

# CRYSTAL FORMS@BOLOGNA

**The 6<sup>th</sup> Workshop on Crystal Forms**

**19-21 January 2012**



The quest for new crystal forms has become one of the most challenging issues in the solid state sciences with impacts on the production, marketing and intellectual property protection of molecular materials such as active pharmaceutical ingredients.

The workshop will bring together top-notch scientists from industry and academy to discuss in a friendly and informal atmosphere issues at the frontier of this burgeoning field of research, from crystal structure prediction, crystal engineering, synthesis of new crystal forms, polymorphs, solvates and co-crystals screening to the intellectual property issues of interest to pharma companies.

The three-day meeting is organized by the group of Molecular Crystal Engineering (Prof. Dario Braga - University of Bologna) and by PolyCrystalLine s.r.l., the company expert on crystal forms.

**Sponsored by:**



**PANalytical**

**NETZSCH**



**Agilent Technologies**



## CF@BO PROGRAMME

### Thursday 19<sup>th</sup> January

**13:00 Registration**

14:00 *Polymorphs, co-crystals and salts in the context of the structural landscape.*  
**Gautam Desiraju**, Indian Institute of Science

14:30 *Polymorphism of Active Pharmaceutical Ingredients: the border between a real quality issue and an effective patent tool.*  
**Pietro Allegrini**, Dipharma Francis

15:00 *Solid state squaramides: a robust synthon.*  
**Cristina Puigjaner**, Universitat de Barcelona

15:30 *Getting your Solid State related inventions patented, particularly, in Europe*  
**Bertrand Gellie**, European Patent Office

**16:00 Coffee break**

16:30 *Theoretical study of the properties of bistable molecular crystals using first-principles methods.*  
**Juan J. Novoa**, University of Barcelona

17:00 *New protocol for high resolution XR-PD and analytical Technology developed by Zach –Zambon Chemicals and Synchrotron Elettra of Trieste Italy.*  
*R. Brescello, M. Verzini, M. Polentarutti, A. Smaniotto and L. Cotarca*  
**Livius Cotarca**, Zach System

17:30 *Methyl paraben: news about an old polymorphic system.*  
**Ulrich Griesser**, University of Innsbruck

18:00 *Crystal engineering & Racetam compounds.*  
**Luc Quéré**, UCB Pharma S.A.

**19:30 Social Dinner**

## **Friday 20<sup>th</sup> January**

- 9:00 *Computed crystal energy landscapes as an aid to polymorph screening .*  
**Sally Price**, University College London
- 9:30 *Crystal structure determination and refinement exploiting texture: a case in between powder and single crystal diffraction.*  
**Luca Lutterotti**, University of Trento
- 10:00 *Solid-state problems: how dispersion corrected Density Functional Theory calculations can help.*  
**Jacco van de Streek**, Avant-garde Materials Simulation Freiburg im Breisgau
- 10:30 Coffee break**
- 11:00 *Prediction and Stability of Polymorphic Forms: Virtual Crystallography, Thermodynamics and Kinetics.*  
**Erwin Marti**, APCh Marti Consulting Spa
- 11:30 *From crystals to soft matter and return.*  
**Fabrizia Grepioni**, University of Bologna
- 12:00 *Co-crystals, Salts and Polymorph screening of o-Desmethyl Venlafaxine and other APIs.*  
**Chiara Capuccini**, PolyCrystalLine
- 12:30 *On-line crystallization monitoring by X-Ray diffraction.*  
**Fabio Masiello**, Panalytical
- 13:00 Lunch**
- 14:30 *Crystal engineering of multiple component crystalline solids.*  
**Mike Zaworotko**, University of South Florida
- 15:00 *What can powder diffraction tell you about the structure of molecular cocrystals?*  
**Maryjane Tremayne**, University of Birmingham
- 15:30 *Challenges in API Form Control: Case Study Examples .*  
**Peter Karpinsky**, Novartis
- 16:00 *Putting the squeeze on pharmaceuticals - using high pressure to explore polymorphism*

*and solvate formation.*

**Colin Pulham**, The University of Edinburgh, Scotland, UK

**16:30 Coffee break**

17:00 *EXPO: a powerful tool for solving powder crystal structures in direct and reciprocal space.*

**Anna Moliterni**, IC-CNR Bari

17:30 *Crystal Forms and Patents in the Pharmaceutical Industry.*

**Heinz Josef Deussen**, LEO-Pharma

18:00 *Synthon Interference: Co-crystals, Salts and Polymorphs*

**Kumar Biradha**, Indian Institute of Technology

18:30 *High Throughput Screening: An Advanced Tool in the Search for Polymorphic Forms, Salts and Co-Crystals.*

**Andrea Decker**, Solvias AG

**Poster Section**

*Posters will be available for discussion throughout the conference in a space close to the meeting room. No specific poster session is allotted but posters will be discussed at coffee breaks and during free time.*

*Please send the abstract (max. 1 A4 page) to the workshop secretary before December 31.*

***The best poster will be awarded by a special prize from Panalytical.***

*Please note also that space available for each poster is 70 (height) x 50 cm (width) and that no printing facilities are available on site. For further details please contact the workshop secretary.*

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## **Saturday 21<sup>st</sup> January**

- 9:00 *SDPD – the ideal analytical partner for co-crystallisation by grinding.*  
**Kenneth Shankland**, University of Reading
- 9:30 *Metal-organic Materials by Mechanochemistry.*  
**James Stuart**, Queen’s University Belfast
- 10:00 *Organic structures from powder data: Challenges and limitations.*  
**Martin Schmidt**, Johann Wolfgang Goethe Universität Frankfurt
- 10:30 Coffee break**
- 11:00 *SSNMR Studies of Weak Interactions and Polymorphic Forms.*  
**Roberto Gobetto**, University of Torino
- 11:30 *The amorphous form in drug development.*  
**Giordani Antonio**, Rottapharm Madaus
- 12:00 *Analysis of element impurities (heavy metal) in pharmaceutical materials and fingerprint identification by ED-XRF.*  
**Eugenio Casini**, Panalytical
- 12:15 **Poster Prize**
- 12:30 *More Adventures in Polymorphland.*  
**Joel Bernstein**, Ben-Gurion University of the Negev
- 13:00 Concluding Remarks**

## **Location**

Bologna is a perfect location for International conferences and events, offering a cultural and academic atmosphere alongside great food and hospitality.

The city of Bologna was founded about 1000 years B.C. and was very prosperous during the Middle Ages, the urban lay out and many buildings of that epoch are still preserved nowadays. There are a number of churches and museums which are well worth of a visit - detailed information will be provided to participants.

## **Accommodation**

Novotel Fiera is a modern four-star hotel located in a strategic position in the heart of the Bologna Trade Fair district; 3 Km from the historical center and train station and 7 Km from the airport.

The conference will be held in a large hall located on the ground floor of the hotel. WiFi Internet connection is provided everywhere in the hotel and some PC workstations will be available for guests.

### **NOVOTEL BOLOGNA FIERA**

Via Michelino 73, 40127 BOLOGNA ITALY  
Tel (+39)051/637771 Fax (+39)051/519224

## **Registration**

Registrations are open on the conference web site: [www.pcl-workshop.com](http://www.pcl-workshop.com)

### **Early-bird registrations before 30 November 2011:**

- 500 € company
- 400 € additional participants from the same company
- 300 € academics
- 150 € students and Ph.D. students

### **Registrations after 30 November 2011**

- 600 € company
- 400 € additional participants from the same company
- 400 € academics
- 200 € students and Ph.D. students

## **Contacts**

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