed<sup>1</sup>; <sup>1</sup>The City University of Hong Kong

### Poster Board #42

(346) **Metal Ablation by Laser Irradiation Under Different Ambient Conditions**; Ahmed Elsieid<sup>1</sup>, Paysoon Dieffenbach<sup>1</sup>, Prasoon Diwakar<sup>1</sup>, Ahmed Hassanein<sup>1</sup>; <sup>1</sup>Purdue University

### Poster Board #43

(347) **Characterization and Classification of Pharmaceutical Tablet Coating by Laser-Induced Breakdown Spectroscopy (LIBS)**; Lanfeng Zou<sup>1</sup>, Xiaodong Bu<sup>1</sup>, Brittany Kassim<sup>1</sup>, Yun Mao<sup>1</sup>; <sup>1</sup>Merck & Co., Inc.

### Poster Board #44

(348) **Latest Advances in Tandem LA – LIBS Instrumentation: Leading the Innovation in Laser Ablation Chemical Analysis with Simultaneous LIBS and LA-ICP-MS**; Chunyi Liu<sup>1</sup>; <sup>1</sup>Applied Spectra, Inc.

### Poster Board #45

(349) **Ultrafast LIBS for 3D Chemical Imaging of Li-Ion Batteries**; Huaming Hou<sup>1,2</sup>, Rick Russo<sup>1</sup>, Vassilia Zorba<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory; <sup>2</sup>The Peac Institute of Multiscale Sciences

**11:40 AM – 1:10 PM**

**WHAT'S HOT VENDOR PRESENTATIONS, Exhibit Hall**

Presider: Brian Dable, *Arete Associates*

Free lunch in exhibit hall for all conferees, ticket required

- 11:40 **BaySpec** “High Performance Portable Mass Spectrometers for Rapid Screening of Trace Residues and Novel Aerial Hyperspectral Imagers for the Full Spectral Range of 400-1700nm”
- 11:50 **Thermo Fisher Scientific**
- 12:00 **Ocean Optics**
- 12:10 **HORIBA Scientific** “Raman Imaging: Finally...Speed & Clarity You've Been Waiting For”
- 12:20 **Kaiser Optical Systems** “Using Fiber-Optic Probes in Raman Spectroscopy to Achieve Representative Sampling in Batch or Continuous Processes”
- 12:30 **Innovative Photonic Solutions** “Lasers and Technologies Enabling Next Generation Raman Spectroscopy”
- 12:40 **Renishaw**
- 12:50 **Princeton Instruments** “Easy, Aberration-free Spectroscopy with the FERGIE Spectroscopy System”
- 1:00 **Ibsen Photonics** “Ultra-compact OEM Spectrometers for LIBS and Raman”

**Tuesday Afternoon, Crystal 4**

**17AES01: MICRO-SCALE ELECTROPORATION AND ELECTROKINETIC STUDY OF CELLS AND BIOMOLECULES**

Organizers and Presiders: Mei He, Mark Hayes

- 1:30 PM (350) **Microfluidic Electroporation for Gene Delivery and Cellular Analysis**; Chang Lu<sup>1</sup>; <sup>1</sup>Virginia Tech
- 1:50 PM (351) **High Throughput Microfluidic Genetic Transformation**; Paulo Garcia<sup>1</sup>, Rameech McCormack<sup>1</sup>, Cullen Buie<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology
- 2:10 PM (352) **Tunable Insulator-Based Dielectrophoresis for Biomolecule and Bioparticle Pre-Concentration and Separation**; Alexandra Ros<sup>1,2</sup>, Daihyun Kim<sup>1,2</sup>; <sup>1</sup>Arizona State University; <sup>2</sup>The Biodesign Institute
- 2:30 PM (353) **Condensed Phase Separation Science and Microfluidics**; Mark Hayes<sup>1</sup>; <sup>1</sup>Arizona State University
- 2:50 PM (354) **Microfluidic Analysis of 3D-Culture Derived Extracellular Vesicles**; Mei He<sup>1</sup>, John Sibbitt<sup>1</sup>, Zhao Zheng<sup>1</sup>; <sup>1</sup>Kansas State University

**Tuesday Afternoon, Crystal 2**

**17ATOM05: EXCITATION AND IONIZATION TECHNIQUES FOR ATOMIC AND MOLECULAR SPECTROSCOPY**

Organizer and Presider: Joachim Franzke

- 1:30 PM (355) **Spatio-Temporal Detection of Arsenic in a Dielectric Barrier Discharge by Optical Emission Spectroscopy**; Sebastian Burhenn<sup>1</sup>, Jan Kratzer<sup>2</sup>, Joachim Franzke<sup>1</sup>; <sup>1</sup>ISAS; <sup>2</sup>Analytical Chemistry CAS



## TECHNICAL PROGRAM – TUESDAY

**Orals 1:30 – 3:10 pm**

1:50 PM (356) **Comparison of LTP-, FAPA-, and LA-hFAPA-MS for Direct Surface Analysis;** Christopher Kuhlmann<sup>1</sup>, Jacob T. Shelley<sup>2</sup>, Carsten Engelhard<sup>1</sup>; <sup>1</sup>University of Siegen; <sup>2</sup>Rensselaer Polytechnic Institute

2:10 PM (357) **Recent Advances in Solution-Cathode Glow Discharge Mass Spectrometry;** Andrew Schwartz<sup>1</sup>, Jacob Shelley<sup>2</sup>, Courtney Walton<sup>2</sup>, Kelsey Williams<sup>1</sup>, Gary Hieftje<sup>3</sup>; <sup>1</sup>State University of New York at Buffalo; <sup>2</sup>Rensselaer Polytechnic Institute; <sup>3</sup>Indiana University

2:30 PM (358) **Filamentary Discharges in DBDI Lead to Soft Ionization for Mass Spectrometry;** Luzia Gyr<sup>1</sup>, Felix David Klute<sup>2</sup>, Joachim Franzke<sup>2</sup>, Renato Zenobi<sup>1</sup>; <sup>1</sup>ETH Zurich; <sup>2</sup>Leibniz-Institut für Analy. Wissenschaften - ISAS

2:50 PM (359) **Development of an Ambient Air Micro Discharge for soft Ionisation – The Flexible Tube Micro Plasma Ionisation (FTμPI);** Sebastian Brandt<sup>1</sup>, Felix David Klute<sup>1</sup>, Alexander Schütz<sup>1</sup>, Carolin Drees<sup>1</sup>, Wolfgang Vautz<sup>1</sup>, Joachim Franzke<sup>1</sup>; <sup>1</sup>ISAS

### Tuesday Afternoon, *Crystal 1*

#### 17AWD05: COBLENTZ CRAVER AWARD SYMPOSIUM HONORING MARTIN ZANNI

Organizer: Martin Zanni; Presider: Mark Drury

1:30 PM (360) **1D- and 2D-Time-resolved Spectroscopic Studies in Conventional and Supercritical Fluids;** Mike George<sup>1</sup>; <sup>1</sup>University of Nottingham

1:50 PM (361) **Probing the Instantaneous Ion Binding Configurations K+ Ion Channel Selectivity Filter Using 2D IR Spectroscopy;** Huong Kratochvil<sup>1</sup>, Martin Zanni<sup>1</sup>, Alvin Annen<sup>3</sup>, Kim Matulef<sup>3</sup>, Jared Ostmeyer<sup>2</sup>, Eduardo Perozo<sup>2</sup>, Benoit Roux<sup>2</sup>, Francis Valiaveetil<sup>3</sup>, Martin Zanni<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

2:10 PM (362) **2D IR Vibrational Probe Pairs for Determining Structure and Dynamics in Biomolecules;** Matthew Tucker<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

2:30 PM (363) **Probing Systems at the Interface of Biology and Nanotechnology with 2D IR Spectroscopy;** Lauren Buchanan<sup>1</sup>; <sup>1</sup>Vanderbilt University

2:50 PM (364) **Direct Charge Transfer across Organic Semiconductor and Metal Interfaces;** Wei Xiong<sup>1</sup>, Bo Xiang<sup>1</sup>, Yingmin Li<sup>1</sup>, Huy Pham<sup>1</sup>, Francesco Paesani<sup>1</sup>; <sup>1</sup>University of California - San Diego

### Tuesday Afternoon, *Crystal 5*

#### 17CTP02: DIVERSITY, EQUITY, AND INCLUSION IN ANALYTICAL CHEMISTRY

Organizers and Presiders: Anna Donnell, Ingeborg Ipping Petterson

1:30 PM (365) **The Chemistry Diversity Initiative: A Graduate Student Program for Success at Purdue University;** Jean Chmielewski, Colby Adolph<sup>1</sup>, Stella Betancourt<sup>1</sup>, Reena Blade<sup>1</sup>, Chris Pulliam<sup>1</sup>; <sup>1</sup>Purdue University

1:50 PM (366) **Retaining Underrepresented Groups at Both the Undergraduate and Graduate Level;** Susan Olesik, Terry Gustafson<sup>1</sup>, Thomas Magliery<sup>1</sup>; <sup>1</sup>The Ohio State University

2:10 PM (367) **Global Initiatives for Conducting Medicine Anti-Counterfeiting Research: Working with multidisciplinary Backgrounds Worldwide;** Sulaf Assi<sup>1</sup>; <sup>1</sup>Bournemouth University

2:30 PM (368) **Diversity, Equity, and Inclusion in Analytical Chemistry;** Megan Schmale<sup>1</sup>; <sup>1</sup>University of Cincinnati

### Tuesday Afternoon, *Carson 1*

#### 17IR06: QUANTUM CASCADE LASERS - II

Organizer: Bernhard Lendl; Presider: Bernhard Lendl, Gerard Wysocki

1:30 PM (369) **Label-Free Tissue Classification by QCL Based IR-Imaging;** Klaus Gerwert<sup>1</sup>; <sup>1</sup>Ruhr-University Bochum

1:50 PM (370) **Quantum Cascade Laser (QCL) Hyperspectral Imaging Applied to Live Cell Analysis;** Bayden Wood<sup>1</sup>, Dale Christensen<sup>1</sup>, Ellen Lowry<sup>1</sup>, Philip Heraud<sup>1</sup>, David Perez-Guaita<sup>1</sup>; <sup>1</sup>Monash University

2:10 PM (371) **On-Chip Quantum Cascade Laser/Detector System for Remote Gas Sensing;** Rolf Szedlak<sup>1</sup>, Andreas Harrer<sup>1</sup>, Benedikt Schwarz<sup>1</sup>, Martin Holzbauer<sup>1</sup>, Johannes Paul Waclawek<sup>2</sup>, Hermann Detz<sup>3</sup>, Aaron Maxwell Andrews<sup>1</sup>, Werner Schrenk<sup>1</sup>, Bernhard Lendl<sup>2</sup>, Gottfried Strasser<sup>1</sup>; <sup>1</sup>Institute of Solid State Electronics, TU Wien; <sup>2</sup>Institute of Chemical Technologies, TU Wien; <sup>3</sup>Austrian Academy of Sciences

2:30 PM (372) **Time-Resolved Spectroscopy of Biological Samples Using QCL Dual-Comb Technique;** Markus Geiser<sup>1,2</sup>, Markus Mangold<sup>1</sup>, Pitt Allmendinger<sup>1</sup>, Andreas Hugi<sup>1</sup>, Filipp Kapsalidis<sup>2</sup>, Pierre Jouy<sup>2</sup>, Jérôme Faist<sup>2</sup>; <sup>1</sup>IRsweep AG, Auguste-Piccard-Hof 1, 8093 Zurich, CH; <sup>2</sup>ETH Zurich, IQE, Auguste-Piccard-Hof 1

2:50 PM (373) **Field-Resolved Spectroscopy in the Mid-Infrared Region: A Highly Sensitive Tool for Molecular Fingerprinting;** Marinus Huber<sup>1,2</sup>, Wolfgang Schweinberger<sup>2,3</sup>, Liudmila Voronina<sup>1,2</sup>, Syed Ali Hussain<sup>2</sup>, Christina Hofer<sup>1,2</sup>, Michael Trubetskov<sup>1</sup>, Mihaela Zigman<sup>1,2</sup>, Ferenc Krausz<sup>1,2</sup>, Ioachim Pupeza<sup>1,2</sup>; <sup>1</sup>Max-Planck-Institut für Quantenoptik; <sup>2</sup>Ludwig-Maximilians-Universität München; <sup>3</sup>King Saud University

### Tuesday Afternoon, *Crystal 3*

#### 17LIBS05: NALIBS: ELEMENTAL MAPPING BY LIBS

Organizer and Presider: Nouredine Melikechi

1:30 PM (374) **Elemental Mapping of Teeth for Anthropological Studies;** Matthieu Baudalet<sup>1</sup>, Mauro Martinez<sup>1</sup>, John Schultz<sup>2</sup>, Michelle Hawkins<sup>2</sup>, Lana Williams<sup>2</sup>, Tosha Dupras<sup>2</sup>; <sup>1</sup>NCFS - University of Central Florida; <sup>2</sup>Anthropology department, UCF

2:10 PM (375) **Digitalization of Drill Core Samples for Mining Exploration Using LIBS;** Francois Doucet<sup>1</sup>, Lutfu Ozcan<sup>1</sup>, Altan Muftuoglu<sup>1</sup>, Dominique Doucet<sup>2</sup>; <sup>1</sup>ELEMISSION Inc.; <sup>2</sup>Sirios Ressource Inc.

2:30 PM (376) **Mapping Analyte Distributions in Surrogate Nuclear Melt Glass Using Laser-Induced Breakdown Spectroscopy and Micro X-Ray Fluorescence;** Michael Shattan<sup>1,4</sup>, Ashley Stowe<sup>2</sup>, Kathryn McIntosh<sup>3</sup>, John Auxier II<sup>1,4</sup>, Christian Parigger<sup>1</sup>, Howard Hall<sup>1,4</sup>; <sup>1</sup>University of Tennessee; <sup>2</sup>Y12 Nuclear Security Site; <sup>3</sup>Los Alamos National Laboratory; <sup>4</sup>Institute for Nuclear Security

2:50 PM (377) **Laser-Induced Breakdown Spectroscopy in Analysis of Elemental Distributions;** Saara Kaski<sup>1</sup>, Sari Romppanen<sup>1</sup>, Heikki Häkkinen<sup>1</sup>; <sup>1</sup>University of Jyväskylä

## TECHNICAL PROGRAM – TUESDAY

**Orals 1:30 – 3:10 pm**

**Tuesday Afternoon, Nevada 7**

### 17MASS02: RECENT DEVELOPMENT IN SINGLE CELL MASS SPECTROMETRY ANALYSIS

Organizer and Presider: Zhibo Yang

- 1:30 PM (378) **Precision Nanopipetting for Single Cell MALDI**; Kermit Murray<sup>1</sup>, Fan Cao<sup>1</sup>, Fabrizio Donnarumma<sup>1</sup>, Randy Duran<sup>1</sup>, Jean-Baptiste Decombe<sup>1</sup>; <sup>1</sup>Louisiana State University
- 1:50 PM (379) **Single-cell Mass Spectrometry: From Subpopulations to Subtypes**; Thanh Do<sup>1</sup>, Troy Comi<sup>1</sup>, Stanislav Rubakhin<sup>1</sup>, Sage Dunham<sup>1</sup>, Jonathan Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign
- 2:10 PM (380) **Cell-by-Cell Metabolic Analysis of the *Xenopus Laevis* Embryo**; Erika Portero<sup>1</sup>, Rosemary Onjiko<sup>1</sup>, Sally Moody<sup>1</sup>, Peter Nemes<sup>1</sup>; <sup>1</sup>The George Washington University
- 2:30 PM (381) **Quantification of Ant-Cancer Compounds in Single Bladder Cancer Cells Using the Single-Probe MS Technique**; Shawna Standke<sup>1</sup>, Ning Pan<sup>1</sup>, Naga Rama Kothapalli<sup>1</sup>, Anh Le<sup>1</sup>, Anthony Burgett<sup>1</sup>, Zhibo Yang<sup>1</sup>; <sup>1</sup>University of Oklahoma
- 2:50 PM (382) **Cellular and Sub-cellular Level Localization of Lipids and Metabolites Using Two- and Three-Dimensional High-Spatial Resolution MALDI Mass Spectrometry Imaging**; Maria Emilia Dueñas<sup>1</sup>, Adam Klein<sup>1</sup>, Liza Alexander<sup>1</sup>, Marna Yandeau-Nelson<sup>1</sup>, Basil Nikolau<sup>1</sup>, Jeffrey Essner<sup>1</sup>, Young-Jin Lee<sup>1</sup>; <sup>1</sup>Iowa State University

**Tuesday Afternoon, Nevada 6**

### 17PAT04: ONLINE ANALYSIS OF INDUSTRIAL PROCESSES AND REACTIONS - IMPROVEMENTS AND BEST PRACTICES

Organizers and Presiders: Anna Sandlin, JD Tate

- 1:30 PM (383) **Comparison of Lab, Portable and Process Gas Chromatographs for On-Line Analysis of R&D Reactions**; Eric Schmidt<sup>1</sup>, Anna Sandlin<sup>1</sup>, Linda Heinicke<sup>1</sup>; <sup>1</sup>The Dow Chemical Company, Freeport, TX
- 1:50 PM (384) **Conventional Gas Detection Technology and the Challenges in Industrial Applications**; John Wilson<sup>1</sup>, Ulf Ostermann<sup>1</sup>; <sup>1</sup>Draeger Inc.
- 2:10 PM (385) **Open Path UVDOAS Ambient Air Monitoring for Petrochemical Applications**; William (Bill) Pearman, J.D. Tate; <sup>1</sup>The Dow Chemical Company
- 2:30 PM (386) **FT-MRR for Trace Chemical Detection and Chiral Characterization in Reaction Solutions**; Justin Neill<sup>1</sup>, Brent Harris<sup>1</sup>, Robin Pulliam<sup>1</sup>, Matt Muckle<sup>1</sup>, Shelby Fields<sup>1</sup>; <sup>1</sup>BrightSpec, Inc.
- 2:50 PM (387) **Comprehensive GC x GC Analyses Using a Process GC**; Anna Sandlin<sup>1</sup>, Ademola Idowu<sup>2</sup>, Bill Winniford<sup>1</sup>, Eric Schmidt<sup>1</sup>, JD Tate<sup>3</sup>, Linda Heinicke<sup>1</sup>; <sup>1</sup>Dow Chemical Company, Analytical Sciences; <sup>2</sup>Dow Chemical Company, Polyurethanes R&D; <sup>3</sup>Dow Chemical Company, Analytical Technology Center

**Tuesday Afternoon, Carson 2**

### 17PMA05: RECENT ADVANCES IN THE MODE OF ACTION OF BIOPHARMACEUTICALS

Organizer and Presider: John Wasylkyk

- 1:30 PM (388) **Protein Dynamics via a Non-perturbing Site-specific Infrared Probe**; Farzaneh Chalyavi<sup>1</sup>, Andrew Schmitz<sup>1</sup>, David Hogle<sup>1</sup>, Matthew Tucker<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

- 1:50 PM (389) **Label-Free Quantification of IgG1 and IgG4 in Mixtures Using Raman Spectroscopy**; Mekhala Spencer<sup>1</sup>, Yun Xu<sup>1</sup>, John Welsh<sup>2</sup>, Peter Levison<sup>2</sup>; <sup>1</sup>University of Manchester; <sup>2</sup>Pall Life Sciences

- 2:10 PM (390) **Confocal Raman Microscopy for Investigation of Bilayer-Analyte Interactions at Nanopore Supported Phospholipid Bilayers**; David Bryce<sup>1</sup>, Jay Kitt<sup>1</sup>, Joel Harris<sup>1</sup>; <sup>1</sup>University of Utah dept. of Chemistry

- 2:30 PM (391) **Metal Induced Folding Patterns of  $\alpha$ -Synuclein Assemblies**; Heather Lucas<sup>1</sup>; <sup>1</sup>Virginia Commonwealth University

- 2:50 PM (392) **Towards a Rapid and Selective Nanoparticle-Based Assay for the Assessment of Biopharmaceutical Glycosylation**; Craig Ward<sup>1</sup>, Karen Faulds<sup>1</sup>, Daniel Bracewell<sup>2</sup>, Duncan Graham<sup>1</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>University College London

**Tuesday Afternoon, Carson 3**

### 17RAM09: TRANSMISSION RAMAN SPECTROSCOPY

Organizer and Presider: Mark Mabry

- 1:30 PM (393) **Time-Gated Raman spectroscopy and 3D Data Analysis for Quantifying Fluorescent Pharmaceuticals**; Tiina Lipiäinen<sup>1</sup>, Jenni Pessi<sup>1</sup>, Parisa Movahedi<sup>2</sup>, Tapio Pahikkala<sup>2</sup>, Jukka Heikkonen<sup>2</sup>, Mari Tenhunen<sup>3</sup>, Lauri Kurki<sup>3</sup>, Jouko Yliruusi<sup>1</sup>, Anne M. Juppo<sup>1</sup>, Clare Strachan<sup>1</sup>; <sup>1</sup>University of Helsinki, Finland; <sup>2</sup>University of Turku, Finland; <sup>3</sup>TimeGate Instruments, Finland

- 1:50 PM (394) **Evaluation of Transmission Raman Spectroscopy for Detection and Quantification of Low Level Drug Content in Pharmaceutical Tablets**; Rajesh Morampudi<sup>1</sup>; <sup>1</sup>Amneal Pharmaceutical

- 2:10 PM (395) **Crystalline Content Determination in Solid Dispersions by Raman Spectroscopy –Effect of the Analyzed Sample Volume on Qualitative and Quantitative Results**; Fran Adar<sup>1</sup>, Mathieu Boiret<sup>1</sup>, L Netchacovitch<sup>2</sup>, E. Ziemons<sup>2</sup>; <sup>1</sup>HORIBA Scientific; <sup>2</sup>University of Liege

- 2:30 PM (396) **0°, 180° - Why the Scattering Geometry Makes a Difference When Applying Raman Spectroscopy**; Sean J. Gilliam<sup>1</sup>, Francis Esmonde-White<sup>1</sup>, David Strachan<sup>1</sup>, Ian R. Lewis<sup>1</sup>; <sup>1</sup>Kaiser Optical Systems, Inc.

- 2:50 PM (397) **Determination of Propensity to Crystallize of Amorphous Solid Dispersions by Transmission Raman Spectroscopy**; Holger van Lishaut<sup>1</sup>, Frank Theil<sup>1</sup>, Sankaran Anantharaman<sup>1</sup>, Johanna Milsman<sup>1</sup>; <sup>1</sup>AbbVie Deutschland, NCE Analytical R&D

**Tuesday Afternoon, Carson 4**

### 17RAM18: NANO IR / NANO-RAMAN I

Organizers: Curtis Marcott, Andrew Whitley;  
Presider Curtis Marcott

- 1:30 PM (398) **Hyperspectral AFM-IR Imaging of Malaria Infected Cells**; David Perez-Guiata<sup>1</sup>, Bayden Wood<sup>1</sup>, Philip Heraud<sup>1</sup>, Shirley Espinoza Herrera<sup>2</sup>, Christian Doerig<sup>1</sup>, Jose Garcia-Bustos, Kamila Kochan<sup>1</sup>, Don McNaughton<sup>1</sup>; <sup>1</sup>Monash University; <sup>2</sup>Institute of Physics Czech Academy of Science

- 1:50 PM (399) **Tip-Enhanced Raman Spectroscopy: An Emergent Tool for Probing Biology and Electrochemistry at the Nanoscale**; Dmitry Kurouski, Igor Lednev, Tanja Deckert-Gaudig, Volker Deckert, Michael Mattei, Richard Van Duyne; <sup>1</sup>Texas A&M University

## TECHNICAL PROGRAM – TUESDAY

**Orals 1:30 – 3:10 pm & 3:50 – 5:30 pm**

- 2:10 PM (400) **Synchrotron Infrared Nano Spectroscopy and Applications of SINS in Biology, Physics, Catalysis, and More;** Michael C. Martin<sup>1</sup>; <sup>1</sup>Advanced Light Source, LBNL
- 2:30 PM (401) **Nanoscale Chemical and Electronic Mapping of Carboxyl Graphene Oxide Using Combined Tip-Enhanced Raman Spectroscopy & Kelvin Probe Force Microscopy;** Marc CHAIGNEAU<sup>1</sup>, Weitao Su<sup>4</sup>, Naresh Kumar<sup>3</sup>, Andrey Krayev<sup>2</sup>; <sup>1</sup>HORIBA Scientific; <sup>2</sup>AIST-NT; <sup>3</sup>National Physical Laboratory; <sup>4</sup>Hangzhou Dianzi University
- 2:50 PM (402) **Polymeric Nanoparticle Chemical Analysis Using Tapping AFM-IR;** Alexandre Dazzi<sup>1</sup>, Jérémie Mathurin<sup>1</sup>, Ariane Deniset-Besseau<sup>1</sup>, Elisabetta Pancani<sup>1</sup>, Ruxanda Gref<sup>1</sup>, Kevin Kjoller<sup>2</sup>, Craig Prater<sup>2</sup>; <sup>1</sup>Université Paris-Sud; <sup>2</sup>Anasys Instruments

### Tuesday Afternoon, Nevada 5 17SPR03: NEXT GENERATION PLASMONICS

Organizers: Emilie Ringe, Jean-Francois Masson;  
President: Emilie Ringe

- 1:30 PM (403) **A Statistical Investigation of the Properties of Plasmonic Single Particles;** Alexandre Brolo<sup>1</sup>, Regivaldo Sobral Filho<sup>1</sup>, XiaoYing Zhang<sup>1</sup>; <sup>1</sup>University of Victoria, Dept of Chemistry
- 1:50 PM (404) **Plasmonic Nanostructures for Trapping and Sensing Single Molecules;** Sang-Hyun Oh<sup>1</sup>; <sup>1</sup>University of Minnesota, Minneapolis
- 2:10 PM (405) **Synthesis of Copper-Silica Core-Shell Nanostructures with Sharp and Stable Localized Surface Plasmon Resonance;** Jingyi Chen; <sup>1</sup>University of Arkansas
- 2:30 PM (406) **Structural Analysis by Enhanced Raman Scattering;** Steven Demers<sup>1</sup>, James Matthews<sup>1</sup>, Cyna Shirazinejad<sup>1</sup>, Grace Isakson<sup>1</sup>, Jason Hafner<sup>1</sup>; <sup>1</sup>Rice University
- 2:50 PM (407) **Photoexcitation of On-Surface Core-Shell Fluorescent Plasmonic Nanoparticles by Grazing Waveguides;** Alexandre Grégoire<sup>1</sup>, Jean-Philippe Bérubé<sup>2</sup>, Réal Vallée<sup>2</sup>, Denis Boudreau<sup>1</sup>; <sup>1</sup>Université Laval, Département de chimie et COPL; <sup>2</sup>Université Laval, Département de physique et COPL

**3:10 PM Poster Session and Coffee Break, SciX Exhibit Hall**

### Tuesday Afternoon, Crystal 4 17AES04: DESIGNER (NANO)STRUCTURES AND MOLECULES FOR SEPARATIONS AND ANALYSIS

Organizer: Rebecca Whelan; President: Jason Dwyer

- 3:50 PM (408) **Coupling Ion Channels to Mobile Nanofluidic Devices (Nanopipettes);** Lane Baker<sup>1</sup>; <sup>1</sup>Indiana University
- 4:10 PM (409) **Chromatographic Properties of Ordered Carbon Nanomaterials;** Susan Olesik<sup>1</sup>; <sup>1</sup>The Ohio State University
- 4:30 PM (410) **Multifunctional Nanomaterials to Screen and Select Proteins;** Lisa Holland; <sup>1</sup>West Virginia University Chemistry
- 4:50 PM (411) **Exploring Media for electrophoretic separation of DNA by Sequence in Microfluidic Chips;** Linda McGown, Wyatt Stevens, Jia Zhao; <sup>1</sup>Rensselaer Polytechnic Institute
- 5:10 PM (412) **Single Molecule Biopolymer Analysis Using Interface-Tailored Nanopore Sensing;** Jason Dwyer<sup>1</sup>, Buddini Karawadeniya<sup>1</sup>, Nuwan Bandara<sup>1</sup>, Jonathan Nichols<sup>1</sup>, Robert Chevalier<sup>1</sup>; <sup>1</sup>University of Rhode Island

### Tuesday Afternoon, Crystal 2 17ATOM06: LASER ABLATION-ICP-MS II

Organizer and Presider: Jorge Pisonero Castro

- 3:50 PM (413) **LA-ICP-MS Analysis and Characterization of Adhesive Tapes as Forensic Evidence;** Jose Almirall, Claudia Martinez-Lopez; <sup>1</sup>Florida International University
- 4:10 PM (414) **LA-ICP-MS Imaging for Anthropological Samples;** Matthieu Baudet<sup>1</sup>; <sup>1</sup>UCF - NCFS
- 4:30 PM (415) **Single-Shot Laser-Ionization Mass Spectrometry for Direct Atomic Analysis;** Jose M Vadillo<sup>1</sup>, J. Javier Laserna<sup>1</sup>; <sup>1</sup>University of Malaga, UMALASERLAB
- 4:50 PM (416) **Effect of Nanoparticles on Laser Sampling and Plasma Emission;** Alessandro De Giacomo<sup>1,2</sup>, Rim Alrifai<sup>1</sup>, Gabriele Valenza<sup>1</sup>, Marcella Dell'Aglio<sup>2</sup>; <sup>1</sup>University of Bari; <sup>2</sup>CNR-NANOTEC
- 5:10 PM (417) **Effect of Topological Charge on Femtosecond Laser-Induced Breakdown Spectroscopy with Optical Vortex Beams;** Jason Becker<sup>1,2</sup>, Xianglei Mao<sup>1</sup>, Richard Russo<sup>1</sup>, Costas Grigoropoulos<sup>2</sup>, Vassilia Zorba<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory; <sup>2</sup>UC Berkeley

### 17CTP03 Tuesday Afternoon, Crystal 5 17CTP03: INNOVATIVE APPROACHES TO TEACHING ANALYTICAL CHEMISTRY

Organizers: Rebecca Airmet, Anna Donnell;  
President: Rebecca Airmet

- 3:50 PM (418) **Teaching Students to Navigate Design Problems: Translating Fundamental Tools for Real-Time Learning;** Barbara Smith<sup>1</sup>, Emma Frow<sup>1</sup>; <sup>1</sup>Arizona State University
- 4:10 PM (419) **Engaging Learners of All Ages with Inquiry Based Environmental Science Education Through Inscied Out;** Seth K. Thompson<sup>1</sup>, Christopher Pierret<sup>2</sup>; <sup>1</sup>University of Minnesota-Twin Cities; <sup>2</sup>Mayo Clinic
- 4:30 PM (420) **Where is Reflection's Place in the Chemistry Classroom?;** Anna Donnell<sup>1</sup>; <sup>1</sup>University of Cincinnati
- 4:50 PM (421) **Experimenting with "Build your Own Instrument" Kits: A Lab for an Analytical Chemistry Course;** Ingeborg Petterson<sup>1</sup>; <sup>1</sup>Goucher College
- 5:10 PM (422) **Research-Based Experiments in Teaching-Labs: How the Chemistry of Food Can Engage Students in Analytical and Physical Chemistry;** Natasja A. Swartz<sup>1</sup>, Paige W. Hall<sup>2</sup>, Rob Jensen<sup>1</sup>, Sam Danforth<sup>3</sup>; <sup>1</sup>Reed College; <sup>2</sup>Pacific University; <sup>3</sup>Western Washington University

### Tuesday Afternoon, Nevada 6 17FORENS02: FOOD FORENSICS

Organizer and Presider: Betsy Jean Yakes

- 3:50 PM (423) **Exposing the Hidden Dangers of Dietary Supplements;** Connie Ruzicka; <sup>1</sup>US Food and Drug Administration
- 4:10 PM (424) **LIBS and Raman Applications for Food Safety and Quality;** Ismail Boyaci<sup>1,2</sup>; <sup>1</sup>Department of Food Engineering; <sup>2</sup>Hacettepe University
- 4:30 PM (425) **Rapid Isolation of Pathogenic Listeria Serovars;** Claire Crowther<sup>1</sup>, Mark Hayes<sup>1</sup>; <sup>1</sup>Arizona State University
- 4:50 PM (426) **Data-Driven Strategies to Focus Food Fraud Prevention Resources;** Karen Everstine<sup>1</sup>; <sup>1</sup>United States Pharmacopeia



## TECHNICAL PROGRAM – TUESDAY

**Orals 3:50 – 5:30 pm**

5:10 PM (427) **Authentication of Turkish Honey Using a Portable Raman System Spectrometry;** Mei-Ling Shotts<sup>1</sup>; <sup>1</sup>The Ohio State University

### Tuesday Afternoon, *Carson 4* 17IR01: NANOIR/NANO-RAMAN II

Organizers: Curtis Marcott, Andrew Whitley;  
President: Andrew Whitley

3:50 PM (428) **Complex Electron Transfer Pathway at a Microelectrode Captured by in situ TERS;** Ivan LUCAS<sup>1</sup>, Thomas Touzalin<sup>1</sup>, Suzanne Joiret<sup>1</sup>, Emmanuel Maisonhaute<sup>1</sup>; <sup>1</sup>LISE laboratory - Sorbonne Universities - UPMC

4:10 PM (429) **Applications of Nanoscale Chemical Imaging to Polyolefins;** Mark Rickard<sup>1</sup>, Gregory Meyers<sup>1</sup>, Carl Reinhardt<sup>1</sup>, Jamie Stanley<sup>1</sup>; <sup>1</sup>Dow Chemical

4:30 PM (430) **Tip-Enhanced Raman Spectroscopy as a New Platform for Plasmon-Induced Polymerization;** Marie Richard-Lacroix<sup>1,2</sup>, Zhenglong Zhang<sup>1,2</sup>, Volker Deckert<sup>1,2</sup>; <sup>1</sup>Leibniz Institute of Photonic Technology (IPHT); <sup>2</sup>Institute of Physical Chemistry (IPC), Jena

4:50 PM (431) **Recent Advances in Nanoscale IR Spectroscopy: Hyperspectral and Tapping AFM-IR Imaging;** Curtis Marcott<sup>1</sup>, Eoghan Dillon<sup>2</sup>, Kevin Kjoller<sup>2</sup>, Craig Prater<sup>2</sup>; <sup>1</sup>Light Light Solutions; <sup>2</sup>Anasys Instruments

5:10 PM (432) **Enabling Discoveries: TERS Imaging of the Grain Boundaries and Unexpected Nanoscale Heterogeneities in 2D Semiconductors.;** Andrey Kravayev<sup>1</sup>; <sup>1</sup>AIST-NT Inc

### Tuesday Afternoon, *Nevada 7* 17MASS03: NOVEL AMBIENT MASS SPECTROMETRY TECHNIQUES FOR FORENSIC SCIENCE ANALYSIS

Organizer and President: Candice Bridge

3:50 PM (433) **Laser Ablation DART Imaging Mass Spectrometry (LADI-MS)—Applications to Forensics;** Rabi Musah<sup>1</sup>, Kristen Fowble<sup>1</sup>; <sup>1</sup>State University of New York

4:10 PM (434) **Pyrolysis -Vacuum Assisted Plasma Ionization Ion Mobility-Mass Spectrometry for Insoluble Polymer Analysis.;** Stephen Zambrzycki<sup>1</sup>, Matthew Bernier<sup>1</sup>, James Bradshaw<sup>2</sup>, Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology; <sup>2</sup>Y-12 National Security Complex

4:30 PM TBA

4:50 PM (436) **Linking Smokeless Powder Residues to Pre-Burn Smokeless Powders Using DART-TOTMS and GC-MS;** Emily Lennert<sup>1</sup>, Candice Bridge<sup>1</sup>; <sup>1</sup>UCF/NCFS

5:10 PM (437) **The Development of a Lab-on-a-Chip Device for the Track Side Detection of Equine Performance Enhancement;** Kim Quayle<sup>1</sup>, Egan H. Doeven<sup>1</sup>, Richard Alexander<sup>1</sup>, Yi Heng Nai<sup>1</sup>, Giorgio M. De Guzman<sup>1</sup>, Paul S. Francis<sup>2</sup>, Xavier A. Conlan<sup>2</sup>, Stephen J. Haswell<sup>1</sup>; <sup>1</sup>Deakin University, CeRRF; <sup>2</sup>Deakin University, CCB

### Tuesday Afternoon, *Carson 2* 17PMA06: PAT IN BIOPHARMACEUTICAL MANUFACTURING

Organizer and President: Myra Coufal

3:50 PM (438) **Building on a Real-time Multivariate Monitoring Platform for Biopharmaceutical Manufacturing Operations: How to Teach an Old Dog New Tricks;** Christopher Garvin<sup>1</sup>, Cenk Undey<sup>1</sup>; <sup>1</sup>Amgen, Inc.

4:10 PM (439) **Validation of Control Strategies Based on Advanced Sensors;** Saly Romero-Torres<sup>1</sup>; <sup>1</sup>Biogen

4:30 PM (440) **Process Analytical Technology (PAT) in Continuous Bioprocessing;** Edita Botonjic-Sehic<sup>1</sup>, Steven Harris<sup>1</sup>; <sup>1</sup>Pall Life Sciences

4:50 PM (441) **Development of Generic Raman Models for Process Monitoring;** Thaddaeus Webster<sup>1</sup>, Colin Jaques<sup>1</sup>, Carrie Mason<sup>1</sup>; <sup>1</sup>Lonza Biologics

5:10 PM (442) **Raman-Based Bioreactor Control: Building Sustainable Applications;** John Bobiak<sup>1</sup>, Dimuthu Jayawickrama<sup>1</sup>, Nobel Vale<sup>1</sup>, George Armenante<sup>1</sup>, Greg Lane<sup>1</sup>, Matthew Rehmann<sup>1</sup>; <sup>1</sup>Bristol Myers Squibb

### Tuesday Afternoon, *Carson 3* 17RAM19: GENERAL RAMAN

Organizers: Ian Lewis, Duncan Graham, Pavel Matousek;  
President: Pavel Matousek

3:50 PM (443) **Combined Raman and Morphological Analysis of Fluorescent Propellants and Organic Gunshot Residue;** Steven Bell, Yen Cheng Ho<sup>2</sup>, Wendy Lee<sup>1</sup>; <sup>1</sup>Queen's University Belfast; <sup>2</sup>New Taipei City Police Department

4:10 PM (444) **Standoff Explosive Detection Using an Eye-Safe, Wide-Area Hyperspectral Raman Sensor;** Nathaniel Gomer<sup>1</sup>, Charles Gardner<sup>1</sup>, Matthew Nelson<sup>1</sup>; <sup>1</sup>ChemImage Sensor Systems

4:30 PM (445) **See Through Raman Spectroscopy;** Jun Zhao<sup>1</sup>, Jack Zhou<sup>1</sup>; <sup>1</sup>B&W Tek

4:50 PM (446) **Silver-Gold Bimetallic Nanostructure Incorporated Nickel Foam as a Rugged and Reliable SERS Substrate;** Tung Duy Vu<sup>1</sup>, Hueil Chung<sup>1</sup>; <sup>1</sup>Hanyang University

5:10 PM (447) **N-Heterocyclic Carbenes as a Surface Modifier for Analysis by Surface-Enhanced Raman Scattering;** Michael Trujillo<sup>1</sup>, Joseph DeJesus<sup>2</sup>, Chaoxiong Ma<sup>1</sup>, David Jenkins<sup>2</sup>, Jon Camden<sup>1</sup>; <sup>1</sup>University of Notre Dame; <sup>2</sup>University of Tennessee

### Tuesday Afternoon, *Carson 1* 17RSC02: RSC SENSORS FOR CANCER DIAGNOSTICS

Organizer and President: Maria Southall

3:50 PM (448) **Electrophoretic Separation of Single Molecules using Thermoplastic Nanocolumns: Applications in Single-Molecule Sequencing;** Steven Soper<sup>1</sup>; <sup>1</sup>University of Kansas

4:10 PM (449) **Infrared Spectral Histopathology Using (H&E) Stained Glass Slides: A Route to Clinical Translation;** Peter Gardner<sup>1</sup>, Michael Pilling<sup>1</sup>, Alex Henderson<sup>1</sup>, Jonathan Shanks<sup>2</sup>, Michael Brown<sup>3</sup>, Noel Clarke<sup>3</sup>; <sup>1</sup>Manchester Institute of Biotechnology, University; <sup>2</sup>Department of Pathology, Christie Hospital, Manche; <sup>3</sup>Genito Urinary Cancer Research Group, Division of



## TECHNICAL PROGRAM – TUESDAY

**Orals 3:50 – 5:30 pm**

4:30 PM (450) **Designing a 3D Culture Platform for Scalable Quantitative Drug Screens**; Amanda Hummon<sup>1</sup>, Gabriel LaBonia<sup>1</sup>, Matthew Boyce<sup>2</sup>, Matthew Lockett<sup>2</sup>; <sup>1</sup>University of Notre Dame; <sup>2</sup>University of North Carolina, Chapel Hill

4:50 PM (451) **After the Diagnosis: Monitoring Cancer Therapies with SPR Sensors**; Jean-Francois Masson<sup>1</sup>; <sup>1</sup>Universite de Montreal

5:10 PM (452) **Mechano-NPS for Cancer Diagnostics**; Lydia Sohn<sup>1</sup>; <sup>1</sup>University of California, Berkeley

**Tuesday Afternoon, Nevada 5**

### 17SPR02: PLASMONIC NANOPARTICLES - BEYOND SPHERE

Organizer: Amanda Haes; Presider: Emilie Ringe

3:50 PM (453) **Bioanalytical and Nanomedicine Applications of Gold Nanorods, Nanostars, and Magnetic Nanoclusters**; Alexander Wei<sup>1</sup>; <sup>1</sup>Purdue University

4:10 PM (454) **Gold Nanostars for Promoting Molecular Adsorption of Non-Thiolated Molecules**; Amanda Haes<sup>1</sup>; <sup>1</sup>University of Iowa

4:30 PM (455) **Gold Nanostars: Can Cinderella Become a Princess?**; Laura Fabris<sup>1</sup>, Supriya Atta<sup>1</sup>, Ted V. Tsoulos<sup>1</sup>; <sup>1</sup>Rutgers University

4:50 PM (456) **Beyond the Nanostar's Plasmon**; Sean Burrows<sup>1</sup>, Lixia Zhou<sup>1</sup>; <sup>1</sup>Oregon State University

5:10 PM (457) **Chiro-Optical Activity of Symmetric and Asymmetric Dimer Plasmonic Nanocrescents**; Jennifer Shumaker-Parry<sup>1</sup>, Peter Stevenson<sup>1</sup>, Mark Swartz<sup>1</sup>, Caitlin Coplan<sup>1</sup>, Venkata Ananth Tamma<sup>2</sup>, Vartkess Ara Apkarian<sup>2</sup>; <sup>1</sup>University of Utah; <sup>2</sup>University of California-Irvine

**TECHNICAL PROGRAM – WEDNESDAY**  
**Awards Presentations - 7:50 am; Plenary Lectures - 8:00 am; Tahoe Ballroom**  
**President: Karen Esmonde-White**



**8:00 am – Applied Spectroscopy Meggers Award**  
**(475) Infrared Response of Sub-Micron-Scale Structures of Poly(Oxymethylene): Surface Polaritons in Polymers;** Naoto Nagai<sup>1</sup>, Makoto Okawara<sup>1</sup>, Yuta Kijima<sup>1</sup>; <sup>1</sup>Industrial Research Institute of Niigata Prefecture



**8:30 am – Lester W. Strock Award**  
**(476) The Wonderful World of High-Precision Isotopic Analysis Using Multi-Collector ICP-MS;** Frank Vanhaecke<sup>1,2</sup>; <sup>1</sup>Ghent University; <sup>2</sup>Department of Analytical Chemistry

**Orals 9:15 – 10:55 am**

**Wednesday Morning, Crystal 2**  
**17ATOM08: ICP-MS FOR BIOMEDICAL APPLICATIONS**  
 Organizer and President: Martin Resano

- 9:15 AM (477) **Chemical Resolution in Tandem ICP- Mass Spectrometry: Application for Multi-Element Analysis in Microsamples of Biological Fluids;** Eduardo Bolea-Fernandez<sup>1</sup>, Kim Phan<sup>1</sup>, Lieve Balcaen<sup>1</sup>, Martin Resano<sup>2</sup>, Frank Vanhaecke<sup>1</sup>; <sup>1</sup>Ghent University; <sup>2</sup>University of Zaragoza
- 9:35 AM (478) **Transient signal Approaches in Sector-Field ICPMS for Fast and Sensitive Trace Element and Isotopic Analysis;** Christophe Pecheyran<sup>1</sup>, Sylvain Beraïl<sup>1</sup>, Oriol Baltrons<sup>1</sup>, Martin Resano<sup>2</sup>, Maïté Aramendia Marzo<sup>2</sup>, Loïc Martin<sup>3</sup>, Chantal Tribolo<sup>3</sup>, Norbert Mercier<sup>3</sup>, Bénédicte Lelievre<sup>4</sup>; <sup>1</sup>University of Pau; <sup>2</sup>University of Zaragoza; <sup>3</sup>University Bordeaux Montaigne; <sup>4</sup>Centre Hospitalier d'Angers
- 9:55 AM (479) **A High Temperature Torch Integrated Sample Introduction System for Characterization of Nanoparticles in Biological Samples;** Martin Resano<sup>1</sup>, Esperanza García-Ruiz<sup>1</sup>, Maite Aramendia<sup>2</sup>, Diego Leite<sup>1</sup>, Águeda Cañabate<sup>3</sup>, José Luis Todolí<sup>3</sup>; <sup>1</sup>Universidad de Zaragoza; <sup>2</sup>Centro Universitario de la Defensa, Universidad de; <sup>3</sup>Universidad de Alicante
- 10:15 AM (480) **Advances for the Determination of Elemental Impurities in Pharmaceutical Products;** Erico Flores<sup>1</sup>; <sup>1</sup>Universidade Federal de Santa Maria
- 10:35 AM (481) **Role of Plasma Techniques in Petroleum Business;** Francisco Lopez-Linares<sup>1</sup>, Jenny Nelson<sup>2</sup>, Estrella Rogel<sup>1</sup>, Cesar Ovalles<sup>1</sup>, Laura Poirier<sup>1</sup>; <sup>1</sup>Chevron Energy Technology Company; <sup>2</sup>Agilent

**Wednesday Morning, Crystal 1**  
**17AWD01: WILLIAM F. MEGGERS AWARD SYMPOSIUM HONORING NAOTO NAGAI**  
 Organizer and President: Naoto Nagai

- 9:15 AM (482) **Application of 2D Correlation Spectroscopy in Characterization of Thin Film of Biodegradable Polymer;** Young Mee Jung<sup>1</sup>, Yujing Chen<sup>1</sup>, Yeonju Park<sup>1</sup>, Isao Noda<sup>2,3</sup>; <sup>1</sup>Kangwon National University; <sup>2</sup>University of Delaware; <sup>3</sup>Danimer Scientific
- 9:35 AM (483) **Two-Trace Two-Dimensional (2T2D) Correlation Spectroscopy – a Method for Extracting Useful Information from Only a Pair of Spectra;** Isao Noda<sup>1</sup>; <sup>1</sup>University of Delaware
- 9:55 AM (484) **Vibrational Spectroscopy with Handheld Instruments: Recent Advances and Future Aspects;** Heinz Siesler<sup>1</sup>; <sup>1</sup>University of Duisburg-Essen
- 10:15 AM (485) **IR Spectroscopy: A Powerful Tool for Analysis of Perfluoroalkyl Compounds;** Takeshi Hasegawa<sup>1</sup>; <sup>1</sup>ICR, Kyoto University
- 10:35 AM (486) **Investigation for Coordination Bond in Li+-Poly(ethylene glycol) Complex by Attenuated Total Reflectance Spectroscopy in the FUV Region.;** Yusuke Morisawa<sup>1</sup>, Nami Ueno<sup>1</sup>, Tomonari Wakabayashi<sup>1</sup>; <sup>1</sup>Kindai University

**Wednesday Morning, Nevada 7**  
**17BIM04: ENDOSCOPY**  
 Organizer and President: Rohith Reddy

- 9:15 AM (487) **Reflectance Confocal and Fluorescence Lifetime Endoscopy in the Oral Cavity;** Kristen Maitland<sup>1</sup>, Javier Jo<sup>1</sup>, Yi-Shing Lisa Cheng<sup>2</sup>; <sup>1</sup>Texas A&M University; <sup>2</sup>Texas A&M College of Dentistry
- 9:35 AM (488) **Development of CARS System with Dual-Wavelength Oscillation Electronically Tuned Ti:Sapphire Laser;** Hidetoshi Sato<sup>1</sup>, Bibin Andriana<sup>1</sup>, Hiroko Matsuyoshi<sup>1</sup>, Yasuhiro Maeda<sup>2</sup>, Satoshi Wada<sup>2</sup>; <sup>1</sup>Kwansei Gakuin University; <sup>2</sup>RIKEN
- 9:55 AM (489) **A Systems Pathology Approach to Spectroscopic Colon Cancer Diagnosis;** Saumya Tiwari<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana Champaign
- 10:15 AM (490) **Synergy of Multispectral Fiber Spectroscopy;** Viacheslav Artyushenko<sup>1</sup>, Urszula Zabarylo<sup>2</sup>, Olga Bibikova<sup>1</sup>, Andrey Bogomolov<sup>1</sup>, Francesco Bianco<sup>1</sup>, Iskander Usenov<sup>1,3</sup>, Tatiana Sakharova<sup>1</sup>, Olaf Minet<sup>2</sup>, Svetlana Tonevitskaia<sup>1</sup>, Hans Joachim Eichler<sup>2</sup>; <sup>1</sup>art photonics GmbH; <sup>2</sup>Charité Universitätsmedizin Berlin; <sup>3</sup>Technical University of Berlin
- 10:35 AM (491) **Decoding Breast Cancer-Induced Stromal Adaptations in Pre-Metastatic Lungs with Label-Free Raman Spectroscopy;** Santosh Paidi<sup>1</sup>, Asif Rizwan<sup>2</sup>, Chao Zheng<sup>1,3</sup>, Menglin Cheng<sup>2</sup>, Kristine Glunde<sup>2</sup>, Ishan Barman<sup>1,2</sup>; <sup>1</sup>Johns Hopkins University; <sup>2</sup>The Johns Hopkins University School of Medicine; <sup>3</sup>The Second Hospital of Shandong University

**Wednesday Morning, Crystal 5**  
**17CTP04: MAKING THE LEAP: PATHWAYS FROM GRADUATE SCHOOL TO A PERMANENT POSITION (PANEL DISCUSSION)**

Organizer and President: Anthony Stender

- 9:15 AM (492) **Making the Jump from Graduate School to the Workforce;** Anthony Stender<sup>1</sup>, Alex Nemiroski, Karen Esmond-White, Barbara Smith, Alex Scheeline, Katelyn Mason, Colin Ingram; <sup>1</sup>Ohio University

**Wednesday Morning, Carson 1**  
**17IR09: ULTRAFAST TWO-DIMENSIONAL SPECTROSCOPY - I**

Organizer and President: Kyle Czech

- 9:15 AM (493) **Monolayer Dynamics at the Air/Water Interface;** Michael Fayer<sup>1</sup>; <sup>1</sup>Stanford University
- 9:55 AM (494) **Spectroscopic Observation of Triplet Separation as a Driving Force of Singlet Fission;** Daniel Turner<sup>1</sup>; <sup>1</sup>New York University
- 10:15 AM (495) **Fully Coherent Electronic-Vibrational Spectroscopy of Transition Metal Complexes;** John Wright, Jonathan Handali, Nathan Neff-Mallon, Erin Boyle; <sup>1</sup>University of Wisconsin-Madison
- 10:35 AM (496) **4D Coherent Electronic-Vibrational Spectroscopy: Theory and Applications;** Elad Harel<sup>1</sup>; <sup>1</sup>Northwestern University

## TECHNICAL PROGRAM – WEDNESDAY

**Orals 9:15 – 10:55 am**

### Wednesday Morning, *Crystal 3* 17LIBS07: NALIBS: LIBS DATA ANALYSIS Organizer and Presider: François R. Doucet

- 9:15 AM (497) **Cancer Diagnosis using LIBS and Machine Learning Tools: Progress and Challenges;** Noureddine Melikechi<sup>1</sup>, Rosalba Guadiuso<sup>1</sup>, Ebo Ewusi-Annan<sup>1</sup>; <sup>1</sup>University of Massachusetts Lowell
- 9:35 AM (498) **Using Portable LIBS to Inform Field Archaeology;** Mary Kate Donais<sup>1</sup>, Luke Douglass<sup>1</sup>, David George<sup>2</sup>; <sup>1</sup>Saint Anselm College Chemistry Department; <sup>2</sup>Saint Anselm College Classics Department
- 9:55 AM (499) **Spatio-Temporal Mapping of Laser Ablation Plumes Using Laser-Induced Fluorescence;** Kyle Hartig<sup>1,2</sup>, Mark Phillips<sup>1</sup>, Sivanandan Harilal<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>University of Florida
- 10:15 AM (500) **Argon Fluoride LA-LEAF for Arsenic: Toward Selective Measurements in Rice;** Jonathan Merten<sup>1</sup>, Patrick Tribbett<sup>1</sup>, Christopher Jones<sup>1</sup>; <sup>1</sup>Arkansas State University
- 10:35 AM (501) **Analysis of High Silicon Content Samples by Laser-Induced Breakdown Spectrometry: Fusion Process to Match the Sample Matrix.;** Alexandrina Carvalho<sup>1</sup>, Maciel Luz<sup>2</sup>, Cassiana Nomura<sup>1</sup>; <sup>1</sup>Universidade de São Paulo; <sup>2</sup>Centro de Tecnologia em Metalurgia e Materiais

### Wednesday Morning, *Nevada 6* 17PAT05: ADVANCES IN ON-LINE PROCESS ANALYSIS Organizer and Presider: Alison Nordon

- 9:15 AM (502) **In-situ Ultrasonic Imaging of Dynamic Process Streams: System Calibration and Image Processing;** Marcus Ingram<sup>1</sup>, Anthony Gachagan<sup>1</sup>, Alison Nordon<sup>1</sup>, Anthony Mulholland<sup>1</sup>, Carmelo Mineo<sup>1</sup>, Martin Hegarty<sup>2</sup>, Edo Becker<sup>2</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>BP Chemicals Ltd
- 9:35 AM (503) **Towards Quantitative Process Monitoring Using SABRE Enhanced Benchtop NMR;** Andrew Parrott<sup>1</sup>, Peter Richardson<sup>2</sup>, Meghan Halse<sup>2</sup>, Alison Nordon<sup>1</sup>, Simon Duckett<sup>2</sup>; <sup>1</sup>University of Strathclyde; <sup>2</sup>University of York
- 9:55 AM (504) **Implementation of Terahertz Spectroscopy as a PAT Tool for Powder Compact Density Assessment;** Shikhar Mohan<sup>1</sup>, Md. Anik Alam<sup>1</sup>, James Drennen, III<sup>1</sup>, Carl Anderson<sup>1</sup>; <sup>1</sup>Duquesne University
- 10:15 AM (505) **Robustness Evaluation of Transmission and Backscattered Modalities for Measuring Content Uniformity of Pharmaceutical Tablets with Raman Spectroscopy;** Md. Nayeem Hossain<sup>1</sup>, Md Anik Alam<sup>1</sup>, Douglas Steinbach<sup>1</sup>, James Drennen<sup>1</sup>, Carl Anderson<sup>1</sup>; <sup>1</sup>Duquesne University
- 10:35 AM (506) **Approaches to Multiblock Modeling and Dimension Reduction for Combining Disparate Data Types;** Heather Brooke<sup>1</sup>, Frank Westad<sup>1</sup>; <sup>1</sup>CAMO Software Inc

### Wednesday Morning, *Carson 2* 17PMA07: SPECTROSCOPIC APPLICATIONS IN THE WORLD OF BIOPHARMACEUTICALS Organizer and Presider: John Bobiak

- 9:15 AM (507) **Fourier-Transform Infrared Spectroscopy for Characterization of Enzymatic Protein Chain Reductions in Industrial Bioprocesses;** Sileshi Gizachew Wubshet<sup>1</sup>, Ulrike Böcker<sup>1</sup>, Diana Lindberg<sup>1</sup>,

Kenneth Aase Kristoffersen<sup>1</sup>, Ingrid Måge<sup>1</sup>, Nils Kristian Afseth<sup>1</sup>; <sup>1</sup>Nofima AS

- 9:35 AM (508) **Near Infrared Solutions for Biopharmaceutical Development and Manufacturing;** Adam J. Hopkins<sup>1</sup>; <sup>1</sup>Metrohm USA
- 9:55 AM (509) **Analytical Tools for Physicochemical Characterization of Biopharmaceuticals;** Sergey Arzhantsev<sup>1</sup>; <sup>1</sup>US FDA
- 10:15 AM (510) **Designing a Calibration Set in Spectral Space for Efficient Development of an NIR Method for Tablet Analysis;** Md Anik Alam<sup>1</sup>, Md Nayeem Hossain<sup>1</sup>, Douglas Steinbach<sup>1</sup>, James Drennen<sup>1</sup>, Carl Anderson<sup>1</sup>; <sup>1</sup>Duquesne University
- 10:35 AM (511) **A Novel Fingerprint and High Wavenumber Raman Spectroscopy System for Hydration Quantification;** Laura Masson<sup>1</sup>, Anita Mahadevan-Jansen<sup>1</sup>; <sup>1</sup>Vanderbilt University

### Wednesday Morning, *Nevada 5* 17SPR06: PLASMONIC-POWERED PROCESSES: SENSING, IMAGING, CATALYSIS, AND BEYOND Organizer and Presider: Wei-Chuan Shih

- 9:15 AM TBA
- 9:35 AM (513) **Fiber Sensors for Chemical and Biochemical Detection Based on Surface Enhanced Raman Scattering;** Jin Zhang<sup>1</sup>; <sup>1</sup>University of California Santa Cruz
- 9:55 AM (514) **Novel Plasmonic Enable Solar-to-Chemical Energy Conversion Systems;** Syed Mubeen<sup>1</sup>, Wei-Chuan Shih<sup>2</sup>, Wei Cheng<sup>1</sup>, Jonathan Koonce<sup>1</sup>, Abdul Sattar Al-Saedi<sup>1</sup>; <sup>1</sup>University of Iowa; <sup>2</sup>University of Houston
- 10:15 AM (515) **Hot Electron Enhanced Thermionic Emission (HEETE) Converters for All-Metal Optical Power Generation;** Matthew Sheldon<sup>1</sup>; <sup>1</sup>Texas A&M University
- 10:35 AM (516) **Far-Field and Near-Field Plasmonic Coupling in Disordered Nanoparticle Arrays and Applications in Ultra-Sensitive Biosensing and Super-Resolution Histopathology;** Wei-Chuan Shih<sup>1</sup>, Fusheng Zhao<sup>1</sup>, Masud Arnob<sup>1</sup>, Jingting Li<sup>1</sup>, Camille Artur<sup>1</sup>, Jason Eriksen<sup>1</sup>, David Mayerich<sup>1</sup>; <sup>1</sup>University of Houston

### Wednesday Morning, *Crystal 4* 17SURFACE01: APPLICATION OF SURFACE SPECTROSCOPIC TECHNIQUES TO ANALYSIS OF NANOMATERIALS AND DEVICES Organizer and Presider: Kateryna Artyushkova

- 9:15 AM (517) **Bridging the Pressure and Materials Gaps: Methanol Oxidation on Perovskite Thin-Films and Powders;** David Mullins<sup>1</sup>, Yafen Zhang<sup>1</sup>, Michelle Kidder<sup>1</sup>, Steven Overbury<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory
- 9:35 AM (518) **Using Tender Ambient Pressure XPS to probe Solid/Liquid Electrochemical Interfaces;** Ethan Crumlin<sup>1</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory
- 9:55 AM (519) **The Surface Chemistry of Water at Solid and Liquid Ionic Interfaces;** Alicia Broderick<sup>1</sup>, John Newberg<sup>1</sup>; <sup>1</sup>University of Delaware
- 10:15 AM (520) **XPS Analysis of Surface-Bound Biomolecules Provides Insight on their Surface Interactions and Dissociative Properties;** Kenan Fears<sup>1</sup>; <sup>1</sup>U.S. Naval Research Laboratory

## TECHNICAL PROGRAM – WEDNESDAY

Orals 9:15 – 10:55 am

Poster Sessions and Coffee Breaks

11:00 am – 12:00 pm & 3:10 – 3:50 pm, *SciX Exhibit Hall*

10:35 AM (521) **Observation of Oxygen Binding on PGM-free Electrocatalysts by Ambient Pressure XPS and XAS;** Kateryna Artyushkova<sup>1</sup>, Elisabeth Weiler<sup>1</sup>, Michael Dzara<sup>2</sup>, Svitlana Pylypenko<sup>2</sup>, Plamen Atanasov<sup>1</sup>; <sup>1</sup>University of New Mexico; <sup>2</sup>Colorado School of Mines

All Wednesday posters should be put up between 9:00 – 10:45 am and removed by 3:50 pm

### 17WPATOM: Wednesday Posters - Atomic Spectroscopy

#### Poster Board #1

(522) **Plasma Assisted Reaction Chemical Ionization using a Dielectric Barrier Discharge for High Sensitivity Elemental Quantification of Environmental Contaminants Separated by Gas Chromatography;** Kunyu Zheng<sup>1</sup>, Peter Haferl<sup>1</sup>, Michael Dolan<sup>1</sup>, Hamid Badiei<sup>2</sup>, Kaveh Jorabchi<sup>1</sup>; <sup>1</sup>Georgetown University; <sup>2</sup>PerkinElmer Inc.

#### Poster Board #2

(523) **Determination of Magnesium, Aluminum, and Calcium in Red Spruce Foliage and Surrounding Soil from Alarka Laurel, North Carolina;** David Butcher<sup>1</sup>; <sup>1</sup>Western Carolina University

#### Poster Board #3

(524) **Optical Emission Hyperspectral Imaging Plasma Diagnostics of Atmospheric Pressure  $\mu$ DBD Optimized for Surface Substrate Erosion Sampling;** Songyue Shi<sup>1</sup>, Xiaoxia Gong<sup>1</sup>, Gerardo Gamez<sup>1</sup>; <sup>1</sup>Texas Tech University

#### Poster Board #4

(525) **Optimizing LA-LEAF for Arsenic in Metals Using a Tunable ArF Laser;** Patrick Tribbett<sup>1</sup>, Christopher Jones<sup>1</sup>, Jonathan Merten<sup>1</sup>; <sup>1</sup>Arkansas State University

#### Poster Board #5

(526) **Agglomeration of Nanoparticle Structures in the Stagnation of Colliding Carbon Plasma;** John Oliver<sup>1</sup>, Tatyana Sizyuk<sup>1</sup>, Prasoon Diwakar<sup>1</sup>; <sup>1</sup>Purdue University

#### Poster Board #6

(527) **Benefits of ICP-MS with 10 Times Higher Sensitivity and 1/2 of Argon Consumption;** Oliver Büttel<sup>1</sup>, Oliver Büttel<sup>1</sup>; <sup>1</sup>Analytik Jena

#### Poster Board #7

(528) **Simulation of Argon Velocity Distribution Directly in Front of the Skimmer Cone of an ICP-MS;** Ross Spencer<sup>1</sup>; <sup>1</sup>Brigham Young University

#### Poster Board #8

(529) **High Temperature Total Sample Consumption Coupled to Inductively Coupled Plasma Mass Spectrometry for the Multielement Analysis of Cerebrospinal Fluid;** Esperanza Garcia-Ruiz<sup>2</sup>, Agueda Cañabate<sup>1</sup>, Martin Resano<sup>2</sup>, Jose Luis Todoli<sup>1</sup>; <sup>1</sup>University of Alicante; <sup>2</sup>University of Zaragoza

#### Poster Board #9

(530) **Hydrodynamic Chromatography Coupled to ICP-MS: Rethinking the Technique for the Analysis of Nanomaterials;** Francisco Laborda<sup>1</sup>, Maria S. Jimenez<sup>1</sup>, Daniel Isabal<sup>1</sup>, Maria T. Gomez<sup>1</sup>, Juan R. Castillo<sup>1</sup>; <sup>1</sup>University of Zaragoza

#### Poster Board #10

(531) **Detection, Characterization and Quantification of Titanium Dioxide Nanoparticles in Complex Samples by AF4-ICP-MS;** Francisco Laborda<sup>1</sup>, David Ojeda<sup>1</sup>, Vanesa Taboada-Lopez<sup>2</sup>, Eduardo Bolea<sup>1,2</sup>, Antonio Moreda<sup>2</sup>, Pilar Bermejo<sup>2</sup>, Juan R. Castillo<sup>1</sup>; <sup>1</sup>University of Zaragoza; <sup>2</sup>University of Santiago de Compostela

#### Poster Board #11

(532) **Role of Clusters for Non-Metal Ionization in ICP-Based Plasma Assisted Reaction Chemical Ionization (PARCI);** Joseph Lesniewski<sup>1</sup>, Kaveh Jorabchi<sup>1</sup>; <sup>1</sup>Georgetown University

#### Poster Board #12

(533) **Ultrasonic Autosampler to Reduce Nanoparticle Aggregation for ICPMS Analysis;** Derrick Quarles<sup>1</sup>, Jared Kaser<sup>1</sup>, Mason Spilinek<sup>1</sup>, Kyle Uhlmeier<sup>1</sup>, Daniel Wiederin<sup>1</sup>; <sup>1</sup>Elemental Scientific

#### Poster Board #13

(534) **Stable Isotope Amount Ratio Analysis by Using High-Resolution Continuum Source Graphite Furnace Molecular Absorption Spectrometry;** Carlos Abad<sup>1,2,3</sup>, Stefan Florek<sup>2</sup>, Helmut Becker-Ross<sup>2</sup>, Mao-Dong Huang<sup>2</sup>, Hans-Joachim Heinrich<sup>1</sup>, Sebastian Recknagel<sup>1</sup>, Jochen Vogl<sup>1</sup>, Norbert Jakubowski<sup>1,3</sup>, Ulrich Panne<sup>1,3</sup>; <sup>1</sup>Bundesanstalt für Materialforschung und -prüfung; <sup>2</sup>Leibniz-Institut für Analytische Wissenschaften; <sup>3</sup>Humboldt-Universität zu Berlin - SALSA

#### Poster Board #14

(535) **Towards Quantitative Analysis of Metallic and Metal Oxide Nanoparticles Using Microsecond Time-Resolved Single-Particle ICP-MS;** Ingo Streng<sup>1</sup>, Antonio R. Montoro Bustos<sup>1</sup>, Karen E. Murphy<sup>1</sup>, Michael R. Winchester<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

### 17WPIR: Wednesday Posters - Infrared Spectroscopy

#### Poster Board #15

(536) **Validation of ATR Correction and Reverse ATR Correction Algorithms, Improved by Optimized Corrections;** Gregory M. Banik<sup>1</sup>, Michelle D'Souza<sup>1</sup>, Keith Kunitsky<sup>1</sup>, Robin O'Connor<sup>1</sup>; <sup>1</sup>Bio-Rad Laboratories

#### Poster Board #16

(537) **Eliminating Fringes from Hyperspectral Data to Localize Chemically Distinct Macromolecules;** Ghazal Azarfar<sup>1</sup>, Ebrahim Aboulizadeh, Nick Walter<sup>1</sup>, Achim Kohler<sup>2</sup>, Carol Hirschmugl<sup>1</sup>; <sup>1</sup>University of Wisconsin Milwaukee; <sup>2</sup>Norwegian University of Life Sciences

#### Poster Board #17

(538) **Quantitative Analysis of Water Content in Polymer Samples by Terahertz Spectroscopy;** Hiromichi Hoshina<sup>1</sup>, Yoh Iwasaki<sup>1</sup>, Eriko Kometani<sup>2</sup>, Makoto Okamoto<sup>2</sup>, Chiko Otani<sup>1</sup>; <sup>1</sup>RIKEN; <sup>2</sup>Kuraray Co. Ltd.

#### Poster Board #18

(539) **Structural Analysis of the Bound Water in Poly(ethylene-vinylalcohol copolymers) by Terahertz Two-Dimensional Correlation Spectroscopy;** Hiromichi Hoshina<sup>1</sup>, Yoh Iwasaki<sup>1</sup>, Eriko Kometani<sup>2</sup>, Makoto Okamoto<sup>2</sup>, Chiko Otani<sup>2</sup>; <sup>1</sup>RIKEN; <sup>2</sup>Kuraray Co. Ltd



**TECHNICAL PROGRAM – WEDNESDAY**  
**Poster Sessions 11:00 am – 12:00 pm & 3:10 – 3:50 pm, SciX Exhibit Hall**

**Poster Board #19**

(540) **2D Correlation Analysis of Surface Reaction on LiFePO<sub>4</sub> Cathode During Charging-Discharging Process Using in-situ Raman Spectroscopy;** Young Mee Jung<sup>1</sup>, Yeonju Park<sup>1</sup>, Su Min Kim<sup>1</sup>, Sila Jin<sup>1</sup>;  
<sup>1</sup>Kangwon National University

**Poster Board #20**

(541) **Theoretical Modeling of Vibrational Coupling between Cyano- and Azido- Reporters;** David Hogle<sup>1</sup>, Ryan Gustafson<sup>1</sup>, Matthew Tucker<sup>1</sup>;  
<sup>1</sup>University of Nevada Reno

**Poster Board #21**

(542) **Spectroscopic Methods for Quantifying Diesel Particulate Matter;** David Parks<sup>1</sup>, Arthur Miller<sup>1</sup>, Peter Griffiths<sup>2</sup>; <sup>1</sup>CDC/NIOSH; <sup>2</sup>Griffiths Consulting LLC

**Poster Board #22**

(543) **Enhancement of Spectral Discrimination Among Samples Using Spectroscopic Mapping Over a Drop-and-Dry Spot;** Daun Seol<sup>1</sup>, Eunjin Jang<sup>1</sup>, Hoeil Chung<sup>1</sup>; <sup>1</sup>Hanyang University

**Poster Board #23**

(544) **Mass Balance and Unit Process Efficiency for the Refinement of Natural Products are Revealed via Spectroscopic Chemical Imaging;** Mark Boatwright<sup>1</sup>, David Wetzel<sup>1</sup>; <sup>1</sup>Kansas State University

**Poster Board #24**

(545) **Determination of Total Petroleum Hydrocarbons (TPH) in Soil by Portable Mid - ATR System;** Toni Miao, Natasha Sihota; <sup>1</sup>Chevron

**Poster Board #25**

(546) **Application of Infrared Microscopy to the Forensic Examination of Automotive Paint Smears;** Barry Lavine<sup>1</sup>, Undugodage Perera<sup>1</sup>, Kaan Kalkan<sup>2</sup>, Linqi Zhang<sup>2</sup>; <sup>1</sup>Department of Chemistry, Oklahoma State University; <sup>2</sup>Department of Mechanical & Aerospace Engineering

**Poster Board #26**

(547) **Differentiation of Bovine, Porcine, and Fish Gelatins by Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) Spectroscopy Coupled with Pattern Recognition;** Ahmet Kemal Aloglu<sup>1</sup>, Peter de B. Harrington<sup>1</sup>; <sup>1</sup>Ohio University

**Poster Board #27**

(548) **Water Solubility Measurements with FTIR for Carbon Capture and Sequestration Relevant Gas Mixtures;** Christopher Wiseall<sup>1</sup>; <sup>1</sup>University of Nottingham

**Poster Board #28**

(549) **Quest ATR Spectroscopy: Fast and Repeatable Analysis of Pharmaceuticals, Drugs and Forensic Samples;** Jeff D'Agostino<sup>1</sup>, Fawzi Abou-Chahine<sup>1</sup>, Mia Abbott<sup>2</sup>, Ben Schazmann<sup>2</sup>; <sup>1</sup>Specac; <sup>2</sup>Dublin Institute of Technology; <sup>3</sup>Staffordshire Univ

**Poster Board #29**

(550) **Measurement of Crystalline Silica Aerosol Using Quantum Cascade Laser-Based Infrared Spectroscopy;** Kevin Ashley<sup>1</sup>, Shijun Wei<sup>1,2</sup>, Pramod Kulkarni<sup>1</sup>, Lina Zheng<sup>1</sup>; <sup>1</sup>CDC/NIOSH; <sup>2</sup>University of Cincinnati

**Poster Board #30**

(551) **Analysis of Diffuse Reflectance Spectra of Dye in Milk Using Representative Layer Theory;** Akihiro Nojima, Takuya Kambayashi<sup>1</sup>, Shin-ichi Taniguchi<sup>1</sup>;  
<sup>1</sup>Hitachi, Ltd.

**Poster Board #31**

(552) **Precise Recovery of Coordinates by Image Processing Algorithm for FTIR Micro-Spectroscopy Limited Angle Computed Tomography;** Sugato Ray<sup>1</sup>, Nicholas Walter<sup>1</sup>, Alexander Schofield<sup>1</sup>, Ghazal Azarfar<sup>1</sup>, Reinhold Blumel<sup>3</sup>, Achim Kohler<sup>2</sup>, Carol Hirschmugl<sup>1</sup>; <sup>1</sup>University of Wisconsin Milwaukee (UWM); <sup>2</sup>Norwegian University of Life Sciences (NMBU); <sup>3</sup>Wesleyan University

**Poster Board #32**

(553) **Mid-Infrared Dispersion Spectroscopy for Trace Gas Sensing;** Jakob Hayden<sup>1</sup>, Pedro Martin-Mateos<sup>2</sup>, Pablo Acedo<sup>2</sup>, Bernhard Lendl<sup>1</sup>; <sup>1</sup>Technische Universitaet Wien; <sup>2</sup>Universidad Carlos III de Madrid

**Poster Board #33**

(554) **Environmental and Industrial Gas Applications of Integrated Cavity Output Spectroscopy;** Diane Errigo<sup>1</sup>, Frédéric Despagne<sup>1</sup>, Steven M. Barnett<sup>2</sup>; <sup>1</sup>ABB; <sup>2</sup>Barnett Technical Services

**Poster Board #34**

(555) **Determination of Domain Stability Using High Throughput-Developability and Comparability Assessment (HT-DCA) Platform and 2D IR and Co-Distribution Correlation Spectroscopies;** Belinda Pastrana<sup>1</sup>; <sup>1</sup>Protein Dynamic Solutions, LLC.

**Poster Board #35**

(556) **Fano Resonances in Infrared Spectroscopy;** Alex Schofield<sup>1</sup>, Reinhold Blumel<sup>2</sup>, Achim Kohler<sup>3</sup>, Rozalia Lukas<sup>3</sup>, Carol Hirschmugl<sup>1</sup>; <sup>1</sup>University of Wisconsin-Milwaukee; <sup>2</sup>Wesleyan University; <sup>3</sup>Norwegian University of Life Sciences

**Poster Board #36**

(557) **Determination of Water and Glycol Concentration in Engine Oil via Induced Emulsification";** Torrey Holland<sup>1</sup>, Ali Mazin Abdul-Munaim<sup>2</sup>, Dennis Watson<sup>3</sup>, Poopalasingam Sivakumar<sup>4</sup>; <sup>1</sup>Southern Illinois University Carbondale; <sup>2</sup>Southern Illinois University Carbondale; <sup>3</sup>Southern Illinois University Carbondale; <sup>4</sup>Southern Illinois University Carbondale

**Poster Board #37**

(558) **Ultrafast Angle-Resolved Photoemission Studies of Cuprate High-Temperature Superconductors;** Christopher Smallwood;  
<sup>1</sup>University of Michigan

**17WPMISC: Wednesday Posters**

**Poster Board 38#**

(559) **Fluorescence Optical Rotary Dispersion for Surface-Specific Chiral Analysis;** Garth J. Simpson<sup>1</sup>, Fengyuan Deng<sup>1</sup>, James R. W. Ulcickas<sup>1</sup>; <sup>1</sup>Purdue University

**Poster Board #39**

(560) **Exciton Correlation in Monolayer MoS<sub>2</sub> revealed by 2D Electronic Spectroscopy;** Liang Guo<sup>1,2</sup>, Daniele Monahan<sup>1</sup>, Graham Fleming<sup>1</sup>; <sup>1</sup>UC Berkeley; <sup>2</sup>Southern Univ of Science & Tech, China

**Poster Board #40**

(561) **Characterization of Ionic Liquids Used in Liquid-Liquid Extraction Processes by Raman Spectroscopy.;** Teresa Alejandra Razo Lazcano<sup>1</sup>, María del Pilar González Muñoz<sup>1</sup>, Mario Ávila Rodríguez<sup>1</sup>, Mercy Suguey Dzul Erosa<sup>1</sup>; <sup>1</sup>Guanajuato University

## TECHNICAL PROGRAM – WEDNESDAY

Poster Sessions 11:00 am – 12:00 pm & 3:10 – 3:50 pm, *SciX Exhibit Hall*

What's Hot Vendor Presentations ♦ Orals 1:30 – 3:10 pm

### Poster Board #41

(562) Interactions Between Ionic Liquids and Liposomes Studied by Differential Scanning Calorimetry; Antti Rantamäki<sup>1</sup>, Suvi-Katriina Ruokonen<sup>1</sup>, Alistair King<sup>1</sup>, Susanne Wiedmer<sup>1</sup>; <sup>1</sup>University of Helsinki

### Poster Board #42

(563) Spectrophotometric Determination of the Concentration of Zn (II), Eu(III), Lu (III), and La (III) with Eriochrome Black T; Daniela Tapia Pitzzu<sup>1</sup>, Jorge H.S.K. Monteiro<sup>1</sup>, Ana de Bettencourt-Dias<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

### Poster Board #43

(564) Multiple Simultaneous Spectroscopic Measurements with a Single Spectrometer; Claudio Egalon<sup>1</sup>; <sup>1</sup>Egalon Consultoria

### Poster Board #44

(565) Molecular Recognition of Muramyl Dipeptide Occurs in the Leucine-rich Repeat Domain of Nod2; Mackenzie Lauro<sup>1</sup>, Brian Bahnson<sup>1</sup>, Catherine Grimes<sup>1</sup>; <sup>1</sup>University of Delaware

11:40 AM – 1:10 PM

**WHAT'S HOT VENDOR PRESENTATIONS, Exhibit Hall**

Presider: Brian Dable, *Arete Associates*

Free lunch in exhibit hall for all conferees, ticket required

- 11:40 **Applied Spectra** “J200 Tandem Clarity – Gateway to Powerful LIBS and LA-ICP-MS Data Analysis”
- 11:50 **BioTools** “Disruptive Vibrational Spectroscopy: RAMAN, FT-IR, VCD & ROA”
- 12:00 **B&W Tek** “Seeing More and Identifying Rapidly with Raman: the i-Raman Pro ST”
- 12:10 **Metrohm USA** “Accelerated Results and Improved Reliability with Metrohm Spectroscopy”
- 12:20 **Ondax** “Rapid Discovery in Industrial Applications: High Throughput Screening with THz-Raman®”
- 12:30 **Flash Analysis** “Innovative Sensing Solutions from Flash Photonics”
- 12:40 **Necsel** “Narrow Linewidth Laser Modules for RAMAN Spectroscopy in Hazardous Environments”
- 12:50 **Wasatch** “Raman – Lowest Limit of Detection in the palm of your hand”
- 1:00 **HORIBA Scientific** “NanoRaman™ Platform: Physical and Chemical Imaging at the Nanoscale”

**Wednesday Afternoon, Crystal 2**

**17ATOM09: ICP-MS FOR THE ANALYSIS OF NANOMATERIALS**

Organizers and Presiders: Jose Manuel Costa, Francisco Laborda

- 1:30 PM (566) ICP-MS Based Methods for the Analysis of Nanomaterials; Francisco Laborda<sup>1</sup>, Eduardo Bolea<sup>1</sup>, Maria T. Gomez<sup>1</sup>, Maria S. Jimenez<sup>1</sup>, Juan R. Castillo<sup>1</sup>; <sup>1</sup>University of Zaragoza
- 1:50 PM (567) New Nanometrology Approaches for Examining Nanomaterials Released from Products Undergoing Weathering; James Ranvile<sup>1</sup>, Katie Challis<sup>1</sup>, Ronald Lankone<sup>2</sup>, Jing Jing Wang<sup>1</sup>, Howard Fairbrother<sup>2</sup>, Paul Westerhoff<sup>3</sup>; <sup>1</sup>Colorado School of Mines; <sup>2</sup>Johns Hopkins University; <sup>3</sup>Arizona State University
- 2:10 PM (568) Achieving Si Traceability for Number Concentration of Inorganic Nanoparticles Using SP-ICPMS; Susana Cuello-Nunez<sup>1</sup>, Dorota Bartczak<sup>1</sup>, Heidi Goenaga-Infante<sup>1</sup>; <sup>1</sup>LGC

- 2:30 PM (569) Metrological Traceability and Validation of Single Particle ICP-MS Measurements of Nanoparticle Size and Number Size Distribution using High - Resolution Scanning Electron Microscopy as Reference Method; Antonio R. Montoro Bustos<sup>1</sup>, Kavuri P. Purushotham<sup>1</sup>, Natalia Farkas<sup>1</sup>, Antonio Possolo<sup>1</sup>, András E. Vladár<sup>1</sup>, Karen E. Murphy<sup>1</sup>, Michael R. Winchester<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

- 2:50 PM (570) Field-Flow Fractionation Coupled to ICP-QQQ for Characterization of Functionalized Inorganic Nanoparticles; Jose Manuel Costa-Fernandez<sup>1</sup>; <sup>1</sup>University of Oviedo

**Wednesday Afternoon, Crystal 1**

**17AWD02: LESTER STROCK AWARD SYMPOSIUM HONORING FRANK VANHAECKE**

Organizer and Presider: Frank Vanhaecke

- 1:30 PM (571) Frank Vanhaecke: The Man in the ICP; Martin Resano<sup>1</sup>; <sup>1</sup>Universidad de Zaragoza
- 1:50 PM (572) Tracing Mercury Pollution in and Unraveling Exposure Pathways for Marine Species via High-Precision Isotopic Analysis with Multi-Collector ICP- Mass Spectrometry; Eduardo Bolea-Fernandez<sup>1</sup>, Ana Rua-Ibarz<sup>1</sup>, Amund Maage<sup>2</sup>, Sylvia Frantzen<sup>2</sup>, Jörg Feldmann<sup>3</sup>, Eva M. Krupp<sup>3</sup>, Frank Vanhaecke<sup>1</sup>; <sup>1</sup>Ghent University; <sup>2</sup>National Institute of Nutrition and Seafood Resea; <sup>3</sup>University of Aberdeen
- 2:10 PM (573) Green Sample Preparation Methods for Trace Element Determination by ICP-based Techniques; Erico Flores; <sup>1</sup>Universidade Federal de Santa Maria
- 2:30 PM (574) Characterization of SiO<sub>2</sub> Nanoparticles by Single Particle – Inductively Coupled Plasma – Tandem Mass Spectroscopy (SP-ICP-MS/MS); Maite Aramendia<sup>1,3</sup>, Eduardo Bolea-Fernandez<sup>2</sup>, Diego Leite<sup>3</sup>, Ana Rua-Ibarz<sup>2</sup>, Lieve Balcaen<sup>2</sup>, Martín Resano<sup>3</sup>, Frank Vanhaecke<sup>2</sup>; <sup>1</sup>Centro Universitario de la Defensa; <sup>2</sup>Ghent University; <sup>3</sup>University of Zaragoza
- 2:50 PM (575) LA-ICP-MS: Theoretical Considerations on and Perspectives for its Future Development.; Stijn J. M. Van Malderen<sup>1</sup>, Frank Vanhaecke<sup>1</sup>, Olga Borovinskaya<sup>2</sup>; <sup>1</sup>Ghent University; <sup>2</sup>TOFWERK AG

**Wednesday Afternoon, Nevada 7**

**17BIM05: BIG DATA IN BIOMEDICAL ANALYSES**

Organizer and Presider: David Mayerich

- 1:30 PM (576) Turning Chemical Imaging Data to Useful Information; Rohit Bhargava<sup>1</sup>, Shachi Mittal<sup>1</sup>, Kevin Yeh<sup>1</sup>; <sup>1</sup>University of Illinois at Urbana-Champaign
- 1:50 PM (577) Does Every Image Pixel Matter in TB-sized Images?; Peter Bajcsy<sup>1</sup>; <sup>1</sup>NIST
- 2:10 PM (578) Chemometric Concepts Applied to Digital Signal Processing; Garth Simpson<sup>1</sup>, Scott Griffin<sup>1</sup>, Scott R. Griffin, Gregory Eakins, Fengyuan Deng, Atanu Sangupta; <sup>1</sup>Purdue University
- 2:30 PM (579) Rethinking the Classification Process with Data Fusion; John Kalivas<sup>1</sup>, Brett Brownfield<sup>1</sup>; <sup>1</sup>Idaho State University
- 2:50 PM (580) New Methodolgy for Finding Optimal Spectral Matches in Reference Databases; Dr. Gregory M. Banik<sup>1</sup>, Karl Nedwed<sup>1</sup>, Ty Abshear<sup>1</sup>; <sup>1</sup>Bio-Rad Laboratories, Informatics Division

# TECHNICAL PROGRAM – WENDESDAY

Orals 1:30 – 3:10 pm

## Wednesday Afternoon, *Crystal 5*

### 17CTP05: FOOD SAFETY AND ANALYSIS: ISSUES AND SOLUTIONS IN IMPLEMENTATION IN THE DEVELOPING WORLD

Organizer and Presider: Janie Dubois

- 1:30 PM (581) **The FDA Food & Veterinary Medicine Science and Research Program: In Search of Partnerships to Develop Innovative Food Safety Applications;** Palmer A. Orlandi<sup>1</sup>, Janie Dubois<sup>2</sup>; <sup>1</sup>US FDA, Office of Foods and Veterinary Medicine; <sup>2</sup>University of Maryland, JIFSAN
- 2:10 PM (582) **“My Method is Valid” – Can You Prove That in Court?;** DeAnn Benesh<sup>1</sup>; <sup>3</sup>M
- 2:30 PM (583) **Use of Chemometrics to Identify Marker Compounds for Food Authentication;** Zhengfang Wang<sup>1</sup>; <sup>1</sup>University of Maryland

## 17IR10 Wednesday Afternoon, *Carson 1*

### 17IR10: ULTRAFAST TWO-DIMENSIONAL SPECTROSCOPY - II

Organizer and Presider: Kyle Czech

- 1:30 PM (584) **Pathway Selective CMDs for Revealing Weak Interactions in Complex Systems;** Jeffrey Davis<sup>1</sup>, Jonathan Tollerud<sup>1</sup>, Fabio Novelli<sup>1</sup>; <sup>1</sup>Swinburne University of Technology
- 2:10 PM (585) **2D Spectroscopy of 2D Materials: Insight into Exciton Dynamics in Atomically Thin Semiconductors;** Galan Moody<sup>1</sup>; <sup>1</sup>National Institute of Standards & Technology
- 2:30 PM (586) **2D Transient Absorption Spectroscopy of Transition Metal Dichalcogenide Heterostructures;** Kyle Czech<sup>1</sup>, Zach Matusinec<sup>1</sup>, John Wright<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison
- 2:50 PM (587) **Global Analysis of Transient Grating and Transient Absorption Spectra of PbSe Quantum Dots;** Daniel Kohler<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

## Wednesday Afternoon, *Crystal 3*

### 17LIBS08: NALIBS: FUNDAMENTALS OF LASER-INDUCED PLASMAS

Organizer and Presider: Prasoon Diwakar

- 1:30 PM (588) **Ultrafast Laser-Induced Plasma Diffusion and Mixing Processes at Interfaces;** Vassilia Zorba, Ran Hai, Xianglei Mao, Rick Russo; <sup>1</sup>Lawrence Berkeley National Laboratory
- 1:50 PM (589) **Fundamental Aspects and Applications of Laser-Induced Plasma Under Water in a Range of Pressure Between 1-150 Bar.;** Alessandro De Giacomo<sup>1,2</sup>, Marcella Dell'Aglio<sup>2</sup>, Antonio Santagata<sup>3</sup>, Gabriele Valenza<sup>1</sup>; <sup>1</sup>University of Bari; <sup>2</sup>CNR-NANOTEC; <sup>3</sup>CNR-ISM
- 2:10 PM (590) **Isotopic Analysis of Uranium Using Laser Induced Fluorescence of LIBS Plumes;** Sivanandan Harilal<sup>1</sup>, Kyle Hartig<sup>1,2,4</sup>, Brian Brumfield<sup>1</sup>, Igor Jovanovic<sup>3</sup>, Mark Phillips<sup>1</sup>; <sup>1</sup>PNNL; <sup>2</sup>The Pennsylvania State University; <sup>3</sup>University of Michigan, Ann Arbor; <sup>4</sup>University of Florida
- 2:30 PM (591) **Comprehensive Ultrashort Laser -Metal Ablation at Terawatt Laser Power;** Ahmed Elsieid<sup>1</sup>, Prasoon Diwakar<sup>1</sup>, Ahmed Hassanein<sup>1</sup>; <sup>1</sup>Purdue Univ
- 2:50 PM (592) **Plasma Dynamics Following Femtosecond Filament Interactions with Solids in Single and Multiple Filament Regimes;** Patrick Skrodzki<sup>1</sup>, Milos Burger<sup>1</sup>, Igor Jovanovic<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI

## Wednesday Afternoon, *Nevada 6*

### 17PAT06: PROCESS MONITORING ENABLED FLOW API AND CONTINUOUS PRODUCT MANUFACTURE

Organizer and Presider: Jim Rydzak

- 1:30 PM (593) **Development of Continuous Flow Chemistry Using Online PAT;** Eric Fang<sup>1</sup>; <sup>1</sup>Snapdragon Chemistry, Inc
- 1:50 PM (594) **Continuous Processing Strategies for Global Health Targets;** Katherine Belecki<sup>1</sup>; <sup>1</sup>Virginia Commonwealth University
- 2:30 PM (595) **Advanced Process Control and PAT – Criticality of Attribute Measurement on a Continuous Tableting Line – Feed Monitoring Example.;** Benoit Igne<sup>1</sup>; <sup>1</sup>GlaxoSmithKline
- 2:50 PM (596) **Integrating Sensors for Monitoring Blend Content in a Pharmaceutical Continuous Manufacturing Plant;** Savitha Panikar<sup>1</sup>, Jingzhe Li<sup>1</sup>, Varsha Rane<sup>1</sup>, Sean Gilliam<sup>2</sup>, Gerardo Callegari<sup>1</sup>, Fernando Muzzio<sup>1</sup>; <sup>1</sup>Rutgers University; <sup>2</sup>Kaiser Optical Systems

## Wednesday Afternoon, *Carson 2*

### 17PMA08: BIOLOGICS CHARACTERIZATION FROM EARLY TO LATE STAGE DEVELOPMENT

Organizer and Presider: Gurusamy Balakrishnan

- 1:30 PM (597) **Identification of Subvisible Particles in Biopharmaceutical Formulations: Raman Spectroscopy and More;** Miguel Saggu<sup>1</sup>, Ankit Patel<sup>1</sup>; <sup>1</sup>Genentech
- 1:50 PM (598) **Analytical Methods and Characterization Techniques for Drug/Device Combination Products;** Sundaravel "Ananth" Ananthavel<sup>1</sup>; <sup>1</sup>AcelRx Pharmaceuticals
- 2:10 PM (599) **Monitoring Oxidation of Methionine Residues in Biotherapeutic Proteins Using Raman and FTIR Spectroscopy;** Gurusamy Balakrishnan<sup>1</sup>, Gregory Barnett<sup>1</sup>, Tapan Das<sup>1</sup>, Sambit Kar<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb
- 2:30 PM (600) **Raman Spectroscopy for Monitoring Bispecific Antibody Assembly;** Andrew Maier<sup>1</sup>; <sup>1</sup>Genentech
- 2:50 PM (601) **Field Flow Fractionation Characterization of the NIST Monoclonal Antibody Standard RM 8671;** Robert Reed<sup>1</sup>, Soheyl Tadjiki<sup>1</sup>, Thorsten Klein<sup>2</sup>; <sup>1</sup>Postnova Analytics Inc.; <sup>2</sup>Postnova Analytics GmbH

## Wednesday Afternoon, *Carson 4*

### 17RAM12: PORTABLE RAMAN

Organizer and Presider: Neil Shand

- 1:30 PM (602) **Use of Portable Raman Spectroscopy in Low Resource Settings;** Matt Keller<sup>1</sup>, Changwon Lee<sup>1</sup>, Wenbo Wang<sup>1</sup>, Jim Stafford<sup>1</sup>, Ben Wilson<sup>1</sup>; <sup>1</sup>Intellectual Ventures Laboratory
- 1:50 PM (603) **Extending Raman;** David Creasey<sup>1</sup>; <sup>1</sup>Wasatch Photonics
- 2:10 PM (604) **Dual Wavelength Applications in Portable Raman Spectroscopy;** Robert Chiment<sup>1</sup>; <sup>1</sup>Innovative Photonic Solutions
- 2:30 PM (605) **Ocean Optics Miniature Raman Spectrometer Development;** Joseph Bonvallet<sup>1</sup>, Bryan Auz<sup>1</sup>, Doug Anderson<sup>1</sup>, Ty Olmstead<sup>1</sup>; <sup>1</sup>Ocean Optics Inc
- 2:50 PM (606) **Raman Imaging for Drugs & Explosives Particle Detection with a High Throughput Virtual Slit;** Edward Gooding<sup>1</sup>, Erik Deutsch<sup>1</sup>, Joseph Huehnerhoff<sup>1</sup>, Jason Lozo<sup>1</sup>, Courtney Johnson<sup>1</sup>, Arsen Hajian<sup>1</sup>; <sup>1</sup>Hindsight Imaging, Inc.



## TECHNICAL PROGRAM – WEDNESDAY

**Orals 1:30 – 3:10 pm & 3:50 – 5:30 pm**

### Wednesday Afternoon, *Carson 3*

#### 17RAM14: INDUSTRIAL RAMAN SPECTROSCOPY

Organizer and President: Karen Esmonde-White

- 1:30 PM (607) **Real Time Measurements of Polymer Properties by Raman Spectroscopy**; Patrice Bourson<sup>1</sup>, David Chaprob<sup>1</sup>, Elise Dropsit<sup>1</sup>, Isabelle Royaud<sup>2</sup>, Marc Poncot<sup>2</sup>, Abdessalam Dahoun<sup>2</sup>, Alain Durand<sup>3</sup>, Sandrine Hoppe<sup>4</sup>, Sarah Saidi<sup>1</sup>, <sup>1</sup>LMOPS CentraleSupélec, University of Lorraine; <sup>2</sup>Institut Jean Lamour - UMR 7198 CNRS - Université; <sup>3</sup>LPMC University of Lorraine; <sup>4</sup>LRGP, University of Lorraine
- 1:50 PM (608) **Chemometric Model Development and Maintenance – An Industry Case Study**; Michael F. Roberto<sup>1</sup>, Randy J Pell<sup>1</sup>; <sup>1</sup>Infometrix, Inc.
- 2:10 PM (609) **Crystallinity and Density Assessment of Layered Polyethylene Using Confocal Raman Microscopy**; Mohammed Ibrahim<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific
- 2:30 PM (610) **Raman Analysis of Multiple Melting Peaks of Polyethylene**; Young Jong Lee<sup>1</sup>, Ying Jin<sup>1</sup>, Anthony Kotula<sup>1</sup>, Chad Snyder<sup>1</sup>, Angela Hight Walker<sup>1</sup>, Klamann Migler<sup>1</sup>; <sup>1</sup>National Institute of Standards and Technology

### Wednesday Afternoon, *Nevada 5*

#### 17SPR05: PLASMON-ENHANCED TECHNIQUES

Organizer and President: Jean-Francois Masson

- 1:30 PM (611) **Plasmon Driven Reactivity**; Zachary Schultz<sup>1</sup>, Darby Nelson<sup>1</sup>, Zhicong Zeng<sup>1</sup>, Hao Wang<sup>1</sup>; <sup>1</sup>University of Notre Dame
- 1:50 PM (612) **Biocompatible, Liposome-Based Surface Enhanced Raman Spectroscopy (SERS) Substrates**; Laura Sagie<sup>1</sup>, William Lum<sup>1</sup>, Ian Bruzas<sup>1</sup>, Zohre Gorunmez<sup>2</sup>; <sup>1</sup>University of Cincinnati, Chemistry Department; <sup>2</sup>University of Cincinnati, Physics Department
- 2:10 PM (613) **Plasmon-Enhanced Fluorescence and Energy Transfer in Composite Nanoparticles and Applications to Sensitive Chemical Detection**; Denis Boudreau<sup>1</sup>, Jeremie Asselin<sup>1</sup>, Nicolas Fontaine<sup>1</sup>, Rihab Bouchareb<sup>1</sup>, Mazeyar Parvinzadeh Gashfi<sup>1</sup>, Simon Labrecque<sup>1</sup>, Paul De Koninck<sup>1</sup>, Jesse Greener<sup>1</sup>, Patrick Mathieu<sup>1</sup>; <sup>1</sup>Université Laval
- 2:30 PM (614) **Plasmonic Nanoparticle Probes for Optical Spectroscopy**; Andrea Tao<sup>1</sup>, Tyler Dill<sup>1</sup>, Yuan Zheng<sup>1</sup>; <sup>1</sup>UC San Diego
- 2:50 PM (615) **Plasmonic Enhancement of Fluorescence as a Tool in Single-Particle Analysis of Ion Concentrations**; Jeremie Asselin<sup>1</sup>, Nicolas Fontaine<sup>1</sup>, Simon Labrecque<sup>2</sup>, Paul De Koninck<sup>2</sup>, Denis Boudreau<sup>1</sup>; <sup>1</sup>Université Laval; <sup>2</sup>IUSMQ

### Wednesday Afternoon, *Crystal 4*

#### 17SURFACE02: MICROSCOPIC METHODS FOR SURFACE SCIENCE PROBLEMS

Organizer and President: Svitlana Pylypenko

- 1:30 PM (616) **Integrating Novel Microscopy into Battery Research: From Atomic Resolution to In Situ and Functional Imaging**; Miaofang Chi; <sup>1</sup>Oak Ridge National Laboratory
- 1:50 PM (617) **Recent Developments in AFM Analysis of Soft Materials at the Nanoscale**; Igor Sokolov<sup>1</sup>, Maxim Dokukin<sup>1</sup>; <sup>1</sup>Tufts University
- 2:10 PM (618) **Materials Science at Surfaces - 2D Materials and Nanospheres**; Petra Reinke<sup>1</sup>, Cameron Volders<sup>1</sup>, Ehsan Monazami<sup>1</sup>, Gopalakrishnan Ramalingam<sup>1</sup>,

John Brandon McClimon<sup>2</sup>; <sup>1</sup>University of Virginia; <sup>2</sup>University of Pennsylvania

- 2:30 PM (619) **Analysis of Nanoscale Semiconductor Devices Using Advanced Scanning Probe Microscopy Techniques**; Phil Kaszuba<sup>1</sup>; <sup>1</sup>Globalfoundries
- 2:50 PM (620) **Nanoscale Chemical Analysis with Photo-Induced Force Microscopy**; Sung Park<sup>1</sup>; <sup>1</sup>Molecular Vista, Inc.

### 3:10 PM Poster Session and Coffee Break, *SciX Exhibit Hall*

### Wednesday Afternoon, *Crystal 2*

#### 17ATOM10: ATMOSPHERIC-PRESSURE PLASMAS FOR OPTICAL MASS SPECTROMETRIES

Organizer and President: Jacob T. Shelley

- 3:50 PM (621) **High Analytical Power Density with the Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD) Microplasma**; High Analytical Power Density with the Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD) Microplasma; R. Kenneth Marcus<sup>1</sup>; <sup>1</sup>Clemson University
- 4:10 PM (622) **Chemical, Electrical, and Spectroscopic Studies of a Solution-Cathode Glow Discharge**; Michael Webb<sup>1</sup>, Denise Moon<sup>2</sup>, Scott Crowe<sup>1</sup>; <sup>1</sup>University of North Carolina Wilmington; <sup>2</sup>ChemImage
- 4:30 PM (623) **Charge Controlled Electrospray Ionization and Plasma Ionization via Triboelectric Nanogenerator (TENG)**; Anyin Li<sup>1</sup>, Yunlong Zi<sup>1</sup>, Zhong Lin Wang<sup>1</sup>, Facundo Fernandez<sup>1</sup>; <sup>1</sup>Georgia Institute of Technology
- 4:50 PM (624) **Soft Argon-Propane Dielectric Barrier Discharge for Mass Spectrometry**; Alexander Schütz<sup>1</sup>, Felix David Klute<sup>1</sup>, Sebastian Brandt<sup>1</sup>, Joachim Franzke<sup>1</sup>; <sup>1</sup>ISAS
- 5:10 PM (625) **Analysis of Nanomaterials Using CE-spICP-MS with Microsecond Dwell Times**; Carsten Engelhard<sup>1</sup>; <sup>1</sup>University of Siegen

### Wednesday Afternoon, *Crystal 1*

#### 17AWD10: BRUCE R. KOWALSKI AWARD IN CHEMOMETRICS SYMPOSIUM HONORING JOSEPH SMITH

Organizer and President: Barry Lavine

- 3:50 PM (626) **Analysis of Lipoprotein and Cholesterol Content Using Chemometrics and Deep-Ultraviolet Resonance Raman Spectroscopy**; Renee JiJi<sup>1</sup>, Michael Eagleburger<sup>1</sup>; <sup>1</sup>University of Missouri
- 4:10 PM (627) **Chemometric Applications of Walsh-Hadamard Filter Functions**; Timothy Corcoran<sup>1</sup>; <sup>1</sup>California State Polytechnic University Pomona
- 4:30 PM (628) **Multivariate Analysis and Raman Microspectroscopic Imaging: Implications for the Search for Life on Mars**; Joseph Smith<sup>1</sup>, Frank Smith<sup>1</sup>, Karl Booksh<sup>1</sup>; <sup>1</sup>University of Delaware
- 4:50 PM (629) **Variable Selection to Improve Reliability and to Reduce Cost of Ownership for Classifications and Calibrations**; Undugodage Perera Perera<sup>1</sup>, Matthew Allen<sup>1</sup>, Joshua Ottaway<sup>2</sup>, Kristl Adams<sup>2</sup>, Chance Carter<sup>2</sup>, Steven Brown<sup>3</sup>, Karl Booksh<sup>3</sup>; <sup>1</sup>Oklahoma State University; <sup>2</sup>Lawrence Livermore National Laboratory; <sup>3</sup>University of Delaware
- 5:10 PM (630) **Modeling Microalgal Biosediment Formation based on FTIR-ATR Monitoring**; Frank Vogt<sup>1</sup>, Zachary Ogburn<sup>1</sup>; <sup>1</sup>University of Tennessee - Chemistry Department



# TECHNICAL PROGRAM – WEDNESDAY

Orals 3:50 – 5:30 pm

## Wednesday Afternoon, Nevada 7

### 17BIM06: SPECTRAL ANALYSIS OF COLLAGENOUS TISSUES

Organizer and Presider: Katherine Cilwa

- 3:50 PM (631) **Rapid and Accurate Peripheral Nerve Imaging by Multipoint Raman Spectroscopy;** Yasuaki Kumamoto<sup>1</sup>, Yoshinori Harada<sup>1</sup>, Hideo Tanaka<sup>1</sup>, Tetsuro Takamatsu<sup>1</sup>; <sup>1</sup>Kyoto Pref. Univ. of Medicine
- 4:10 PM (632) **Spectroscopic Evaluation of Collagen Fibrosis in Post-Myocardial Infarction Cardiac Tissue;** Kathleen Gough<sup>1</sup>, Negar Atefi<sup>1</sup>, Richard Wiens<sup>1</sup>, Ian Dixon<sup>1</sup>; <sup>1</sup>University of Manitoba
- 4:30 PM (633) **Challenges in Infrared Spectroscopic Data Collection and Processing from Collagen-Containing Tissues;** Mugdha Padalkar<sup>1</sup>, Rutvin Kyada<sup>1</sup>, Farzad Yousefi<sup>1</sup>, Ramya Ailavajhala<sup>1</sup>, Jessica Falcon<sup>1</sup>, Nancy Pleshko<sup>1</sup>; <sup>1</sup>Temple University
- 4:50 PM (634) **Quantification of Differences in Bone Mineral Phosphate Peak Positions and Relative Intensities in Transmission vs. ATR Spectroscopic Data Collection;** William Querido<sup>1</sup>, Ramyasri Ailavajhala<sup>1</sup>, Mugdha Padalkar<sup>1</sup>, Nancy Pleshko<sup>1</sup>; <sup>1</sup>Temple University
- 5:10 PM (635) **Carbonate in Bone Mineral: Discriminating the Structural Changes Simultaneously Imposed by Carbonate in A and B Sites of Apatite;** Mary Tecklenburg<sup>1</sup>, Honey Madupalli<sup>1</sup>; <sup>1</sup>Central Michigan University

## Wednesday Afternoon, Nevada 6

### 17FORENS03: PROTEOMICS FOR FORENSIC ANALYSIS

Organizer and Presider: Katelyn Mason

- 3:50 PM (636) **Overview of Proteomic Approaches to Forensics at LLNL;** Katelyn Mason<sup>1</sup>, Deon Anex<sup>1</sup>, Glendon Parker<sup>1,3</sup>, Bradley Hart<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory; <sup>2</sup>Protein Based Identification Technologies; <sup>3</sup>University of California Davis
- 4:10 PM (637) **Proteomic Approaches to Increasing the Value of Hair Shaft Evidence;** Robert Rice<sup>1</sup>, Pei-Wen Wu<sup>1</sup>, Tempest Plott<sup>1</sup>, Zachary Goecker<sup>1</sup>, Glendon Parker<sup>1</sup>; <sup>1</sup>University of California Davis
- 4:30 PM (638) **Combining Mass Spectrometry Protein Analysis and DNA PCR-STR Testing for Contact Traces;** Mechthild Prinz<sup>1</sup>, Steven Kranes<sup>1</sup>, Stacey Ann Sterling<sup>1</sup>, Glendon Parker<sup>2</sup>, Katelyn Mason<sup>3</sup>, Deon Anex<sup>3</sup>, Bradley Hart<sup>3</sup>; <sup>1</sup>John Jay College of Criminal Justice; <sup>2</sup>UC Davis; <sup>3</sup>Lawrence Livermore National Laboratory
- 4:50 PM (639) **“NextGen Serology: Leveraging Mass Spectrometry for Protein Based Human Body Fluid Identification;** Phillip Danielson<sup>1</sup>, Kevin Legg<sup>2</sup>, Heather McKiernan<sup>1,2</sup>; <sup>1</sup>University of Denver; <sup>2</sup>Center for Forensic Science Research and Education
- 5:10 PM (640) **High-Throughput Screening for Lipid Biomarker Discovery in Novel Arabidopsis Thaliana Signaling Pathway;** Rebecca Hansen<sup>1</sup>, Hongqing Guo<sup>1</sup>, Yanhai Yin<sup>1</sup>, Young-Jin Lee<sup>1</sup>; <sup>1</sup>Iowa State University

## Wednesday Afternoon, Carson 1

### 17IR11: ULTRAFAST TWO-DIMENSIONAL SPECTROSCOPY-III

Organizer and Presider: Kyle Czech

- 3:50 PM (641) **Analytical Solutions to the Finite-Pulse Bloch Model for Multidimensional Coherent Spectroscopy;** Christopher Smallwood<sup>1,2</sup>, Travis Autry<sup>2,3</sup>, Steven Cundiff<sup>1,2,3</sup>; <sup>1</sup>University of Michigan; <sup>2</sup>JILA (University of Colorado & NIST); <sup>3</sup>University of Colorado
- 4:10 PM (642) **Simulating Vibrational Spectroscopic Experiments with Wilson;** Magnus Ringholm<sup>1</sup>; <sup>1</sup>UiT The Arctic University of Norway
- 4:30 PM (643) **Many-Body Theory of Quasiparticle-Resolving Spectroscopies;** Mackillo Kira<sup>1</sup>; <sup>1</sup>University of Michigan-Ann Arbor
- 5:10 PM (644) **Round Table Discussion;** Kyle Czech<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

## Wednesday Afternoon, Crystal 3

### 17LIBS09: NALIBS: NEW METHODS AND ADVANCEMENTS IN LIBS

Organizer and Presider: Vassilia Zorba

- 3:50 PM (645) **Spectral Identification in the Attogram Regime through Laser-Induced Breakdown Spectroscopy of Single Optically-Trapped Nanoparticles in Air;** Javier Laserna<sup>1</sup>, Pablo Purohit<sup>1</sup>; <sup>1</sup>Universidad de Malaga
- 4:10 PM (646) **Femtosecond LIBS with Optical Vortex Beams;** Vassilia Zorba<sup>1</sup>, Jason R. Becker<sup>1,2</sup>, Xianglei Mao<sup>1</sup>, Rick Russo<sup>1</sup>, Costas P. Grigoropoulos<sup>2</sup>; <sup>1</sup>Lawrence Berkeley National Laboratory; <sup>2</sup>University of California, Berkeley
- 4:30 PM (647) **Calibration-Free Monte Carlo Method for Laser-Induced Breakdown Spectroscopy;** Igor Gornushkin, Alexander Kazakov<sup>2</sup>, Ulrich Panne<sup>1</sup>, Norbert Huber<sup>3</sup>, Johannes Pedarnig<sup>3</sup>, Simon Eschböck-Fuchs<sup>4</sup>, Roman Rössler<sup>4</sup>; <sup>1</sup>BAM; <sup>2</sup>Saint Petersburg State University of Aerospace In; <sup>3</sup>Institute of Applied Physics, Johannes Kepler Uni; <sup>4</sup>voestalpine Stahl GmbH, 4020 Linz, Austria
- 4:50 PM (648) **Exploiting UV-femtosecond LIBS in Single- and Double-Pulse Modes for the Sensitive Analysis of Aerosols and Thin Films;** Demetrios Anglos<sup>1,2</sup>, Konstantinos Marmatakis<sup>1,2</sup>, Nikos Giannakaris<sup>1,2</sup>, Panayiotis Siozos<sup>1</sup>; <sup>1</sup>IESL-FORTH; <sup>2</sup>Dept. of Chemistry, Univ. of Crete
- 5:10 PM (649) **Advances in LIBS and Challenges;** Mohamad Sabsabi<sup>1</sup>; <sup>1</sup>National Research Council Canada (NRC)

## Wednesday Afternoon, Carson 2

### 17PMA09: ADVANCES IN MICRO-ANALYSIS OF BIOLOGICS

Organizers: Lydia Breckenridge, Rina Dukor

Presiders: John Wasylyk, Anna Luczak

- 3:50 PM (650) **Chemical Denaturation of Bovine Serum Albumin Observed by DUV Photoelectron Yield Spectroscopy Combined with IR-Laser Ablation of Droplet Beam;** Hiroya Asami<sup>1</sup>, Tomoko Hasegawa<sup>1</sup>, Jun-ya Kohno<sup>1</sup>; <sup>1</sup>Gakushuin University
- 4:10 PM (651) **Vibrational Spectroscopy Studies of the Interaction of Cytochrome c with Cardiolipin in Phospholipid Membranes;** Jay Kitt<sup>1</sup>, David Bryce<sup>1</sup>, Joel Harris<sup>1</sup>; <sup>1</sup>University of Utah

## TECHNICAL PROGRAM – WEDNESDAY

**Orals 3:50 – 5:30 pm**

- 4:30 PM (652) **Structure and Stability of BioPharmaceuticals with Raman and ROA spectroscopy**; Rina Dukor<sup>1</sup>, Juanita Sanchez<sup>1</sup>, Carolina Carballo<sup>1</sup>, Laurence Nafie<sup>1,2</sup>; <sup>1</sup>BioTools Inc; <sup>2</sup>Syracuse University
- 4:50 PM (653) **Deconvolution of Vibrational Spectra for Analysis of Protein Secondary Structure**; John Wasyluk<sup>1</sup>, Mary Krause<sup>1</sup>, Daniel Fichana<sup>1</sup>, Ming Huang<sup>1</sup>, Robert Wethman<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Co.
- 5:10 PM (654) **Biopharmaceutical Applications of ICP-MS**; Lydia Breckenridge, Masano Huang<sup>1</sup>, Mary Krause<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

### Wednesday Afternoon, Carson 3

#### 17RAM13: PHARMACEUTICAL AND BIOTECHNOLOGY INDUSTRIAL APPLICATIONS OF RAMAN SPECTROSCOPY

Organizer and Presider: Karen Esmonde-White

- 3:50 PM (655) **Process Optimization Strategies for Cell Culture Bioreactors Using Raman Spectroscopy and Multivariate Analysis**; Karin Balss<sup>1</sup>, Ann Edwards<sup>1</sup>, Wan Su<sup>1</sup>, Carl Rafferty<sup>1</sup>, Dan Trout<sup>1</sup>, Steve Mehrman<sup>1</sup>, Priya Ramachandral<sup>1</sup>, Raghunath Shivappa<sup>1</sup>, Olav Lyngberg<sup>1</sup>; <sup>1</sup>Janssen Pharmaceuticals
- 4:10 PM (656) **Use of PAT in the Selection of a Design Space based on Process Understanding: A Case Study**; Antonio Ramirez<sup>1</sup>, Daniel Hallow<sup>2</sup>, Michaël Fenster<sup>1</sup>, Sha Lou<sup>1</sup>, Nathan Domagalski<sup>1</sup>, Srinivas Tummala<sup>1</sup>, Sushil Srivastava<sup>1</sup>, Lindsay Hobson<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb Company; <sup>2</sup>Noramco
- 4:30 PM (657) **Aldehyde Detection, Speciation, and Quantification Using Surface-Enhanced Raman Spectroscopy**; Mark Peterman<sup>1</sup>, Samuel Kleinman<sup>1</sup>, Merwan Benhabib<sup>1</sup>; <sup>1</sup>OndaVia, Inc.
- 4:50 PM (658) **Label Free Approach to Monitor Ultra-Violet Radiation Induced Changes in Skin Cells**; Surya Singh<sup>1</sup>, Jeon Woong Kang<sup>1</sup>, Ramachandra Rao Dasari<sup>1</sup>; <sup>1</sup>Massachusetts Institute of Technology
- 5:10 PM (659) **Substrate Evaluation Using Single Molecule SERS**; Alexandre Brolo, MuYang Zhang<sup>1</sup>; <sup>1</sup>University of Victoria, Dept of Chemistry

### Wednesday Afternoon, Carson 4

#### 17RAM20: RAMAN OPTICAL ACTIVITY (ROA)

Organizer and Presider: Christian Johannessen

- 3:50 PM (660) **Raman Optical Activity of Biofluids: Molecular Signature of Health and Disease?**; Vladimír Setnička<sup>1</sup>, Lucie Habartová<sup>1</sup>; <sup>1</sup>University of Chemistry and Technology Prague
- 4:10 PM (661) **Raman Optical Activity: From Carbohydrates to Pharmaceuticals**; Václav Profant<sup>1</sup>, Petr Bouř<sup>2</sup>, Vladimír Baumruk<sup>1</sup>; <sup>1</sup>Charles University; <sup>2</sup>Institute of Organic Chemistry and Biochemistry
- 4:30 PM (662) **Quantitative Analysis of Raman Optical Activity Spectra for the Assignment of Polysaccharide Structure in the Gel Phase**; Steffen Lüdeke<sup>1</sup>, Anja Rütther<sup>1</sup>, Aurelien Forget<sup>1,2</sup>, Anjan Roy<sup>3</sup>, Carolina Carballo<sup>3</sup>, Florian Mießner<sup>1</sup>, Rina K. Dukor<sup>3</sup>, Laurence A. Nafie<sup>3</sup>, Christian Johannessen<sup>4</sup>, V. Prasad Shastri<sup>1</sup>; <sup>1</sup>University of Freiburg; <sup>2</sup>Queensland

University of Technology; <sup>3</sup>BioTools, Inc.; <sup>4</sup>University of Antwerp

- 4:50 PM (663) **Raman Optical Activity of the Hydrogen Out-of-Plane Mode is a Sensitive Probe of Chromophore Distortions in a Photoreceptor Protein**; Masashi Unno<sup>1</sup>; <sup>1</sup>Saga University
- 5:10 PM (664) **Studying the Various Structural Forms of Alpha Synuclein by Means of Raman Optical Activity**; Christian Johannessen<sup>1</sup>, Carl Mensch<sup>1,2</sup>; <sup>1</sup>University of Antwerp; <sup>2</sup>Ghent University

### Wednesday Afternoon, Nevada 5

#### 17SPR04: POINT-OF-CARE PLASMONICS

Organizer and Presider: Jean-Francois Masson

- 3:50 PM (665) **Scalable Nanofabrication of Cost-Effective 3D Plasmonic Chips for Point of Care Applications**; Wei-Chuan Shih<sup>1</sup>; <sup>1</sup>University of Houston
- 4:10 PM (666) **Manipulating Plasmonic Hot Spots as a Strategy for Enhanced Clinical Diagnostics**; Marc Porter, Nicholas Owens<sup>1</sup>, Jason Beck<sup>1</sup>, Michael Granger<sup>1</sup>; <sup>1</sup>University of Utah
- 4:30 PM (667) **A Biogenic Silver Nanoparticle Based Assay for Improved Cancer Diagnostics**; Mark McDermott<sup>1</sup>, Sunil Rajput<sup>1</sup>; <sup>1</sup>University of Alberta
- 4:50 PM (668) **Field-Deployed SPR Sensors Environmental Applications**; Jean-Francois Masson<sup>1</sup>, Thibault Brulé<sup>1</sup>, Geneviève Granger<sup>1</sup>, Natalia Bukar<sup>1</sup>; <sup>1</sup>Université de Montreal
- 5:10 PM (669) **Localized Surface Plasmon Resonance for Studying the Immobilization of Liposomes on Sensor Surfaces**; Susanne Wiedmer<sup>1</sup>, Joanna Witos<sup>1</sup>, Giacomo Russo<sup>1</sup>, Filip Dusa<sup>1</sup>, Wen Chen<sup>1</sup>; <sup>1</sup>University of Helsinki, Department of Chemistry

### Wednesday Afternoon, Crystal 4

#### 17SURFACE03: SURFACE ANALYSIS OF ENVIRONMENTAL INTERFACES AND SYSTEMS

Organizer and Presider: Xiao-Ying Yu

- 3:50 PM (670) **Accessing the Relevant Temporal and Lateral Scale of Interfacial Electrochemistry through Multimodal Approach**; Vijay Murugesan<sup>1,2</sup>, Kee Sung Han<sup>1,2</sup>, Karl T. Mueller<sup>1,2</sup>; <sup>1</sup>Pacific Northwest National Laboratory; <sup>2</sup>Joint Center for Energy Storage Research
- 4:10 PM (671) **Liquid-jet X-ray Photoelectron Spectroscopy as a Probe of Liquid/Gas and Liquid/Solid Interfaces**; John Hemminger<sup>1</sup>; <sup>1</sup>University of California, Irvine
- 4:30 PM (672) **Spectroscopy and Microscopy Investigation of Interfacial Processes Affecting Uranium in Abandoned Mines**; Jose Cerrato, Sumant Avasarala, Lucia Rodriguez, Adrian Brearley, Kateryna Artyushkova, Johanna Blake; <sup>1</sup>University of New Mexico
- 4:50 PM (673) **EnviroESCATM – Routine Surface Analysis under Environmental Conditions**; Thomas Schultmeyer<sup>1</sup>; <sup>1</sup>SPECS Surface Nano Analysis, Inc.
- 5:10 PM (674) **In Situ Chemical Imaging of the Evolving Material Interface in Liquids**; Xiao-Ying Yu<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory

## TECHNICAL PROGRAM – THURSDAY

Awards Presentations - 7:50 am; Plenary Lectures - 8:00 am; *Tahoe Ballroom*

President: Karen Esmonde-White



**8:00 am – ANACHEM Award**  
(700) Development of Ultraviolet Photodissociation Mass Spectrometry for Characterization of Proteins; Jennifer Brodbelt;  
<sup>1</sup>University of Texas at Austin



**8:30 am – AES Mid-Career Award**  
(701) Using Microchip Electrophoresis and Electrochemical Detection to Investigate Cellular Communication; R. Scott Martin<sup>1</sup>; <sup>1</sup>Saint Louis University

### Orals 9:15 – 10:55 am

#### Thursday Morning, *Crystal 2*

#### 17ACS01: RECENT DEVELOPMENTS IN ATOMIC MASS SPECTROMETRY

Organizer and President: Charles Wilkins

- 9:15 AM (702) **Online Elemental Analysis of Airborne Nanoparticles**; Murray Johnston<sup>1</sup>, Justin Krasnomowicz<sup>1</sup>, Andrew Horan<sup>1</sup>; <sup>1</sup>University of Delaware
- 9:35 AM (703) **Airborne Laser Spark Ionization**; Jens Riedel<sup>1</sup>, Andreas Bierstedt<sup>1</sup>; <sup>1</sup>BAM Federal Institute for Materials Research
- 9:55 AM (704) **The Liquid Sampling-Atmospheric Pressure Glow Discharge (LS-APGD): Adding Versatility to Your “Organic” Mass Spectrometer**; R. Kenneth Marcus<sup>1</sup>, Edward Hoegg<sup>1</sup>, Htoo Paing<sup>1</sup>, Tyler Williams<sup>1</sup>; <sup>1</sup>Clemson University
- 10:15 AM (705) **Distance of Flight Mass Spectrometry for Atomic Spectrometry**; Steven Ray<sup>1</sup>, Andrew Schwartz<sup>1</sup>, M. Bonner Denton<sup>2</sup>, Gene Atlas<sup>3</sup>, Jaime Orejas-Ibanez<sup>1</sup>; <sup>1</sup>State University of New York at Buffalo; <sup>2</sup>University of Arizona; <sup>3</sup>Imager Laboratories
- 10:35 AM (706) **Atmospheric-Pressure Glow Discharges As Sources of Spatially Resolved Atomic and Molecular Information**; Jacob Shelley<sup>1</sup>, Sunil Badal<sup>1</sup>, Montwaun Young<sup>1</sup>, Jessica Hellinger<sup>1</sup>, Garrett MacLean<sup>1</sup>, Courtney Walton<sup>1</sup>; <sup>1</sup>Rensselaer Polytechnic Institute

#### Thursday Morning, *Crystal 1*

#### 17AWD03: ANACHEM AWARD SYMPOSIUM HONORING JENNIFER BRODBELT

Organize: Keith Olson; President: Kristina Hakansson

- 9:15 AM (707) **Dual Cleavable Crosslinking Technology (DUCCT): A New Strategy for High Confidence Identification of Crosslinked Peptides**; Saiful Chowdhury<sup>1</sup>, Jayanta Chakrabarty<sup>1</sup>, Abu Hena Kamal<sup>1</sup>; <sup>1</sup>University of Texas at Arlington
- 9:35 AM (708) **Fourier Analysis Method for Analyzing Large, Polydisperse Membrane Protein-Lipid Complexes with Native Ion Mobility-Mass Spectrometry**; James Prell<sup>1</sup>, Sean Cleary<sup>1</sup>; <sup>1</sup>University of Oregon
- 9:55 AM (709) **Characterization of Glycan and Carbohydrate Structures and Conformations using Hydrogen/Deuterium Exchange-Mass Spectrometry**; Elyssia Gallagher<sup>1</sup>, Tara Liyanage<sup>1</sup>, Jamie Kim<sup>1</sup>, Marina Mulenos<sup>1</sup>, Matthew Brantley<sup>1</sup>, Touradj Solouki<sup>1</sup>; <sup>1</sup>Baylor University
- 10:15 AM (710) **The PepSAVI-MS Pipeline for Natural Product Bioactive Peptide Discovery**; Leslie Hicks, Christine Kirkpatrick<sup>1</sup>, Nicole Parsley<sup>1</sup>; <sup>1</sup>University of North Carolina Chapel Hill
- 10:35 AM (711) **Microscale Mass Spectrometry Analysis of Live in vitro Tumors**; Zhibo Yang<sup>1</sup>, Xiang Tian<sup>1</sup>, Mei Sun<sup>1</sup>; <sup>1</sup>University of Oklahoma

#### Thursday Morning, *Crystal 5*

#### 17CHEM04: MULTIBLOCK METHODS: THE KEY TO MEASUREMENT FUSION

Organizer and President: Douglas Rutledge

- 9:15 AM TBA
- 9:55 AM (713) **BIVREGBLS : A New R Package in Method Comparison Studies with Tolerance Intervals and (Correlated)-Errors-in-Variables Regressions**; Marion Berger<sup>1</sup>, Bernard G. Francq<sup>2</sup>; <sup>1</sup>Sanofi, Biostatistics and Programming, CMC Support; <sup>2</sup>GSK, CMC Statistical Sciences, Technical R&D
- 10:15 AM (714) **Combining Independent Components Analysis and Multiblock Data Analysis: Application to Hyperspectral Images**; Benoit Jaillais<sup>1</sup>, Eloise Lancelot<sup>1</sup>, Douglas N. Rutledge<sup>2</sup>; <sup>1</sup>Oniris; <sup>2</sup>AgroParisTech
- 10:35 AM (715) **The Application of Micro-Raman Spectroscopy and Micro-XRF to Analysis of Duct Tapes**; Sergey Mamedov<sup>1</sup>; <sup>1</sup>Horiba Scientific

#### Thursday Morning, *Carson 1*

#### 17IR07: CLINICAL APPLICATIONS OF VIBRATIONAL SPECTROSCOPY

Organizer and President: Matthew Baker

- 9:15 AM (716) **Evidence of Fibrin Accumulation Preceding Altered Collagen Production in Combat Related Heterotopic Ossification Identified via Raman Spectroscopy**; Katherine E Cilwa<sup>1,3</sup>, Benjamin M Wheatley<sup>1,2</sup>, Devaveena Dey<sup>1,3</sup>, Thomas A Davis<sup>1,2</sup>; <sup>1</sup>Naval Medical Research Center; <sup>2</sup>Uniformed Services University and WRNMMC; <sup>3</sup>Henry M. Jackson Foundation
- 9:35 AM (717) **Multi-Centre Raman Imaging for Pathology Classification in Barrett’s Oesophagus**; Gavin Lloyd<sup>1</sup>, Catherine Kendall<sup>1</sup>, Nick Stone<sup>2</sup>, Lauren Denton<sup>2</sup>, Jennifer Dorney<sup>2</sup>, Geaint Thomas<sup>3</sup>, Riana Gaifulina<sup>3</sup>, Aaran Lewis<sup>3</sup>, Martin Isabelle<sup>4</sup>, Ian Bell<sup>4</sup>; <sup>1</sup>Gloucestershire Hospitals NHS Foundation Trust; <sup>2</sup>Univeristy of Exeter; <sup>3</sup>University College London (UCL); <sup>4</sup>Renishaw
- 9:55 AM (718) **Motor Capsules for Esophageal Cancer Screening and Diagnosis**; Rohith Reddy<sup>1,2</sup>, Jing Dong<sup>1,2</sup>, Michalina Gora<sup>1,2</sup>, Metthew Beatty<sup>2</sup>, Kanwarpal Singh<sup>1,2</sup>, Tim Ford<sup>2</sup>, Emilie Beaulieu-Ouellet<sup>2</sup>, Catriona Grant<sup>2</sup>, Mireille Rosenberg<sup>2</sup>, Guillermo Tearney<sup>1,2</sup>; <sup>1</sup>Harvard Medical School; <sup>2</sup>Massachusetts General Hospital



## TECHNICAL PROGRAM – THURSDAY

**Orals 9:15 – 10:55 am**

10:15 AM (719) **Infrared Spectroscopy for Tissue Pathology Imaging: Importance of Location and Resolution of Measurements;** Michael Walsh<sup>1</sup>, Vishal Varma<sup>1</sup>, Hari Sreedhar<sup>1</sup>, Shaiju Nazeer<sup>1</sup>, David Martinez<sup>1</sup>, Christie Massie<sup>1</sup>, Suman Setty<sup>1</sup>, Grace Guzman<sup>1</sup>; <sup>1</sup>University of Illinois at Chicago

10:35 AM (720) **Temporal Diabetes-Mediated Biochemical Changes in Distinctive Mouse Retinal Layers;** Ebrahim Aboulizadeh<sup>1</sup>, Christine Sorenson<sup>2</sup>, Miriam Unger<sup>3</sup>, Nader Sheibani<sup>2</sup>, Carol Hirschmugl<sup>1</sup>; <sup>1</sup>University of Wisconsin-Milwaukee; <sup>2</sup>University of Wisconsin-Madison; <sup>3</sup>Physical Electronics GmbH

### Thursday Morning, Crystal 3

#### 17LIBS04: NALIBS: LIBS FOR PHARMACEUTICAL AND BIOLOGICAL ANALYSIS

Organizer and Presider: Steven Rehse

9:15 AM (721) **Overview of LIBS Analysis of Soft and Hard Tissues;** Pavel Pořizka<sup>1,2</sup>, Prochazka David<sup>1,2</sup>, Jakub Klus<sup>1,2</sup>, Pavlína Škarková<sup>1</sup>, Jan Novotný<sup>1,2</sup>, Jozef Kaiser<sup>1,2</sup>; <sup>1</sup>Central European Institute of Technology; <sup>2</sup>AtomTrace a.s.

9:35 AM (722) **Bio-LIBS and the Role of Trace Metals When Laser-Induced Breakdown Spectroscopy is Used to Study Biological or Biomedical Systems;** Steven Rehse<sup>1</sup>, Alexandra Paulick<sup>1</sup>, Dylan Malenfant<sup>1</sup>, Vlora Riberdy<sup>1</sup>, Siddharth Doshi<sup>2</sup>; <sup>1</sup>University of Windsor; <sup>2</sup>Vellore Institute of Technology

9:55 AM (723) **LIBS and XRF: Complimentary Solid State Analysis Techniques in the Pharmaceutical Lab;** Lydia Breckenridge<sup>1</sup>, Sharla Wood<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

10:15 AM (724) **Quantitative Laser-Induced Breakdown Spectroscopy (LIBS) for Early Detection of Calcification in Aortic Valvular Interstitial Cells (VICs);** Seyyed Ali Davari, Shirin Masjedi, Zannatul Ferdous, Dibyendu Mukherjee; <sup>1</sup>University of Tennessee; <sup>2</sup>Vanderbilt University

10:35 AM (725) **Feasibility of LIBS for Prediction of Minerals in Powdered Infant Formula;** Xavier Cama-Moncunill<sup>1</sup>, Maria Markiewicz-Keszycka<sup>1</sup>, Yash Dixit<sup>1</sup>, Raquel Cama-Moncunill<sup>1</sup>, Maria Casado-Gavaldà<sup>1</sup>, Patrick J. Cullen<sup>1,2</sup>, Carl Sullivan<sup>1</sup>; <sup>1</sup>Dublin Institute of Technology; <sup>2</sup>UNSW Australia

### Thursday Morning, Nevada 7

#### 17MASS04: 'OMICS FRONTIERS: ION MOBILITY AND MASS SPECTROMETRY

Organizer and Presider: Brian Clowers

9:15 AM (726) **Developing Ion Mobility - Hydrogen Deuterium Exchange - Mass Spectrometry Techniques for Rapid Analysis of 'Omics Mixtures;** Hossein Maleki<sup>1</sup>, Megan Maurer<sup>1</sup>, Stephen Valentine<sup>1</sup>; <sup>1</sup>West Virginia University

9:35 AM (727) **Ion Mobility and the Omics: The Challenge of Separating Isomeric Systems;** James Dodds<sup>1</sup>, Jody May<sup>1</sup>, John McLean<sup>1</sup>; <sup>1</sup>Vanderbilt University

9:55 AM (728) **The Evolution of FTMS Based Trapped Ion Mobility Separation;** Michael Easterling<sup>1</sup>, Melvin Park<sup>1</sup>, Christopher Thompson<sup>1</sup>, Mark Ridgeway<sup>1</sup>; <sup>1</sup>Bruker Daltonics Inc.

10:15 AM (729) **Tuning Mobility Separation Factors for Metabolomics via Selective Ion-Neutral Clustering;** Brian Clowers<sup>1</sup>, Pearl Kwantwi-Barima<sup>1</sup>, Zhihao Yu<sup>1</sup>, Christopher Hogan<sup>1,2</sup>; <sup>1</sup>Washington State University; <sup>2</sup>University of Minnesota

10:35 AM (730) **Lipidomics Analysis of Antimicrobial-Resistant Bacteria by HILIC-Ion Mobility-Mass Spectrometry;** Kelly Hines<sup>1</sup>, Brian Werth<sup>1</sup>, Libin Xu<sup>1</sup>; <sup>1</sup>University of Washington

### Thursday Morning, Nevada 5

#### 17NANO04: NANO-FACILITATED SENSING

Organizer and Presider: David E. Thompson

9:15 AM (731) **New Strategies for Surface-Enhanced Sensing: Carbenes as Thiol Replacements and Hyper-Raman Based Detection;** Jon Camden<sup>1</sup>; <sup>1</sup>University of Notre Dame

9:35 AM (732) **Doped Lanthanum Hafnates as Scintillating Materials for High-Energy Photon Detection;** Yuanbing Mao<sup>1</sup>, Kareem Wahid<sup>1</sup>, Madhab Pokhrel<sup>1</sup>; <sup>1</sup>University of Texas Rio Grande Valley

9:55 AM (733) **Mechanically Deforming Nanoparticles and Impressing Deformation Patterns;** Jeffrey Anker<sup>1</sup>, Fathima Ameer<sup>1</sup>, Meenakshi Ranasinghe<sup>1</sup>, Shilpa Varahagiri<sup>1</sup>, Daniel Willet<sup>1</sup>, Yimei Wen<sup>1</sup>, George Chumanov<sup>1</sup>; <sup>1</sup>Clemson University, Chemistry Department

10:15 AM (734) **SERS Headspace Sampling for a Polysulfide Cyanide Antidote;** David Thompson<sup>1</sup>, Md Nure Alam<sup>1</sup>, Reece Thompson<sup>1</sup>, Joie Games<sup>1</sup>; <sup>1</sup>Sam Houston State University

10:35 AM (735) **Planar Array Substrate Based Surface Enhanced Raman Spectroscopy: Effect of Metal Types and Geometries on Enhancement and Thermodynamics of Binding;** Ashish Tripathi<sup>1</sup>, Erik D. Emmons<sup>1</sup>, Augustus W. Fountain III<sup>1</sup>, Jason A. Guicheteau<sup>1</sup>; <sup>1</sup>US Army RDECOM ECBC

### Thursday Morning, Nevada 6

#### 17PAT02: SAS PAT TECHNICAL SECTION: PAT IN THE BIOPHARMACEUTICAL INDUSTRIES - SESSION II

Organizer: Saly Romero; Presider: Dan Hill

9:15 AM (736) **Approach to Multivariate Model Lifecycle Management;** Daniel Hill<sup>1</sup>; <sup>1</sup>Biogen, Inc.

9:35 AM (737) **Towards a Turnkey Process Raman Spectroscopy Analyzer in Upstream Bioprocessing Operations;** Karen Esmonde-White<sup>1</sup>, Maryann Cuellar<sup>1</sup>, Alexander Pitters<sup>2</sup>, Sean Gilliam<sup>1</sup>, David Strachan<sup>1</sup>, Herve Lucas<sup>2</sup>, Bruno Lenain<sup>2</sup>, Ian Lewis<sup>1</sup>; <sup>1</sup>Kaiser Optical Systems, Inc.; <sup>2</sup>Kaiser Optical Systems, SARL

9:55 AM (738) **Model System Based Comparison of NIR and Raman Spectroscopy by the Prediction of the Glucose Concentration of CHO Cell Cultivations;** Bence Kozma<sup>1,2</sup>, László Párta<sup>2</sup>, Szilveszter Gergely<sup>1</sup>, András Salgó<sup>1</sup>; <sup>1</sup>Budapest University of Technology and Economics; <sup>2</sup>Gedeon Richter Plc.

10:15 AM (739) **Detailed Characterization of Culture Media Through the Use of Imaging Technology Leading to Enhanced Understanding and Control of Bioprocesses;** Mark Kemper<sup>1</sup>, Rudy Hofmeister<sup>1</sup>, Scott Tandy<sup>1</sup>; <sup>1</sup>H2Optx, Inc.

10:35 AM (740) **How to Develop and Implement Raman Glucose Control for Biomanufacturing Mammalian Cell Culture Processes;** John Paul Smelko<sup>1</sup>; <sup>1</sup>Biogen, Inc.



## TECHNICAL PROGRAM – THURSDAY

Orals 9:15 – 10:55 am

Poster Sessions and Coffee Breaks

11:00 am – 12:00 pm & 3:10 – 3:50 pm, *Grand Salon*

### Thursday Morning, *Carson 3* 17RAM10: RAMAN MICROSCOPY

Organizers and Presiders: Katsumasa Fujita, Duncan Graham

- 9:15 AM (741) **Lighting Up Non-Fluorescent Molecules with Stimulated Raman Scattering Microscopy**; Dan Fu<sup>1</sup>; <sup>1</sup>University of Washington
- 9:35 AM (742) **Optimized Methods for Spontaneous Raman-Imaging of Immune Cells**; Nicholas Smith<sup>1</sup>, Alison Hobro<sup>1</sup>, Nicolas Pavillon<sup>1</sup>; <sup>1</sup>Osaka University
- 9:55 AM (743) **Confocal Raman Microscopy for Investigating the Internal Surface Chemistry of Porous Particles**; Joel Harris, Jay Kitt<sup>1</sup>, David Bryce<sup>1</sup>; <sup>1</sup>University of Utah
- 10:15 AM (744) **3D Raman Imaging: A Method to Study the Effects of Lubrication on the Microstructure of Tablets**; Shashwat Gupta<sup>1</sup>, Savitha Paniakr<sup>1</sup>, Fernando Muzzio<sup>1</sup>; <sup>1</sup>Rutgers- The State University of New Jersey
- 10:35 AM (745) **Advances in Approaches and Techniques for the Acquisition, Analysis and Post-Processing of Three-Dimensional Raman Imaging Data**; Joachim Koenen<sup>1</sup>, Ute Schmidt<sup>1</sup>, Wei Liu<sup>1</sup>; <sup>1</sup>WITec GmbH

### Thursday Morning, *Carson 4* 17RAM17: SPECIAL PITTCO/FACSS JOINT SESSION: RAMAN SPECTROSCOPY FOR SECURITY AND FORENSICS PURPOSES

Organizer and Presider: Igor Lednev

- 9:15 AM (746) **Trends and Potentials of Raman Spectroscopy in Biological Safety and Security**; Juergen Popp<sup>1,2,3</sup>; <sup>1</sup>Leibniz Institute of Photonic Technology; <sup>2</sup>Friedrich-Schiller-University Jena; <sup>3</sup>Research Campus Infectognostic
- 9:35 AM (747) **Development of Standoff Deep UV Resonance Raman Determination of Trace Explosives**; Sanford Asher<sup>1</sup>, Sergei Bykov<sup>1</sup>, Katie Gares<sup>1</sup>, Kyle Hufziger<sup>1</sup>; <sup>1</sup>University of Pittsburgh
- 9:55 AM (748) **Novel Through-Barrier Detection of Explosives, Narcotics and their Precursors**; Matthew Bloomfield<sup>1</sup>, Robert Stokes<sup>2</sup>; <sup>1</sup>Cobalt Light Systems, Inc; <sup>2</sup>Cobalt Light Systems, Ltd
- 10:15 AM (749) **Universal Detection of Body Fluid Traces In Situ with Raman Hyperspectroscopy for Forensic Purposes**; Marisia Fikiet<sup>1</sup>, Gregory McLaughlin<sup>1</sup>, Masahiro Ando<sup>2</sup>, Hiro-o Hamaguchi<sup>2</sup>, Igor Lednev<sup>1</sup>; <sup>1</sup>University at Albany, SUNY; <sup>2</sup>Spectroscopic Science Laboratory, Co.
- 10:35 AM (750) **Raman Spectroscopy Technique in Toxicology: Detecting and Quantifying Cocaine in Seized Drug Samples from an Amazon State of Brazil**; Landulfo Silveira<sup>1,2</sup>, Ciro Penido<sup>1,2</sup>, Marcos Pacheco<sup>1,2</sup>, Renato Zângaro<sup>1,2</sup>, Igor Lednev<sup>3</sup>; <sup>1</sup>Universidade Anhembi Morumbi - UAM; <sup>2</sup>Center for Innovation, Technology and Education; <sup>3</sup>State University of New York - SUNY

### Thursday Morning, *Crystal 4* 17SPECIAL02: MODERN TECHNIQUES IN MICROSCOPY

Organizer and Presider: Anthony Stender

- 9:15 AM (751) **Super-Resolution Chemical Imaging with SERS and STORM**; Nathan Lindquist<sup>1</sup>, Aeli Olson<sup>1</sup>, Kelsey Spies<sup>1</sup>, Anna Browning<sup>1</sup>, Paula Soneral<sup>1</sup>; <sup>1</sup>Bethel University
- 9:35 AM (752) **Advanced Microscopies for Nanophotonics**; Matthew Sheldon; <sup>1</sup>Texas A&M University
- 9:55 AM (753) **Spatially Resolving Vibrational Couplings for Structure Identification with Hyperspectral 2D Infrared Microscopy**; Joshua Ostrander<sup>1</sup>, Martin Zanni<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison
- 10:15 AM (754) **Multimodal Nonlinear Imaging for Sensitive and Specific Analysis of Multiple Solid State Forms and their Changes on Pharmaceutical Tablets**; Clare Strachan<sup>1</sup>, Dunja Novakovic<sup>1</sup>, Jukka Saarinen<sup>1</sup>, Antti Isomäki<sup>1</sup>, Sara Fraser-Miller<sup>3</sup>, Leena Peltonen<sup>1</sup>, Timo Laaksonen<sup>2</sup>; <sup>1</sup>University of Helsinki; <sup>2</sup>Tampere University of Technology; <sup>3</sup>University of Otago
- 10:35 AM (755) **Spatially Encoded Polarization-Dependent SHG Microscopy of Pharmaceutical Materials**; Garth Simpson<sup>1</sup>, Changqin Ding<sup>1</sup>, James R. W. Ulcickas<sup>1</sup>, Fengyuan Deng<sup>1</sup>, Ellen J. Gualieri<sup>2</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Formulatrix, Inc.

All Thursday posters should be put up between 9:00 – 10:45 am and removed by 3:50 pm

### 17THPFORENS: Thursday Posters – Forensics

#### Poster Board #1

- (756) **Race Differentiation by Raman Spectroscopy of a Bloodstain for Forensic Purposes**; Ewelina Mistek<sup>1</sup>, Lenka Halámková<sup>1</sup>, Kyle Doty<sup>1</sup>, Claire Muro<sup>1</sup>, Igor Lednev<sup>1</sup>; <sup>1</sup>State University of New York at Albany

#### Poster Board #2

- (757) **Detection and Identification of Illicit Substances in Articles of Mail by a Shortwave Infrared (SWIR) Hyperspectral Imager**; Oksana Olkhovik<sup>1</sup>, Nathaniel Gomer<sup>1</sup>, Robert Schweitzer<sup>1</sup>, Jeffrey Beckstead<sup>1</sup>, Matthew Nelson<sup>1</sup>; <sup>1</sup>ChemImage Corporation

#### Poster Board #3

- (758) **Gas Composition Measurements during One-Dimensional Time to Explosion Experiments**; Greg Klunder<sup>1</sup>, Paul Spackman<sup>1</sup>, Fowzia Zaka<sup>1</sup>, Nick Muetterties<sup>1</sup>, Evan Kahl<sup>1</sup>, Peter Hsu<sup>1</sup>; <sup>1</sup>Lawrence Livermore National Laboratory

#### Poster Board #4

- (759) **Calibration of the Likelihood Ratio for the Evaluation of Forensic Glass Evidence**; Ruthmara Corzo<sup>1</sup>, Daniel Ramos<sup>2</sup>, Jose Almirall<sup>1</sup>; <sup>1</sup>Florida International University; <sup>2</sup>Universidad Autonoma de Madrid

**TECHNICAL PROGRAM – THURSDAY**  
**Poster Sessions 11:00 am – 12:00 pm & 3:10 – 3:50 pm, Grand Salon**

**17THPMAS: Thursday Posters - Mass Spectrometry**

**Poster Board #5**

(760) **Monitoring Sulfonate Ester Potential Genotoxic Impurities in Pharmaceuticals by GCMS and LCMS;** Joseph Snodgrass<sup>1</sup>, Shunyan Mo<sup>1</sup>, David Moon<sup>1</sup>, Ricardo Borjas<sup>1</sup>; <sup>1</sup>Vertex Pharmaceuticals, Inc

**Poster Board #6**

(761) **Detailed Molecular Composition Analysis of Middle Distillates Using GC×GC-TOFMS; A Tool to Upgrade Low Value Refinery Streams;** Kalicharan Chattopadhyay<sup>1</sup>, Anil Yadav<sup>1</sup>, Dheer Singh<sup>1</sup>, Anju Chopra<sup>1</sup>, J. Christopher<sup>1</sup>, G. S. Kapur<sup>1</sup>; <sup>1</sup>R & D Centre, Indian Oil Corporation Ltd, India.

**Poster Board #7**

(762) **Charge Transfer Dissociation (CTD) Mass Spectrometry of Sulfated Oligosaccharides;** Zachary Sasiene<sup>1</sup>, Praneeth Mendis<sup>1</sup>, Glen Jackson<sup>1</sup>; <sup>1</sup>West Virginia University

**Poster Board #8**

(763) **Measurement of Material Properties from Levitated Micron Sized Particles;** Matthew Hart<sup>1</sup>, Vasanthi Sivaprakasam<sup>1</sup>, Jozsef Czege<sup>1</sup>, Jay Eversole<sup>1</sup>; <sup>1</sup>Naval Research Laboratory

**Poster Board #9**

(764) **Identification of Streptococcus Gallolyticus Subsp. Gallolyticus TX20005 (biotype I) Competence Stimulating Peptide Pheromone;** Anthony Harrington<sup>1</sup>; <sup>1</sup>University of Nevada, Reno

**Poster Board #10**

(765) **Microwave-Assisted Electrospray Ionization (μAESI);** Maria Rivera<sup>1</sup>, Jaime Orejas-Ibanez<sup>1</sup>, Andrew Schwartz<sup>1</sup>, Steven Ray<sup>1</sup>; <sup>1</sup>University at Buffalo

**Poster Board #11**

(766) **The Use of a Capillary Dielectric Barrier Discharge Ionization (DBDI) Source for Spatially-Resolved Measurements of Cholesterol in Mouse Brains;** Mercede Erickson<sup>1</sup>, Isabella James<sup>1</sup>, Richard Carson<sup>1</sup>, John C. Price<sup>1</sup>, Paul B. Farnsworth<sup>1</sup>; <sup>1</sup>Brigham Young University

**17THPMICRO: Thursday Posters - Microscopy and Imaging**

**Poster Board #12**

(767) **Use of Nonlinear Optics for Materials State Awareness;** James Patterson<sup>1</sup>; <sup>1</sup>Brigham Young University

**Poster Board #13**

(768) **Quantitative Spectroscopic Chemical Imaging Enables Product Purity Assessment Resulting from Operational Changes in Industrial Processing;** David Wetzel<sup>1</sup>, Mark Boatwright<sup>1</sup>; <sup>1</sup>Kansas State University

**Poster Board #14**

(769) **Visible Light Tomography to Define Edges in FTIR Tomographic Reconstructions;** Nicholas Walter<sup>1</sup>, Carol Hirschmugl<sup>1</sup>, Sugato Ray<sup>1</sup>, Ghazal Azarfar<sup>1</sup>, Alex Schofield<sup>1</sup>; <sup>1</sup>University of Wisconsin-Milwaukee

**Poster Board #15**

(770) **Multi-Modal Super-Resolution Microscopy through Super-Resolution Radial Fluctuations (SRRF);** Justin Cooper<sup>1</sup>, Mark Browne<sup>1</sup>, Hugh Gribben<sup>1</sup>, Martin Catney<sup>1</sup>, Colin Coates<sup>1</sup>, Geraint Wilde<sup>1</sup>, Ricardo Henriques<sup>2</sup>; <sup>1</sup>Andor Technology Belfast, UK; <sup>2</sup>University College London, UK

**Poster Board #16**

(771) **True Resolution Enhancement for Optical Spectroscopy;** Jeffrey Oleske<sup>1</sup>, Justin Cooper<sup>1</sup>, Hugh Gribben<sup>1</sup>, Martin Catney<sup>1</sup>, Colin Coates<sup>1</sup>, Geraint Wilde<sup>1</sup>, Ricardo Henriques<sup>2</sup>; <sup>1</sup>Andor Technology Belfast, UK

**Poster Board #17**

(772) **Label-free Imaging of Amphotericin B Interacting with Live Cells Using Transient Absorption Microscopy;** Kevin Higgins<sup>1</sup>, Tessa Calhoun<sup>1</sup>; <sup>1</sup>University of Tennessee, Knoxville

**17THPNANO: Thursday Posters – Nanotechnology**

**Poster Board #18**

(773) **Two Dimensional Silver Nanoparticle Polymer Composites for Organic Vapor Sensing;** Yimei Wen<sup>1</sup>, George Chumanov<sup>1</sup>; <sup>1</sup>Clemson University

**Poster Board #19**

(774) **Interactive Web-Based Visualization Tool for Monitoring Optical Properties of Nanoparticles During Synthesis Reactions;** Bryan Calderón-Jiménez<sup>1</sup>, Gabriel Sarmanho<sup>1</sup>, Karen E. Murphy, Antonio R. Montoro-Bustos<sup>1</sup>, José R. Vega-Baudrit<sup>2</sup>; <sup>1</sup>National Institute of Standards and Technology; <sup>2</sup>National Laboratory of Nanotechnology, CR

**Poster Board #20**

(775) **Algae-Biotemplated Water-Splitting Copper Oxide Nanocatalysts for Hydrogen Production;** Paloma Salazar<sup>1</sup>, Sakr Elsaidi<sup>1</sup>, Marina Avram<sup>1</sup>, Daniel Nde<sup>1</sup>, Wei Zhao<sup>1</sup>; <sup>1</sup>University of Arkansas at Little Rock

**17THPPMA: Thursday Posters - Pharmaceutical Analysis**

**Poster Board #21**

(776) **Calibration-Free Quantification of Trace Crystallinity within Amorphous Solid Dispersions by SHG Microscopy;** Garth J. Simpson<sup>1</sup>, Casey J. Smith<sup>1</sup>, Janny Dinh<sup>1</sup>, Paul Schmitt<sup>3</sup>, Ellen J. Gualtieri<sup>2</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Formulatrix, Inc.; <sup>3</sup>Wabash College

**Poster Board #22**

(777) **Multi-Bounce ATR FTIR Measurement of Live Cells in Response to Anticancer Drugs;** Ali Altharawi<sup>1</sup>; <sup>1</sup>King's College London

**Poster Board #23**

(778) **Quantification of Solid-State Co-Amorphous Mixtures of Crystalline Carbamazepine by Terahertz Spectroscopy;** Yi Li, James K. Drennen, III, Carl A. Anderson<sup>1,2</sup>; <sup>1</sup>Duquesne University Graduate School; <sup>2</sup>Duquesne Center of Pharmaceutical Technology

**Poster Board #24**

(779) **Benefits of Spectroscopic Analysis Over Standard Analytic Techniques within the Laboratory;** Keely Bergqvist<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

**Poster Board #25**

(780) **Applications of UPLC-MSMS in Pharmaceutical Impurity Profiling;** Lynn X. Zhang<sup>1</sup>, Heather Fleming<sup>1</sup>, Jason Batchelor<sup>1</sup>, Rachel Rensing<sup>1</sup>; <sup>1</sup>EAG Laboratories

**Poster Board #26**

(781) **Qualifying ATR Accessories for Use in Pharmaceutical Applications;** Steve Lowry<sup>1</sup>, Garry Ritter<sup>1</sup>; <sup>1</sup>Thermo Fisher Scientific

**TECHNICAL PROGRAM – THURSDAY**  
**Poster Sessions 11:00 am – 12:00 pm & 3:10 – 3:50 pm, Grand Salon**  
**Orals 1:30 – 3:10 pm**

**Poster Board #27**

(782) **Beyond Elemental Impurities Analyses in Pharmaceutical Research: LC-ICP-MS Applications;** Brittany Kassim<sup>1</sup>, Lanfang Zou<sup>1</sup>, Qiang Tu<sup>1</sup>, Xiaodong Bu<sup>1</sup>, Yun Mao<sup>1</sup>; <sup>1</sup>Merck

**Poster Board #28**

(783) **Bioecological Study of Sargassum sp. and its Extract Bioactivity as Anti-MDR Bacteria;** Anggara Mahardika<sup>2</sup>, Rini Pramesti<sup>1</sup>, Wilis A. Setyani, Muhamad Zainuddin<sup>3,4</sup>, AB Susanto<sup>1</sup>; <sup>1</sup>Diponegoro University, Indonesia; <sup>2</sup>Kwansei Gakuin University; <sup>3</sup>University of Islam Nahdlatul Ulama; <sup>4</sup>Universite Bretagne Sud, France

**Poster Board #29**

(784) **Raw Material Identification: Method Driven Raman for Increased Speed and Accuracy;** Adam Hopkins<sup>1</sup>; <sup>1</sup>Metrohm USA

**Poster Board #30**

(785) **Development of Vapor Diffusion Chamber for in situ and High Throughput X-Ray Diffraction Analysis;** Kathleen Sokolowsky<sup>1</sup>, Andrew Brunskill<sup>1</sup>, Alexander Chin<sup>1</sup>, Matthew Hagan<sup>1</sup>, Timothy Rhodes<sup>1</sup>; <sup>1</sup>Merck & Co., Inc.

**Poster Board #31**

(786) **A New Approach to Characterize Crystallization in Complex Transdermal Delivery System (TDS) by Raman Mapping and Modeling;** Teng Xu, Daniel Willett<sup>1</sup>, Sam Raney<sup>1</sup>, Caroline Strasinger<sup>1</sup>, Jason Rodriguez<sup>1</sup>, David Keire<sup>1</sup>, Anna Wokovich<sup>1</sup>; <sup>1</sup>Food and Drug Administration (FDA)

**Poster Board #32**

(787) **Prediction of in vitro Drug Release of a Multiparticulate Dosage Form by Process Analytical Techniques (PAT);** Hanzhou Feng<sup>1</sup>, Shikhar Mohan<sup>1</sup>, James Drennen III<sup>1</sup>, Carl Anderson<sup>1</sup>; <sup>1</sup>Duquesne University

**Poster Board #33**

(788) **Applications of a Multispectral Vision System to Support Development of Pharmaceutical Products;** Brian Marks<sup>1</sup>, Rich Steinbeiser<sup>2</sup>, Simon Hamilton<sup>1</sup>, Megan Mackey<sup>1</sup>, W Peter Wuelfing<sup>1</sup>; <sup>1</sup>Merck Research Labs, Merck & Co. Inc; <sup>2</sup>Merck Manufacturing Division, Merck & Co. Inc

**17THPRAM: Thursday Posters – Raman**

**Poster Board #34**

(789) **Methods for Approaching Substrate Interference in Raman Spectroscopy for Forensic Science;** Marisia Fikiet<sup>2</sup>; <sup>1</sup>Spectroscopic Science Laboratory, Co.; <sup>2</sup>University at Albany, SUNY

**Poster Board #35**

(790) **Confocal Raman Microscopy Investigation of Self-Assembly of Hybrid Supported Phospholipid Bilayers within Individual Porous Silica Chromatographic Particles;** Jay Kitt<sup>1</sup>, David Bryce<sup>1</sup>, Joel Harris<sup>1</sup>; <sup>1</sup>University of Utah

**Poster Board #36**

(791) **Raman Chemical Imaging of Adsorption and Reactions on Surfaces;** Erik Emmons<sup>1</sup>, Ashish Tripathi<sup>1</sup>, Gregory Mogilevsky<sup>2</sup>, Chris Karwacki<sup>1</sup>; <sup>1</sup>U.S. Army ECBC; <sup>2</sup>Leidos, Inc.

**Poster Board #37**

(792) **Swept-Wavelength Raman Spectroscopy for the Detection of Controlled Substances;** Pratima Kunapareddy<sup>1</sup>, Calvin Zulick<sup>1</sup>, Jacob Grun<sup>1</sup>; <sup>1</sup>Naval Research Lab

**Poster Board #38**

(793) **Quantitative Analysis of Saccharides in Kappaphycus Alvarezii Using Raman Imaging;** Anggara Mahardika<sup>1</sup>, AB Susanto<sup>2</sup>, Rini Pramesti<sup>2</sup>, Yusuke Matsuda<sup>1</sup>, Hidetoshi Sato<sup>1</sup>; <sup>1</sup>Kwansei Gakuin University, Japan; <sup>2</sup>Diponegoro University, Indonesia

**Poster Board #39**

(794) **Spectroscopy and DFT Studies of Uranyl Carbonate, UO<sub>2</sub>CO<sub>3</sub>: A Model for Uranium Transport, Carbon Dioxide Sequestration, and Seawater Species;** N. Kalashnyk<sup>1</sup>, D. L. Perry<sup>2</sup>, F. Massuyeau<sup>1</sup>, E. Faulques<sup>1</sup>; <sup>1</sup>Inst. Jean Rouxel (IMN), Nantes University, France; <sup>2</sup>LBNL, University of California, Berkeley, CA

**Poster Board #40**

(795) **Tip-Enhanced Raman Spectroscopy with Plasmon-Resonance Thin-Film Waveguide Probe;** Kaifeng Zhang<sup>1</sup>, Takehiro Tachizaki<sup>2</sup>, Ryota Matsumoto<sup>3</sup>, Toshihiro Okamoto<sup>3</sup>, Masanobu Haraguchi<sup>3</sup>, Shin-ichi Taniguchi<sup>1</sup>; <sup>1</sup>R&D Group, Hitachi, Ltd.; <sup>2</sup>School of Engineering, Tokai University; <sup>3</sup>Graduate School, Tokushima University

**Thursday Afternoon, Crystal 1**

**17AWD06: AES ELECTROPHORESIS AWARD SYMPOSIUM HONORING R. SCOTT MARTIN**

Organizer: Ryan Kelly; President: Jim Rydzak

- 1:30 PM (797) **Bioanalytical Methods for Investigating Dynamic Behavior of Pancreatic Cells;** Michael Roper<sup>1</sup>; <sup>1</sup>Florida State University
- 1:50 PM (798) **Sheath-Flow SERS for Online Chemical Detection;** Zachary Schultz<sup>1</sup>, Emily Peters<sup>1</sup>, Anh Nguyen<sup>1</sup>, Rafael Masitas<sup>1</sup>; <sup>1</sup>University of Notre Dame
- 2:10 PM (799) **Microchip Electrophoresis-Based Methods for Measuring Oxidative Stress;** Susan Lunte<sup>1</sup>; <sup>1</sup>University of Kansas
- 2:30 PM (800) **Metabolomic Analysis of Diabetic Complications using Microfluidics;** Jim Edwards; <sup>1</sup>Saint Louis University
- 2:50 PM (801) **Microfluidics Made Easy: 15 Years of Collaboration with the Martin Group;** Dana Spence<sup>1</sup>; <sup>1</sup>Michigan State University

**Thursday Afternoon, Crystal 5**

**17CHEM05: NEW DEVELOPMENTS IN CALIBRATION METHODS**

Organizer and President: Dongsheng Bu

- 1:30 PM (802) **Robust Selection of Latent Variables for Small NIR Calibration Sets;** Carl Anderson<sup>1</sup>, Anik Alam<sup>1</sup>, James K. Drennen<sup>1</sup>; <sup>1</sup>Duquesne University
- 1:50 PM (803) **Using Advanced Statistics to Increase the Information Content and Usefulness of Radio Frequency Spectroscopy;** Matthew Augustine; <sup>1</sup>UC Davis
- 2:10 PM (804) **Spectroscopic and Chemometrics Applications in Synthetic Drug Substance and Drug Product Development;** Wencan Chen<sup>1</sup>, Yong Xie<sup>1</sup>; <sup>1</sup>Amgine Inc.



## TECHNICAL PROGRAM – THURSDAY

**Orals 1:30 – 3:10 pm**

2:30 PM (805) **Automated Multivariate Calibration & Classification in Portable/Handheld Instruments with Systemic Modeling Approaches**; Christopher Brown<sup>1</sup>; <sup>1</sup>908 Devices

2:50 PM (806) **Calibration Updating by Sample and Feature Augmentation**; Erik Andries<sup>1</sup>, John Kalivas<sup>2</sup>, Anit Gurung<sup>2</sup>; <sup>1</sup>Central New Mexico Community College; <sup>2</sup>Idaho State University

**Thursday Afternoon, Nevada 6**  
**17FORENS04: SPECIAL PITTCO/FACSS JOINT SESSION: FORENSIC ANALYSIS IN THE LAB AND AT THE CRIME SCENE**  
Organizer and Presider: Igor Lednev

1:30 PM (807) **Forensic Science R&D Funding Program at the National Institute of Justice**; Gregory Dutton<sup>1</sup>, Minh Nguyen<sup>1</sup>; <sup>1</sup>National Institute of Justice

1:50 PM (808) **Trace Blood Detection with Infrared Spectroscopy, Infrared Imaging, and Latent Heat Thermography in the Context of Achievable Detection Limits**; Stephen Morgan<sup>1</sup>, Michael Myrick<sup>1</sup>, Raymond Belliveau<sup>1</sup>, Brianna Cassidy<sup>1</sup>, Zhenyu Lu<sup>1</sup>, Stephanie DeJong<sup>1</sup>; <sup>1</sup>University of South Carolina

2:10 PM (809) **On-Site GC/MS Analysis of Drugs: Reasoning, Reliability and Return on Investment**; Glen Jackson<sup>1</sup>; <sup>1</sup>West Virginia University

2:30 PM (810) **Sampling and Analysis of Breath Components for Cannabis Detection Using Capillary Microextraction of Volatiles (CMV)**; William MacCrehan<sup>2</sup>, D'Nisha Hamblin<sup>1,2</sup>, Bruce Benner<sup>2</sup>, Michelle Schantz<sup>2</sup>, Jose Almirall<sup>1</sup>, Mim Young<sup>2</sup>, Sigalit Gura<sup>1</sup>; <sup>1</sup>Department of Chemistry and Biochemistry, Florida; <sup>2</sup>Chemical Sciences, National Institute of Standards

2:50 PM (811) **Analysis of Blood Traces by Attenuated Total Reflection (ATR) Fourier Transform-Infrared (FT-IR) Spectroscopy for Forensic Purposes**; Ewelina Mistek<sup>1</sup>, Igor Lednev<sup>1</sup>; <sup>1</sup>State University of New York at Albany

**Thursday Afternoon, Carson 1**  
**17IR08: TOWARDS POINT-OF-CARE TESTING WITH RAMAN SPECTROSCOPY**  
Organizer and Presider: Ishan Barman

1:30 PM (812) **Raman Applications in Orthopaedics: From Gout to Arthritis**; Ozan Akkus<sup>1</sup>, Mustafa Unal<sup>1</sup>, Bolan Li<sup>1</sup>; <sup>1</sup>Case Western Reserve University

1:50 PM (813) **Resonance Raman Spectroscopy Based Label-Free Approach for HbA1c Detection**; Rishikesh Pandey<sup>1,2</sup>; <sup>1</sup>University of Connecticut School of Medicine; <sup>2</sup>Connecticut Children Medical Center

2:10 PM (814) **Mechanical Trap Surface-Enhanced Raman Spectroscopy for Three-Dimensional Molecular Imaging of Single Live Cells**; Santosh Paidi<sup>1</sup>; <sup>1</sup>Johns Hopkins University

2:30 PM (815) **Monitor reactions by *in situ* IR and Raman Spectroscopy**; Xiaoyun (Shawn) Chen<sup>1</sup>; <sup>1</sup>The Dow Chemical Company

2:50 PM (816) **Surface-enhanced Raman Scattering from Synergistic Contribution of Graphene and Semiconductor in Graphene-TiO<sub>2</sub> Assembly for Stem Cell Related Bioanalysis**; Tingting Zheng, Enduo Feng, Yang Tian; <sup>1</sup>East China Normal University

**Thursday Afternoon, Crystal 3**  
**17LIBS11: NALIBS: FIELD APPLICATION OF LIBS**  
Organizer and Presider: Steve Buckley

1:30 PM (817) **On-Line Monitoring of Materials by Chemometric Methods Applied to LIBS**; Arne Bengtson<sup>1</sup>, Jonas Petersson<sup>1</sup>, Bertrand Noharet<sup>1</sup>, Baptiste Ottino<sup>1</sup>, Mattias Åslund<sup>1</sup>, Tania Irebo Schwartz; <sup>1</sup>Swerea KIMAB

1:50 PM (818) **Effect of Laser Parameters on the Analysis of Precious Metals in Minerals by Laser-Induced Breakdown Spectroscopy (LIBS)**; Daniel Diaz<sup>1,2</sup>, David Hahn<sup>2</sup>, Alejandro Molina<sup>1</sup>; <sup>1</sup>Universidad Nacional de Colombia - Sede Medellin; <sup>2</sup>MAE-University of Florida, Gainesville

2:10 PM (819) **Testing of Carbon and Silicon in Low-Alloy Carbon Steels by Field-Portable Handheld LIBS**; Brendan Connors<sup>1</sup>, David Day<sup>1</sup>; <sup>1</sup>SciAps, Inc.

2:30 PM (820) **Analysis of Glass Pharmaceutical Containers with a Handheld LIBS Spectrometer**; Katherine Bakeev<sup>1</sup>, Qun Li<sup>1</sup>, Dan Liu<sup>1</sup>, Jing Li, Sean Wang<sup>1</sup>; <sup>1</sup>B&W Tek

2:50 PM (821) **Subsurface Mineral Exploration Using LIBS**; Pablo Sobron<sup>1,2</sup>, Kris Zacny<sup>3</sup>; <sup>1</sup>Impossible Sensing; <sup>2</sup>SETI Institute; <sup>3</sup>Honeybee Robotics

**Thursday Afternoon, Nevada 7**  
**17MASS05: RECENT ADVANCES IN OLIGOSACCHARIDE ANALYSIS BY MASS SPECTROMETRY**  
Organizer and Presider: Glen Jackson

1:30 PM (822) **Development of a CE-MS/MS Platform for Sequencing Glycosaminoglycans**; Jon Amster<sup>1</sup>, Patience Sanderson<sup>1</sup>, Morgan Stickney<sup>1</sup>, Franklin Leach<sup>1</sup>, James Xia<sup>3</sup>, Yanlei Yu<sup>2</sup>, Fuming Zhang<sup>2</sup>, Robert Linhardt<sup>2</sup>; <sup>1</sup>University of Georgia; <sup>2</sup>Rensselaer Polytechnic Institute; <sup>3</sup>CMP Scientific Corporation

1:50 PM (823) **Gas-Phase Ion-Electron Reactions for Carbohydrate and Glycopeptide Structural Characterization**; Kristina Hakansson; <sup>1</sup>University of Michigan

2:10 PM (824) **LC-MS/MS Analysis of Glycan and Glycopeptide Isomers**; Yehia Mechref<sup>1</sup>; <sup>1</sup>Texas Tech University, Lubbock, TX

2:30 PM (825) **A Multidimensional Strategy to Resolve Carbohydrate Isomerism in the Gas Phase**; Eric D. Dodds<sup>1</sup>, Katherine N. Schumacher<sup>1</sup>, Jessica L. Minnick<sup>1</sup>, Richard L. Backhus<sup>1</sup>; <sup>1</sup>University of Nebraska - Lincoln

2:50 PM (826) **Mapping the Glycoproteome with Activated Ion Electron Transfer Dissociation**; Nicholas M. Riley<sup>1</sup>, Alexander S. Hebert<sup>1</sup>, Nicholas W. Kwiecien<sup>1</sup>, Michael S. Westphall<sup>1</sup>, Joshua J. Coon<sup>1</sup>; <sup>1</sup>University of Wisconsin-Madison

**Thursday Afternoon, Nevada 5**  
**17NANO05: IMAGING AND SENSING APPLICATIONS OF ATOMIC PRECISION NANOCCLUSERS**  
Organizer and Presider: Gangli Wang

1:30 PM (827) **Dual Emissive Gold Nanoparticles for Ratiometric pH Sensing**; Jie Zheng<sup>1</sup>; <sup>1</sup>The University of Texas at Dallas

1:50 PM (828) **Tailoring Luminescent Nanoparticles in Biology**; Gang Han<sup>1</sup>; <sup>1</sup>University of Massachusetts-Medical School



## TECHNICAL PROGRAM – THURSDAY

Orals 1:30 – 3:10 pm

Innovation Award Symposium 3:50 – 5:10 pm, *Tahoe Ballroom*

2:10 PM (829) **Photoelectrochemistry of Colloidal TiO<sub>2</sub> Nanoparticles: From Aggregates to Single Crystals**; Mario Alpuche-Aviles<sup>1</sup>, Krishna Barakoti<sup>1</sup>, Pushpa Chhetri<sup>1</sup>, Rezvan Kazemi<sup>1</sup>, Nelum Karunathilake<sup>1</sup>, Ganesh Rana<sup>1</sup>; <sup>1</sup>University of Nevada, Reno, Department of Chemistr

2:30 PM TBA

2:50 PM (831) **Near Infrared ElectroChemiluminescence of Gold Nanoclusters for Redox and Metal Ion Sensing**; Gangli Wang<sup>1</sup>; <sup>1</sup>Georgia State University

**Thursday Afternoon, Carson 3**

### 17RAM03: RAMAN IMAGING & MICROSCOPY II

Organizers and Presiders: Pavel Matousek, Ian Lewis, Duncan Graham

1:30 PM (832) **Innovative Applications of Raman Microscopy**; Peng Wang<sup>1</sup>, Thomas Tague<sup>1</sup>, Juergen Sawatzki<sup>2</sup>, Sergey Shilov<sup>1</sup>; <sup>1</sup>Bruker Optics Inc., Billerica, MA; <sup>2</sup>Bruker Optik GmbH, Ettlingen, Germany

1:50 PM (833) **2D and 3D Micro-Raman Imaging of Crystal Transformation due to Indentation of ZrO<sub>2</sub> Ceramic and ZrO<sub>2</sub> Containing Glass Ceramic Materials**; Galan Moore<sup>1</sup>, Charlene Smith<sup>1</sup>, Benjamin Hanson<sup>1</sup>, Sara Cole<sup>1</sup>; <sup>1</sup>Corning Incorporated

2:10 PM (834) **A Novel Wide-Field Raman System for Fast Chemical Imaging**; Haithem Mustafa, Ozan Akkus; <sup>1</sup>Case Western Reserve University

2:30 PM (835) **Raman Chemical Imaging Based Cell Cytometry: Differentiation and Quantification of viable and Gamma Deactivated B. Anthracis Sterne Spore**; Jason Guicheteau<sup>1</sup>, Ashish Tripathi<sup>1</sup>, Erik Emmons<sup>1</sup>, Michael Kim<sup>1</sup>, Phillip Wilcox; <sup>1</sup>USA Army RDECOM Edgewood Chemical Biological Center

2:50 PM (836) **Dynamic Sampling in Raman Microscopy**; Garth Simpson<sup>1</sup>, Shijie Zhang<sup>1</sup>, Zhengtian Song<sup>1</sup>, Azhad U. Chowdhury<sup>1</sup>, G. M. Dilshan P. Godaliyaddab<sup>1</sup>, Dong Hye Ye<sup>1</sup>, Atanu Sengupta<sup>2</sup>, Gregery T. Buzzard<sup>1</sup>, Charles A. Bouman<sup>1</sup>; <sup>1</sup>Purdue University; <sup>2</sup>Dr. Reddy's Laboratory

**Thursday Afternoon, Carson 4**

### 17RAM16: PHARMACEUTICAL RAMAN

Organizer and Presider: Ian Lewis

1:30 PM (837) **Method Development for the Classification of Drugs with Identical API Content Using Raman Spectroscopy**; Md. Naveem Hossain, Carl Anderson<sup>1</sup>, James Drennen<sup>1</sup>; <sup>1</sup>Duquesne University

1:50 PM (838) **Low-Frequency Raman Spectroscopy Can Improve Quantitative Solid-State Analysis of Solid-State Form Mixtures of Pharmaceuticals**; Tiina Lipiäinen<sup>1</sup>, Sara J. Fraser-Miller<sup>2</sup>, Keith C. Gordon<sup>2</sup>, Clare J. Strachan<sup>1</sup>; <sup>1</sup>University of Helsinki, Finland; <sup>2</sup>University of Otago, New Zealand

2:10 PM (839) **Monitoring Form Conversion of Pharmaceutical Drug Using In-line and At-line Raman Spectroscopy**; Ming Huang<sup>1</sup>, John Wasyluk<sup>1</sup>, Robert Wethman<sup>1</sup>; <sup>1</sup>Bristol-Myers Squibb

2:30 PM (840) **Monitoring API Concentration by Raman Spectroscopy**; Zachary Harms<sup>1</sup>, Zhenqi Shi<sup>1</sup>, Rajesh Kulkarni<sup>1</sup>, James Hermiller<sup>1</sup>, David Myers<sup>1</sup>; <sup>1</sup>Eli Lilly and Company

2:50 PM (841) **Quantitative Raman Assays for On-Site Analysis of Stockpiled Drugs**; Daniel Willett<sup>1</sup>, Jason Rodriguez<sup>1</sup>; <sup>1</sup>U.S. Food and Drug Administration

**Thursday Afternoon, Crystal 4**

### 17SPECIAL04: CELEBRATING THE FACSS MEMBERSHIP OF THE AUSTRIAN SOCIETY OF ANALYTICAL CHEMISTRY (ASAC)

Organizer and Presider: Bernhard Lendl

1:30 PM (842) **Fabry-Pérot Photothermal Interferometry (FP-PTI) for Trace Gas Sensing in Small Sample Volumes**; Bernhard Lendl<sup>1</sup>, Jakob Hayden<sup>1</sup>, Johannes Paul Waclawek<sup>1</sup>; <sup>1</sup>Technische Universität Wien

1:50 PM (843) **Analysis of Oxides in Steel Slag and of Trace Elements in Steel by Laser-Induced Breakdown Spectroscopy**; Johannes D. Pedarnig<sup>1</sup>, Simon Eschlböck-Fuchs<sup>1,2</sup>, Ludwig Birkbauer<sup>1</sup>, Christoph M. Ahamer<sup>1</sup>, Wolfgang Gaderbauer<sup>1</sup>, Hubert Duchaczek<sup>2</sup>, Josef Hofstadler<sup>1,2</sup>, Andreas Pissenberger<sup>2</sup>, Roman Rössler<sup>2</sup>, Norbert Huber<sup>1</sup>; <sup>1</sup>Johannes Kepler University Linz / Austria; <sup>2</sup>voestalpine Stahl GmbH, Linz / Austria

2:10 PM (844) **Investigating Li<sub>7</sub>-3xAlxLa<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> Garnets Using Laser Based Spectroscopic Analysis Techniques**; Stefan Smetaczek<sup>1</sup>, Maximilian Bonta<sup>1</sup>, Andreas Wachter-Welzl<sup>1</sup>, Stefanie Taibl<sup>1</sup>, Reinhard Wagner<sup>2</sup>, Daniel Rettenwander<sup>3</sup>, Jürgen Fleig<sup>1</sup>, Andreas Limbeck<sup>1</sup>; <sup>1</sup>TU Wien; <sup>2</sup>University of Salzburg; <sup>3</sup>Massachusetts Institute of Technology

2:30 PM (845) **Mid-Infrared Spectroscopy with Supercontinuum Laser Sources**; Markus Brandstetter<sup>1</sup>, Jakob Kilgus<sup>1</sup>, Christoph Gasser<sup>2</sup>, Bernhard Lendl<sup>1</sup>, Kristina Duswald<sup>1</sup>; <sup>1</sup>Research Center for Non-Destructive Testing; <sup>2</sup>Vienna University of Technology

2:50 PM (846) **Recent Advances of Vibrational Spectroscopy in Phytomics**; Christian Huck<sup>1</sup>; <sup>1</sup>Leopold-Franzens University, Innsbruck, Austria

**3:10 PM Poster Session and Coffee Break, Grand Salon**

**Thursday Afternoon, Tahoe Ballroom**

### 17AWD08: FACSS INNOVATION AWARD SYMPOSIUM

Organizer and Presider: Karen Esmonde-White

3:45 PM Presentation of the FACSS Distinguished Service Award to Diane Parry

3:50 PM (847) **Probing Cancer by Exploiting Spontaneous and Stimulated Raman Scattering**; Ji-Xin Cheng<sup>1</sup>, Chien Sheng Liao<sup>1</sup>; <sup>1</sup>Boston University

4:10 PM (848) **Effective Light Directed Assembly of Building Blocks with Microscale Control**; Chia-Hung Chen<sup>1</sup>; <sup>1</sup>National University of Singapore

4:30 PM (849) **Optical Reflection and Waveguiding of Sound in Free Space**; Daniel Kazal<sup>1</sup>, Ellen Holthoff<sup>2</sup>, Brian Cullum<sup>1</sup>; <sup>1</sup>University of Maryland, Baltimore County; <sup>2</sup>Army Research Laboratory, Adelphi, MD

4:50 PM (850) **Dried Blood Spheroids: A Versatile Paper-Based Biofluid Sample Collection Platform for Improved Analyte Stability**; Abraham Badu-Tawiah<sup>1</sup>, Deidre Damon<sup>1</sup>; <sup>1</sup>The Ohio State University

## FRIDAY MORNING CLOSING SESSION

7:30 – 10:00 AM, Tahoe Ballroom

7:30 AM Continental Breakfast  
8:00 AM **Announcement of 2017 Innovation Award Winner**

8:30 – 10 AM

**The New Vision of Analytical Science by the World**

Organizer and President: Matthieu Baudelet

8:30 AM (851) **The Science of Debunking Misconceptions**; Panayiota Kendeou<sup>1</sup>; <sup>1</sup>University of Minnesota  
9:00 AM (852) **The New 3R's: Risk, Reward, and Regulation**; Fred LaPlant<sup>1</sup>; <sup>1</sup>3M  
9:30 AM (853) **Calling Bullshit in the Age of Big Data**; Jevin West<sup>1</sup>; Carl T. Bergstrom<sup>1</sup>; <sup>1</sup>University of Washington  
10:00 AM **Preview of SciX 2018 Conference in Atlanta**  
10:15 AM Adjourn

**SciX 2018, Atlanta Marriott Marquis, Atlanta, Georgia October 21 - 26**

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**John Wasylyk, Bristol-Myers Squibb**  
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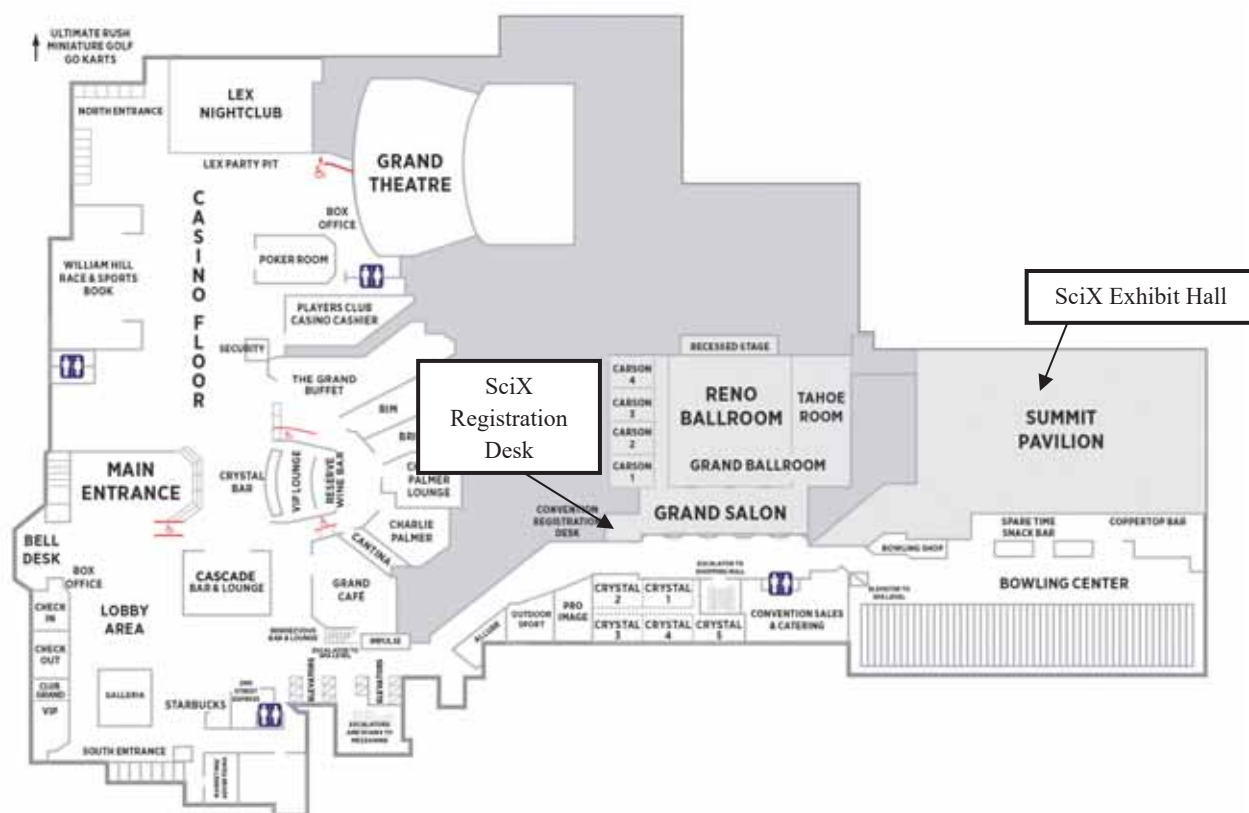
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