EuroSciCon

4th Edition of International conference on

# Advanced Spectroscopy, Crystallography and Applications in Modern Chemistry

April 25-26
Rome, Italy

2019



Crystallography 2019

https://crystallography.euroscicon.com/

# Day 1, Agenda

## General Session

08:00 AM — INTRODUCTION

09:00 AM — PLENARY

10:00 AM — KEYNOTE

**Networking & Refreshments Break @ Foyer**

| | HALL 01 | HALL 02 | HALL 03 |
|---|---|---|---|
| 11:00 AM | Talks On: **Crystallography** | Talks On: **Chemical Crystallography** | Talks On: **Advanced Crystallography** |
| | Talks On: **Small Molecule Crystallography: Novel Structures and General Interest** | Talks On: **Computational Crystallography** | Talks On: **Supermolecular Crystallography** |
| | **SESSION DISCUSSION** | **SESSION DISCUSSION** | **SESSION DISCUSSION** |
| 02:00 PM | Panel Over: **Polymer Crystallization** | Panel Over: **Nano Crystallography** | Panel Over: **Electron Crystallography** |
| | Workshop On: **Crystallization** | Workshop On: **Engineering of Crystalline and Non-crystalline Solids** | Workshop On: **Structure and Properties of Functional Materials** |
| | *Lunch Break @ Restaurant* | *Lunch Break @ Restaurant* | *Lunch Break @ Restaurant* |
| 04:00 PM | Talks On: **Crystallography of Novel Materials** | Talks On: **X-Ray Crystallography** | Talks On: **Chemical Crystallography: General Interest** |
| | Lectures on: **Mounting the Crystal** | Lectures on: **Ions and salts** | Lectures on: **Crystal Growth** |
| 06:00 PM | Session On: **Chemical shift interaction** | Session On: **Vibrational circular dichroism Spectroscopy** | Session On: **Cryo-electron microscopy (cryo-EM)** |
| | **NETWORKING** | **NETWORKING** | **NETWORKING** |

# Day 2, Agenda

## General Session

08:00 AM — INTRODUCTION

09:00 AM — PLENARY

10:00 AM — KEYNOTE

**Networking & Refreshments Break @ Foyer**

| | HALL 01 | HALL 02 | HALL 03 |
|---|---|---|---|
| 11:00 AM | Talks On: **Nuclear Magnetic Resonance Crystallography (NMR crystallography)** | Talks On: **Spectroscopy** | Talks On: **Advances in Neutron Diffraction** |
| | Talks On: **Application of Modern Chemistry** | Talks On: **Metal-Organic Frameworks (MOFs)** | Talks On: **Pharmaceutical Co-crystals** |
| | **SESSION DISCUSSION** | **SESSION DISCUSSION** | **SESSION DISCUSSION** |
| 02:00 PM | Panel Over: **Crystallography Applications** | Panel Over: **Porous and Liquid Crystals** | Panel Over: **Nano-materials and Nanotechnology** |
| | Workshop On: **Crystal Engineering** | Workshop On: **Quasi-crystals** | Workshop On: **Novel crystallization strategies for XFEL studies** |
| | ***Lunch Break @ Restaurant*** | ***Lunch Break @ Restaurant*** | ***Lunch Break @ Restaurant*** |
| 04:00 PM | Talks On: **Biological Structure Determination** | Talks On: **Crystallography in Biology** | Talks On: **NMR Spectroscopy vs. X-Ray Crystallography** |
| | Lectures on: **Spectroscopy Applications** | Lectures on: **Ultraviolet Photoelectron Spectroscopy (UPS)** | Lectures on: **Applications of NMR** |
| 06:00 PM | Session On: **Fiber diffraction** | Session On: **Applications of X-ray diffraction** | Session On: **Diamonds growth** |
| | **NETWORKING** | **NETWORKING** | **NETWORKING** |

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# GLIMPSES OF CRYSTALLOGRAPHY CONFERENCES


















# City Attractions












# City Attractions



Roman Forum



Saint Peter's Square



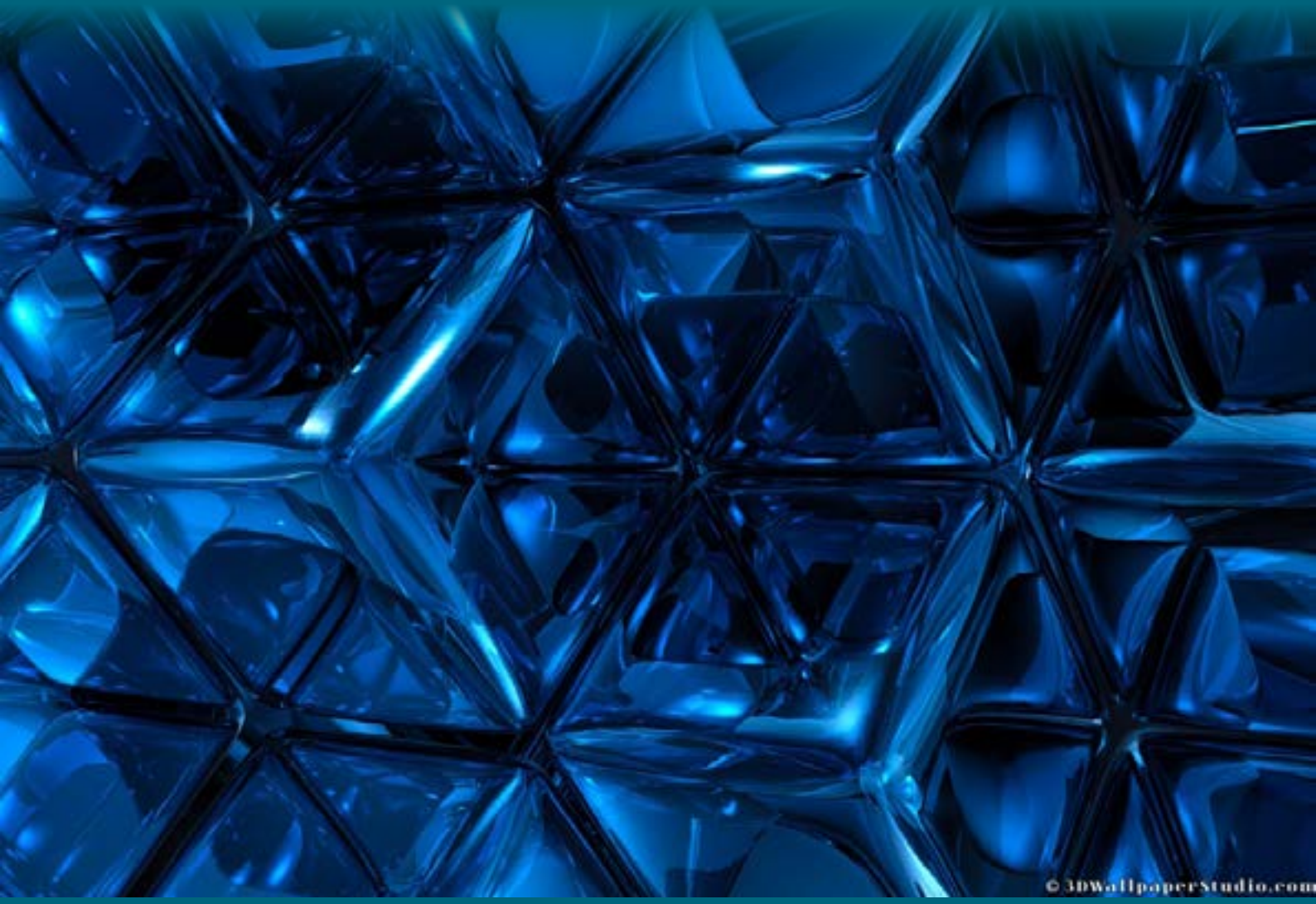
San Giovanni in Laterano



Santa Maria in Trastevere

3rd Edition of International Conference on

# Advanced Spectroscopy Crystallography and Applications in Modern Chemistry




**June 04-05, 2018**
**London, UK**

EuroSciCon

# Crystallography 2018

## Agenda Day 1: June 04, 2018

## Bleriot 2

**09:30-10:00** **Registrations**

10:00-10:25 Opening Ceremony

**Keynote Forum**

10:25-10:30 Introduction

**10:30-11:10** **Title: Phonon assisted oxygen diffusion vs. oxygen and electronic ordering mechanisms in non-stoichiometric correlated oxides**

Werner Paulus, University of Montpellier, France

**Networking & Refreshment Break 11:10-11:25 @ Breakout Area**

**11:25-12:05** **Title: Crystallography of phase transformations in solids and its applications**

Mingxing Zhang, The University of Queensland, Australia

**12:05-12:45** **Title: Advances and applications of neutron scattering and diffraction**

Martin Meven, RWTH Aachen University, Germany

**Lunch Break 12:45-13:30 @ RBG**

**Session Introduction**

**Sessions: Chemical Crystallography | Advanced Crystallography | Crystal Growth | Nuclear Magnetic Resonance Crystallography | Advances in Neutron Diffraction | Biological Structure Determination | Application of Modern Chemistry**

**Session Chair: Henrich H. Paradies,** Jacobs-University, Germany

**Session Co-Chair: Vijeesh Padmanabhan,** The Cochin College, India

**13:30-14:00** **Title: Stereochemistry and anti-inflammatory inhibition: Asymmetry complexes of 4-halogenated mofebutazones derivatives**

Henrich H. Paradies, Jacobs-University, Germany

**14:00-14:30** **Title: Synthesis and characterization of Triglycinesulphate crystals doped with potassium succinate**

Vijeesh Padmanabhan, The Cochin College, India

**14:30-15:00** **Title: Novel magneto-optic behavior from a polysquaraine: structure / property relationship**

Daniel E. Lynch, Exilica Limited, UK

**15:00-15:30** **Title: High-pressure crystallographic studies in diamond anvil cells using X-rays and neutrons**

Andrzej Grzechnik, RWTH Aachen University, Germany

**Networking & Refreshment Break 15:30-15:45 @ Breakout Area**

**15:45-16:15** **Title: NMR Crystallography as a tool for characterization of active sites of solid catalysts**

Olga B. Lapina, Novosibirsk State University, Russia

**16:15-16:45** **Title: Crystallography of oxidized metal(II)- di(phenolate) complexes; Geometric and electronic structures relationship**

Yuichi Shimazaki, Ibaraki University, Japan

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|---|---|
| 16:45-17:15 | **Title: Femtoscope: Atomic Resonance in ATP imposes the necessary and sufficient conditions for cancer efficient radio-therapy**<br>Edward Jimenez, Central University, Ecuador, USA |

# Agenda Day 2: June 05, 2018

## Bleriot 2

**09:00-10:00 Registrations**

**Keynote Forum**

| | |
|---|---|
| 10:00-10:40 | **Title: Solid-State NMR in materials science**<br>Anastasia Vyalykh, TU Bergakademie Freiberg, Germany |

**Networking & Refreshment Break 10:40-10:55 @ Breakout Area**

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|---|---|
| 10:55-11:35 | **Title: Structural features of a new oxygen deficient perovskite $Sr_2ScGaO_5$, a promising oxygen ion conductor at moderate temperature**<br>Monica Ceretti, Institut Charles Gerhardt Montpellier, France |

**Session Introduction**

**Sessions: Crystallography of Novel Materials | Spectroscopy Applications | Crystallography Applications | Crystallography in Biology**

**Session Chair: Marie-Hélène Lemée-Cailleau,** Institut Laue Langevin, France

**Session Co-Chair: Yuichi Shimazaki,** Ibaraki University, Japan

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|---|---|
| 11:35-12:05 | **Title: Neutron Laue and X-ray diffraction study of a new crystallographic superspace phase in n-nonadecane–urea**<br>Marie-Hélène Lemée-Cailleau, Institut Laue Langevin, France |
| 12:05-12:35 | **Title: Fluorination of cuspidine-related phases, $Ln_4Al_2O_9$ (Ln=Sm, Eu, Gd, Tb)**<br>Aroa Morán-Ruiz, University of the Basque Country, Spain |
| 12:35-13:05 | **Title: Fluorescence in quantum systems with violated symmetry**<br>Nikolai N. Bogolubov (Jr.), Mathematical Institute of the RAS, Russia |

**Lunch Break 13:05-13:50**

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|---|---|
| 13:50-14:20 | **Title: Antibody-enabled small molecule drug discovery**<br>Alastair Lawson, UCB, UK |
| 14:20-14:50 | **Title: CrystalCMP – Fast packing comparison of molecular crystals**<br>Jan Rohlíček, Institute of Physics, ASCR, Czech Republic |
| 14:50-15:20 | **Title: Frag Xtal Screen for direct crystallographic fragment screening**<br>Christin Reuter, Jena Bioscience GmbH, Germany |

**Networking & Refreshment Break 15:20-15:35 @ Breakout Area**

**Poster Presentations @Foyer @15:35 onwards**

**Panel Discussion**

**Awards & Closing Ceremony**