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748th Conference

Scientific Program

International Conference on

Applied Crystallography

October 17-19, 2016 Houston, USA



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Day 1 October 17, 2016

08:30-09:30 Registrations

Windsor I

conferenceseries.com 09:30-09:55 **Opening Ceremony**

Keynote Forum

09:55-10:00 **Introduction**

10:00-10:40 **Title: Crystal structure and organic solid-state reactions**

Gerd Kaupp, University of Oldenburg, Germany

Networking and Refreshments Break and Group Photo 10:40-11:00 @ Foyer

Group Photo @ Windsor I

11:00-11:40 **Title: Orientational disorder of dipolar molecules: A key to understand polarity formation in materials**

Jurg Hulliger, University of Berne, Switzerland

Panel Discussion

Sessions: Advanced Crystallography | Crystallography in Biology | Recent development in X-ray studies and Crystallography Applications

Session Chair: Gerd Kaupp, University of Oldenburg, Germany

Session Introduction

11:40-12:05 **Title: Breathing crystals - P,T-induced dynamics of heterospin crystals**

Victor Ovcharenko, International Tomography Center, Russia

12:05-12:30 **Title: Structure-based mechanistic insights into PAM-dependent spacer acquisition for incorporation into the CRISPR array**

Yanli Wang, Chinese Academy of Sciences, China

12:30-12:55 **Title: Two alternative structures of oxygen-evolving complex in photosystem II found by X-ray crystallography at extremely low doses**

Nobuo Kamiya, Osaka City University, Japan

12:55-13:20 **Title: Hydrated Nickel(II) ions- The new secondary building units for the formation of 2D and 3D cationic water networks**

Geeta Hundal, Guru Nanak Dev University, India

Lunch Break 13:20-14:20 @ Churchill

14:20-14:45 **Title: Structural insights into the activation process of the opioid mu receptor**

Helene Demene, Centre of Biochimie Structrale, France

14:45-15:10 **Title: Numerical simulation of liquid phase diffusion growth of SiGe single crystals using fixed and dynamic grid techniques: A comparison**

Mandeep Sekhon, University of California, USA

15:10-15:35 **Title: Structure determination by correlated scattering**

Dilano K Saldin, University of Wisconsin-Milwaukee, USA

Networking and Refreshments Break 15:35-15:55 @ Foyer

15:55-16:20 **Title: Structural insights into mode of regulation of serine protease HtrA2**

Kakoli Bose, Tata Memorial Centre, India

16:20-16:40 **Title: Structure determination from powder diffraction data of self-assembled structures consisting of beta-peptide foldamers**

Jintaek Gong, Korea Advanced Institute Science and Technology, Republic of Korea

Panel Discussion 16:40-17:00

Windsor I

Keynote Forum

Introduction

09:10-09:50 **Title: Attrition-induced deracemization of racemizable crystal-liquid suspensions for the production of industrially relevant compounds**
Richard M. Kellogg, Syncom BV, The Netherlands

09:50-10:30 **Title: Macromolecular computational crystallography: Looking forward (and backward)**
Alexandre Urzhumtsev, Université de Lorraine, France

Networking and Refreshments Break 10:30-10:50 @ Foyer

Crystallography in Materials Science

Session Chair: Andriy Lotnyk, Leibniz Institute of Surface Modification (IOM), Germany

Session Introduction

10:50-11:15 **Title: Local atomic arrangement in Ge-Sb-Te phase-change thin films**
Andriy Lotnyk, Leibniz Institute of Surface Modification (IOM), Germany

11:15-11:40 **Title: NMR Crystallography: when nuclear magnetic resonance and diffraction meet**
Christian BONHOMME, Pierre et Marie Curie University, France

11:40-12:05 **Title: Directionally tunable and mechanically deformable ferroelectric crystals from rotating polar globular ionic molecules**
Tamotsu Inabe, Hokkaido University, Japan

12:05-12:30 **Title: Redox orbital and electronic structure in energy materials by Compton scattering spectroscopy**
Kosuke Suzuki, Gunma University, Japan

12:30-12:55 **Title: Algorithms for generating Coincidence Site Lattices (CSLs) and near-CSLs in arbitrary bravais lattice systems**
Srikanth Patala, North Carolina State University, USA

12:55-13:20 **Title: Synthesis of (doped) ABO2 nanoparticles: Can this work at temperatures ≤ 90 °C without using an additional reducing agent?**
Melanie John, Ludwig-Maximilians-Universität München, Germany

Lunch Break 13:20-14:20 @ Churchill

14:20-14:45 **Title: Crystallographic and molecular packing interaction analysis of cholest-based steroids: A CSD study**
Rajni Kant, University of Jammu, India

14:45-15:10 **Title: Synthesis and applications of porous materials for gas storage**
Li-Xian SUN, Guilin University of Electronic Technology, China

15:10-15:35 **Title: Surfactant-mediated shape evolution of 3D organic molecular architecture**
Myobin Jeon, Korea Advanced Institute Science and Technology, Republic of Korea

Networking and Refreshments Break 15:35-15:55 @ Foyer

15:55-16:20 **Title: A new approach for estimating the density of noncrystalline materials**
Takahiro Sakagami, Ehime University, Japan

16:20-16:45 **Title: Effect of change in structural properties on gas sensing performance of Polyaniline-SrO2 nanocomposites**
Janhavi Talegaonkar, R. L. College, India

16:45-17:10 **Title: Crystal growth of gallium oxide based wide bandgap semiconductors**
Qixin Guo, Saga University, Japan

Panel Discussions 17:10-17:30

Day 3 October 19, 2016

Windsor I

Chemical Crystallography

Session Chair: Jean-Guillaume Eon, Universidade Federal do Rio de Janeiro, Brazil

Session Introduction

10:00-10:25	**Title: Topological features in crystal structures: A quotient graph-assisted analysis of underlying nets and their embeddings** **Jean-Guillaume Eon,** Universidade Federal do Rio de Janeiro, Brazil
10:25-10:50	**Title: X-ray crystal structures of the one-electron oxidized metal–phenolate complexes; Geometric and electronic structures relationship** **Yuichi Shimazaki,** Ibaraki University, Japan

Networking and Refreshments Break 10:50-11:10 @ Foyer

11:10-11:35	**Title: Magnetic ordering, frustration and possible spin liquid state from 1D Cr3-triangles in the TiCrIr2 xOsxB2 series** **Boniface P T Fokwa,** University of California-Riverside, USA
11:35-12:00	**Title: Oxide cluster-surfactant hybrid single crystals toward solid electrolyte** **Takeru Ito,** Tokai University, Japan
12:00-12:25	**Title: The investigation of chemical crystallography and kinetic reactivity of Re(I) tricarbonyl complexes** **Marietjie Schutte-Smith,** University of the Free State, South Africa
12:25-12:50	**Title: Relations between crystal structures and physical properties in the ternary systems cextysnz (t = pd or pt)** **Werner Paschinger,** University of Vienna, Austria

Lunch @ Churchill 12:50 onwards….

Award Ceremony



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