

Dear Friends and Colleagues,

We cordially invite you to attend the 2nd ICSU/IUPAC Workshop on Crystal Engineering, which will be held in Como, Italy on August 30-September 1, 2015. This international workshop will serve as a mid-term meeting of the ICSU project CONVINCE “CONcepts and terMIology in Crystal Engineering” and of the IUPAC project “Basic Terminology of Crystal Engineering” (IUPAC Project No. 2012-044-1-100).

The objective of this workshop is to bring together a large number of scientists working in any areas related to crystal engineering.

In particular, this workshop is directed to:

- Specialists of international standing;
- Scientists from developing countries who will describe the particular practices adopted in their countries;
- Researchers and students concerned with crystal engineering research.

The program will comprise invited lectures by internationally renowned leaders in the field. Posters presentations are also scheduled and opportunities are planned for young scientists' networking with both peers and recognized leaders in the field.

Welcome to the 2nd ICSU/IUPAC Workshop on Crystal Engineering!

*Pierangelo Metrangolo
Giuseppe Resnati*

Speakers

Christer Aakeröy	(USA)
Alessia Bacchi	(Italy)
Len Barbour	(South Africa)
Joel Bernstein	(United Arab Emirates)
Andrew Bond	(Denmark)
Susan Bourne	(South Africa)
Dario Braga	(Italy)
Lee Brammer	(UK)
Carolyn P. Brock	(USA)
Neil Champness	(UK)
Graeme M. Day	(UK)
Gautam R. Desiraju	(India)
Mohamed Eddaoudi	(Saudi Arabia)
Mir Wais Hosseini	(France)
Janusz Lipkowski	(Poland)
Leonard R. MacGillivray	(USA)
Vasuki Ramachandran	(UK)
Giuseppe Resnati	(Italy)
Kari Rissanen	(Finland)
Robin D. Rogers	(USA)
Jonathan W. Steed	(UK)
Michael Zaworotko	(Ireland)

Local Organizing Committee

Chairmen

Pierangelo Metrangolo (Politecnico di Milano)
Giuseppe Resnati (Politecnico di Milano)

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**2nd ICSU/IUPAC
Workshop
on Crystal Engineering**

August 31 - September 1, 2015
Politecnico di Milano
Como - Italy

Scientific Themes

Computational Crystallography
2D Crystal Engineering
Pharmaceutical Co-crystals
Functional Crystals
Supramolecular Crystallography
Biomacromolecules
Metal-Organic Frameworks (MOFs)
Organic Crystals
Inorganic Crystals
Functional Crystals
Industrial Crystallization
Porous Crystals
Liquid Crystals

Program

MONDAY, AUGUST 31, 2015

08:30-09:00 **REGISTRATION**
09:00-09:15 **WELCOME ADDRESSES**
P. Metrangolo

SESSION I

09:15 - 09:45 **NANOINDENTATION IN CRYSTAL ENGINEERING: MECHANICAL PROPERTIES OF MOLECULAR CRYSTALS**
G. R. Desiraju

09:45 - 10:15 **SYNTHONIC ENGINEERING TOOLS FOR RATIONAL DESIGN OF PHARMACEUTICAL PRODUCT FORMULATION**
V. Ramachandran

10:15 - 10:45 **CRYSTALLIZATION AND GELATION: ORTHOGONAL SELF-ASSEMBLY FAR FROM EQUILIBRIUM**
J. W. Steed

10:45 - 11:15 **Coffee Break**

SESSION II

11:15 - 11:45 **STRUCTURAL FLEXIBILITY IN THE SOLID STATE**
L. Barbour

11:45 - 12:15 **MOLECULAR SALTS, IONIC CO-CRYSTALS, MOLECULAR CO-CRYSTALS**
D. Braga

12:15 - 12:45 **COVALENT, SUPRAMOLECULAR...IONIC? USING IONIC LIQUIDS TO DEMONSTRATE MANIPULATION OF THE IONIC BOND; AN UNDERUTILIZED TOOL IN CRYSTAL ENGINEERING**
R. D. Rogers

12:45 - 14:00 **Lunch**

SESSION III

14:00 - 14:30 **CAGING, REACTING AND SEPARATING VIA HALOGEN BONDING**
G. Resnati
14:30 - 15:00 **ANION- π INTERACTIONS IN THE SOLID STATE**
K. Rissanen

15:00 - 15:30 **HYDROGEN- AND HALOGEN-BOND DRIVEN CO-CRYSTAL SYNTHESIS**
C. B. Aakeröy

15:30 - 16:00 **HYDROGEN BONDS AND HALOGEN BONDS IN CRYSTAL ENGINEERING: FROM STRENGTH TO STRENGTH**
L. Brammer

16:00 - 16:30 **Coffee Break**

SESSION IV

16:30 - 17:00 **CRYSTAL ENGINEERING, SUPRAMOLECULAR CHEMISTRY, AND ORGANIC SYNTHESIS**
L. R. MacGillivray

17:00 - 17:30 **COMPUTATIONAL METHODS IN CRYSTAL ENGINEERING: LATTICE ENERGIES AND STRUCTURE PREDICTION**
G. M. Day

17:30 - 18:00 **FACTS AND FICTIONS ABOUT POLYMORPHISM**
J. Bernstein, A. J. Cruz-Cabeza, S. M. Reutzel-Edens

18:00 - 18:30 **INTERMOLECULAR INTERACTION ENERGY FRAMEWORKS**
A. D. Bond

18:30 - 19:00 **PACKING REGULARITIES IN HIGH-Z' STRUCTURES OF ORGANIC MOLECULES**
C. P. Brock

19:00 - 20:30 **POSTER SESSION**
21:00 - 23:00 **Social Dinner**

TUESDAY, SEPTEMBER 1, 2015

08:30 - 09:00 **REGISTRATION**

SESSION V

09:00 - 09:30 **CRYSTAL ENGINEERING OF HYBRID ULTRAMICROPOROUS MATERIALS**
M. J. Zaworotko

09:30 - 10:00 **SUPRAMOLECULAR TOOLS IN CRYSTAL ENGINEERING OF CYCLODEXTRINS**
J. Lipkowski

10:00 - 10:30 **THERMO- AND MECHANOCROMIC BEHAVIOUR IN COORDINATION COMPLEXES AND MOFs**
S. A. Bourne

10:30 - 11:00 **A SUPRAMOLECULAR BUILDING APPROACH FOR THE DESIGN AND CONSTRUCTION OF METAL-ORGANIC FRAMEWORKS**
M. Eddaoudi

11:00 - 11:30 **Coffee Break**

SESSION VI (11:30 - 13:00)

08:30 - 12:00 **MOLECULAR TECTONICS: HIERARCHICAL ORGANIZATION OF MATTER IN THE CRYSTALLINE PHASE**
M. W. Hosseini

09:45 - 10:15 **TRAPPING LIQUID DRUGS INSIDE CRYSTALS**
A. Bacchi

12:30 - 13:00 **ORGANISATION OF MOLECULAR TECTONS ON THE NANOSCALE USING HYDROGEN BONDS**
N. R. Champness

13:00 - 13:30 **CONCLUDING REMARKS**

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