

The 22nd Bruker Crystallographic Users Group Meeting

**January 17-19, 2016
Jacksonville, FL**

presented by



Bruker advisers: Sue Byram, Dan Frankel.
Local chair: Christos Lampropoulos.
Program chair: Ilia Guzei.

At a glance

January 17, 2016, Sunday night, 6:30 PM - 9:00 PM. Opening Reception at [Blackfinn Ameripub](#) (4840 Big Island Drive, Suite 05, Jacksonville, FL, 904-345-3466).

January 18, 2016, Monday. Lecture session topic is "Methods in crystallography" with highlights in the evolution of Bruker AXS software and hardware in the field of single-crystal X-ray diffraction in general, and high-pressure crystallography in particular. The lectures will be held at the [Talon room](#) at the top floor of Building 16 ([Osprey Commons](#)) in the morning. The workshops take place after lunch at the Science and Engineering Building (Building 50).

Shuttle bus service between the Sheraton and conference venue: Pick up at 7:45 AM at the Sheraton. Drop off in front of Building 16, [Osprey Commons](#) (or in Parking Lot 8), where the [Talon room](#) is. Pick up at 4:20 PM in front of the [Science and Engineering Building 50](#), in Parking Lot 7. Drop off at the Sheraton.

January 18, 2016, Monday night. An optional 5:00 PM bus tour to St. Augustine. The bus leaves from the Sheraton hotel.

January 19, 2016, Tuesday. Topic is "Chemistry and Crystallography" with lectures from a number of institutes in Florida.

Shuttle bus service between the Sheraton and conference venue: Pick up at 7:30 AM at the Sheraton. Drop off in front of Building 16, [Osprey Commons](#) (or in Parking Lot 8), where the [Talon room](#) is. Pick up at 2:30 PM in front of Building 16, [Osprey Commons](#) (or in Parking Lot 8). Drop off at the Sheraton.

Both lectures and workshop will be held the [Talon room](#) at the top floor of Building 16 ([Osprey Commons](#)).

There will be only one workshop by George Sheldrick on Tuesday, January 19 after lunch.

The meeting ends at 2:30 PM on January 19, 2016, Tuesday.

Meeting Program (1/2) Sunday and Monday

Sunday, January 17, 2016	
6:30 PM	Opening Reception at Blackfinn Ameripub (4840 Big Island Drive, Suite 05, Jacksonville, FL 32246, 904-345-3466)
Monday, January 18, 2016	
Methods in crystallography	
8:00 AM	Registration.
8:30 AM	Christos Lampropoulos. Welcome.
8:35 AM	Ilia Guzei. Introductory remarks.
8:45 AM	Susan Byram. "What is new at Bruker".
9:10 AM	Roger Durst. "Latest Bruker Technologies for Single-Crystal Diffraction".
9:35 AM	George Sheldrick. "Intrinsic phasing (XT)".
10:00 AM	Coffee break
10:25 AM	Ilia Guzei. "Crystal growing contests: a legacy of the International Year of Crystallography 2014".
10:50 AM	Marcio Siqueira. "An introduction to diamond anvil cells and loading techniques for high pressure experiments".
11:15 AM	Michael Ruf. "Processing High Pressure Data with APEX3".
11:40 AM	Dan Frankel. "What's for lunch".
Workshops below will run in parallel twice. Check workshop schedule on page 4 for your assignment.	
<i>First set of workshops - 1:15 PM</i>	
1:15 PM	Khalil Abboud & Bruce Noll. "Crystal structure determinations: the final touches".
1:15 PM	Joseph Reibenspies & Nattamai Bhuvanesh. "Comparing predicted powder patterns from SCD with observed PXRD patterns".
1:15 PM	Marcio Siqueira & Michael Ruf. "High Pressure Crystallography – Finally Getting your feet wet!"
<i>Second set of workshops - 2:45 PM</i>	
2:45 PM	Khalil Abboud & Bruce Noll. "Crystal structure determinations: the final touches".
2:45 PM	Joseph Reibenspies & Nattamai Bhuvanesh. "Comparing predicted powder patterns from SCD with observed PXRD patterns".
2:45 PM	Marcio Siqueira & Michael Ruf. "High Pressure Crystallography – Finally Getting your feet wet!"
4:15 PM	Scientific program ends
5:00 PM	An optional bus tour to St. Augustine. The bus leaves from the Sheraton hotel.

For workshop assignments, see page 4

Meeting Program (2/2)

Tuesday

Tuesday, January 19, 2016	
Chemistry and Crystallography	
7:45 AM	Registration.
8:05 AM	Ilia Guzei. Introductory remarks.
8:15 AM	Thomas Albrecht-Schmitt. "Taking the Berkelium Leap".
8:40 AM	Joel Mague. "Rare Earth Polyoxotungstates; Some Cautionary Tales".
9:05 AM	Wenyang Gao. "Challenges in Structural Analysis of Metal-Organic Frameworks (MOFs)".
9:30 AM	Coffee break
10:00 AM	Christos Lampropoulos. "The great dependence of cluster chemistry on X-ray crystallography".
10:25 AM	Bruce Noll. "Advanced data collection strategies".
10:50 AM	Ton Spek. "Updates on Validation and SQUEEZE".
11:15 AM	Bob Burrow. "Easy access to the Bruker APEX2/APEX3 PostgreSQL Database".
11:40 AM	Dan Frankel. "Closing remarks".
Workshop for all participants	
1:00 PM	George Sheldrick (University of Goettingen). "Practical guide to SADABS, TWINABS, XT, etc."
2:30 PM	Meeting ends

Poster presentations

Name	Affiliation	Title
Annaliese Thuijs	University of Florida	New approaches for the preparation of high nuclearity Mn-Ce clusters: the highest nuclearity Mn-Ce cluster to date.
Ari Alico	Florida State University	Structural Trends in the Lanthanide Chromates.
Ashley Felts	University of Florida	Modification of a Bruker APEX Duo Diffractometer for Variable Temperature, Solvated Powder X-Ray Diffraction and Synchrotron Screening.
Bob Burrow	Universidade Federal de Santa Maria, Brazil	Using povray to generate X-ray aperture masks for SAINT.
Daisuke Takahashi	University of Florida	Structural and magnetic properties of a family of core-shell-type heterometallic clusters.
Indranil Chakraborty	University of California Santa Cruz	Diverse Topologies Directed by Anionic Interactions in the Supramolecular Assembly of Ag(I) Centers.
Joshua de Groot	University of Iowa	Extending dimensionality in uranyl amino acid metal-organic materials.
Logesh Mathivathanan	Florida International University	Cu(II)-pyrazolato clusters as building units for framework materials.
Maurice Payne	University of Iowa	Towards Novel Hybrid Materials: Synthesis and Characterization of New Uranyl (VI) Complexes Incorporating Zwitterionic Ligands.
Teresa Eaton	Florida State University	Th(VO ₃) ₂ (SeO ₃) and Ln(VO ₃) ₂ (IO ₃) (Ln = Ce, Pr, Nd, Sm, and Eu): Unusual cases of aliovalent substitution.

Workshop assignments

Monday, January 18, 2016		
<i>First set of workshops - 1:15 PM</i>		
Khalil Abboud & Bruce Noll. "Crystal structure determinations: the final touches".	Joseph Reibenspies & Nattamai Bhuvanesh. "Comparing predicted powder patterns from SCD with observed PXRD patterns".	Marcio Siqueira & Michael Ruf. "High Pressure Crystallography – Finally Getting your feet wet!"
Annaliese Thuijs	Ali Arico	Alexander Chemey
Catherine Lavin	Ashley Felts	Allen Hunter
Christos Lampropoulos	Bohari M Yamin	Ilia Guzei
Daisuke Takahashi	Chunqing Zhao	Joshua de Groot
Hannah Johnston	Frankie White	Philip D. Martin
Indranil Chakraborty	James A. Golen	Robert Alan Burrow
Kevin Seidler	Mo Payne	Thomas Pekarek
Logesh Mathivathanan	Peter S White	
Matthew Marsh	Teresa Eaton	
Samantha Brewer	Thayumanasamy Somasundaram	
Tamara Hamilton	Tony Hu	
Valerie Lopez-Diaz		

Monday, January 18, 2016		
<i>Second set of workshops - 2:45 PM</i>		
Khalil Abboud & Bruce Noll. "Crystal structure determinations: the final touches".	Joseph Reibenspies & Nattamai Bhuvanesh. "Comparing predicted powder patterns from SCD with observed PXRD patterns".	Marcio Siqueira & Michael Ruf. "High Pressure Crystallography – Finally Getting your feet wet!"
Alexander Chemey	Catherine Lavin	Annaliese Thuijs
Ali Arico	Daisuke Takahashi	Bohari M Yamin
Ashley Felts	Greg McManus	Christos Lampropoulos
Chunqing Zhao	Ilia Guzei	James A. Golen
Frankie White	John Bacsá	Lev Gasparov
Hazem Ahmed Ghabbour	Joshua de Groot	Matthew Marsh
Li Yongxin	Kevin Seidler	Mo Payne
Philip D. Martin	Logesh Mathivathanan	Teresa Eaton
Rudi Wehmschulte	Michael Lufaso	
Teresa Eaton	Tamara Hamilton	
Tony Hu	Thomas Pekarek	
	Valerie Lopez-Diaz	