MEETING Announcement

GEORGIA SECTION

ACS Chemistry for Life™

Tuesday, October 28th 2014

Dr. John Bacsa

A brief historical tour of chemical X-ray crystallography: from Max von Laue's discovery of diffraction of X-rays to modern change density analysis.

Location:
Maggiano's Little Italy– Buckhead
3368 Peachtree Rd, Atlanta, GA 30326

Directions: **Click Here**

Tuesday, October 28th 2014

6:00 pm Meet and mingle (cash bar)

6:20 pm Dinner

7:30 pm Presentation

Menu (Family Style):

First Course:
Maggiano's Salad & Caesar Salad
Bruschetta & Calamari

Second Course:
Spaghetti Marinara & Four cheese Ravioli
Salmon & Chicken Parmesan

Desserts:
Cheesecake & Profiteroles

**Coffee, Soda & Ice Tea included

RSVP by 4:00 pm on 24 October 2014
to Joel Pollino at joelpollino@gmail.com

Price:
$30 regular; $15 students, K-12 teachers, retired current ACS members
Payment: ***At the door***

Cash, Credit Card, or Check to: "Georgia Section ACS"

Dr. John Bacsa

Facilities Director, X-Ray Diffraction Center
Emory University, Atlanta GA

EMORY UNIVERSITY

Dr. John Bacsa is the Facilities Director, X-ray Diffraction Center at Emory University. The X-ray center's primary function is the complete determination of the three-dimensional arrangement of atoms and molecules in inorganic, organometallic, organic and biological compounds. Laboratories at Emory and elsewhere rely on our service for the unambiguous structural characterization of their products, to establish relative and absolute stereochemistry and to confirm the outcomes of reactions. He holds a PhD from the University of the Witwatersrand, Johannesburg, South Africa (advisor: Prof. J.C.A. Boeyens) where he studied the

effects of steric interactions on rhenium-rhenium bond distances by combination of X-ray crystallography and molecular modelling. With these results he was able to determine the relationships between bond strengths, harmonic force-constants and characteristic bond lengths for these metal-metal bonds. He is interested in determining and analyzing the electron density in molecules from theory and experiment and in determining bond order functions for varied elements in the periodic table. He has approximately 133 publications that have been cited 722 times.

Positions and Honors.

Positions:

1998-01 Managed the X-ray facility, University of Cape Town, South Africa.

2002-02 Research associate of Prof. Mark D. Hollingsworth, Kansas State University.

2002-04 Postdoctoral Research in Inorganic Chemistry, Texas A&M University.

2004-2007 Manager, Toronto Protein Diffraction Facilities, Sickkids Hospital, Toronto, Canada.

2007-2011 Senior Experimental Officer, University of Liverpool, UK.

2004-present Facilities director of the X-ray Diffraction Center at Emory University.

Awards:

2002 Fellowship from National Aeronautics and Space Administration (NASA).

2002-2004 Reviewer, *Inorganic Chemistry*.

2002-present Reviewer, *Acta Crystallographica* Section C.

2012 Research highlighted in *Chemical Engineering News*.

A brief historical tour of chemical X-ray crystallography: from Max von Laue's discovery of diffraction of X-rays to modern change density analysis

Abstract: The aim of this presentation is to give, from a historical perspective, a brief overview of X-ray crystallography. Although Bragg is credited for determining the first atomic resolution structure of a crystal by X-rays, Max von Laue demonstrated that crystals diffract X-rays and was awarded the Nobel Prize for Physics in 1914 for this discovery. Von Laue's X-ray diffraction photos revealed the underlying space-group symmetry of crystals and validated mathematical derivations of the space lattice. Subsequently, Bragg made the connection between wavelength of X-ray light and the spacing between atoms in a crystal, and opened the door to routine structure determinations. The increase in the data quality allowed the nature of chemical interactions to be fundamentally characterized. Charge and energy can now be precisely determined by X-ray crystallography but the exact nature of a chemical bond remains elusive.