2nd ADVANCES IN CRYSTAL ENGINEERING

January 15th, 2016

THE WORKSHOP

Cristal Engineering is a fast growing area of knowledge with implications in both academicals and industrials environment. It can be defined as the rational design and synthesis of functional molecular solids. APIs represent a particularly great challenge to crystal engineers because of applied reasons and their frequent exhibited polymorphism, which can have intellectual property implications.

The aim of this workshop is to review the recent developments in the field of Crystal Engineering by some of the world leading experts. We plan to cover the state-of-the-art in this area, in particular polymorphism, co-crystals, crystal packing analysis, high-pressure crystallography, polymorphic phase transitions, crystal transformations and patents. The workshop intends to create a relaxed atmosphere which will help a personal access to the speakers and an interaction between researchers during the coffee breaks and lunch.

Each speaker will deliver a 1 hour presentation (50 min talk + 10 min of questions).

SPEAKERS

Bernstein Joel, New York University in Shanghai, China.
Braga Dario, University of Bolonia, Italy.
Cruz-Cabeza Aurora J., University of Manchester, United Kingdom.
Grepioni Fabrizia, University of Bolonia, Italy.
Novoa Juan J., University of Barcelona, Spain.
Hunter Chris, Cambridge University
Reutzel-Edens Susan, Eli Lilly & Company, Indianapolis, United States.
Prohens Rafel, Polymorphism and Calorimetry Unit, CCiT, University of Barcelona

REGISTRATION

IQTCUB - XRQTC members: 50 €
Standard registration: 300 €
Academic registration: 150 €
Groups prices available
http://www.xrqtc.com/second-advances-in-crystal-engineering/

ORGANIZERS

GEM² Grup d'Estructura de Materials Moleculars

XRQTC Reference Network on Theoretical and Computational Chemistry

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PROGRAM

FRIDAY, 15th January	
8:30-9:00	Registration
9:00-9:10	**Welcome and starting remarks** Chair's welcome Prof. Juan J. Novoa
9:10-10:10	Joel Bernstein, Professor at the New York University in Shanghai, China: Facts and Fictions of Polymorphism in Pharmaceutical Solids
10:10-11:10	Aurora J. Cruz-Cabeza, Professor at the University of Manchester, United Kingdom: Conformational Polymorphism: From definitions to crystallization and design
11:10-11:30	**Coffee break**
11:30-12:30	Christopher Hunter, Professor at the University of Cambridge, United Kingdom: Quantification of Intermolecular Interactions
12:30-13:30	Prohens Rafel, Senior Researcher at the CCiT, University of Barcelona: Application of Combined Virtual/Experimental Approaches to Solid Form Screening
13:30-15:00	**Lunch break**
15:00-16:00	Dario Braga, Professor at the University of Bolonia, Italy: From molecular co-crystals to mixed crystals and ionic co-crystals
16:00-17:00	Susan Reutzel-Edens, Senior Scientist at Eli Lilly & Company, United States: Turning Molecules into Medicines Through Structure-Based Solid Form Design
17:00-17:20	**Coffee break**
17:20-18:20	Fabrizia Grepioni, Professor at the University of Bolonia, Italy: Light interactions in crystals for interactions with light
18:20-19:20	Juan J.Novoa, University of Barcelona, Spain: Theoretical prediction of polymorphs using pixel intermolecular potentials
19:20-19:30	**Closing remarks**