ESF Research Conferences

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Molecular Crystal Engineering

EuroConference on

Evaluations and Predictions of Solid State Materials Properties

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Helsinki, Finland, 17 – 22 June 2005

Chair: **Kari Rissanen** (University of Jyväskylä, FIN)
Vice-Chair: **Guy Orpen** (University of Bristol, UK)
Co-Chair: **Dario Braga** (University of Bologna, I)

Scientific Committee
Maria J. Calhorda (University of Lisbon, P); **Juan Novoa** (University of Barcelona, E);
Sally Price (IUCL, UK); **Pekka Pyykkö** (University of Helsinki, FIN)

With support from the Finnish Academy

Final Programme

On line at: http://www.esf.org/conferences/pc05191

Friday 17 June

Late afternoon / early evening	Registration at the hotel reception and ESF desk
19.00	Supper
21.00	Welcome drink

Saturday 18 June

Session I: Theoretical Evaluation of Intermolecular Interactions
Chair: Guy Orpen

09.15-09.30	Opening Remarks by **Kari Rissanen**
09.30-10.30	**Pekka Pyykkö** (University of Helsinki, FIN) *The Metallophilic Attraction: Theory*
10.30-11.00	**Coffee break**
11.00-11.45	**Maria-José Calhorda** (University of Lisbon, P) *TD-DFT Studies of Electronic Properties of Polynuclear Species*
11.45-12.30	**Juan Novoa** (University of Barcelona, E) *Theoretical Approach to Inter-ion Interactions in Solids*
13.00	**Lunch**

Chair: Alessia Bacchi

15.30-16.15	**Eric Clot** (University of Montpellier, F) *Counter Ion Effects on Structure and Reactivity from a DFT Perspective*
16.15-17.00	**Coffee break**
17.00-18.00	Flash Presentation n°1 (33 presentations of 2 minutes each) Chaired by **Kari Rissanen**
18.00-19.00	Poster session n°1
19.00	**Dinner**

Sunday 19 June

Session II: Modelling Crystals, Data Mining

Chair: Janet Scott

09.00-09.45	**Roberto Dovesi** (University of Torino, I) *Quantum Mechanical Simulation of Solid State Materials. An ab initio Approach with the CRYSTAL Program*
09.45-10.30	**Angelo Gavezzotti** (University of Milano, I) *Towards a Realistic Crystal Engineering: Quantitative Evaluation of Molecular Recognition Energies beyond the Atom-Atom Level*
10.30-11.00	**Coffee break**
11.00-11.45	**Sally L. Price** (University of London, UK) *Progress in the Computational Prediction of Organic Crystal Structures*
11.45-12.45	**Frank. H. Allen** (Cambridge Crystallographic Data Centre, Cambridge, UK) *Knowledge-Based Approaches to Crystal Design*
13.00	**Lunch**

Chair: Joel Bernstein

	Short talks
15.30-15.45	**Reiko Kuroda** (University of Tokyo , JP) *Solid-state Photochemical Reaction of 2-Arylthio-3-methylcyclohexen-1-one*
15.45-16.00	**Thomas Packianathan** (Bharathidasan University, IN) *Crystal Engineering of Solids of Pharmaceutical Interest: Hydrogen – bonded Supramolecular Motifs formed by Trimethoprim and Pyrimethamine with Carboxylic Acids.*
16.00-16.15	**Elena Kadyshevich** (Research Institute of Atmospheric Physics, Moscow, RU) *A Feasible Mechanism of Origination of Simplest Living Matter: Some Thermodynamic, Structural and Kinetic Aspects*
16.15-16.30	**Chun-Ying Duan** (Nanjing University, CN) *Chiral Coordination Polymers achieved from a Silver-containing Double-helicate*
16.30-17.00	**Coffee break**

17.00-18.00	Flash Presentation n°2 (33 presentations of 2 minutes each) Chaired by **Guy Orpen**
18.00-19.00	Poster session n°2
19.00	**Dinner**

Monday 20 June

Session III: Supramolecular Isomerism and Polymorphism
Chair: Jerry Atwood

09.00-09.45	**Joel Bernstein** (Ben-Gurion University of the Negev , Beer Sheva, IL) *Recent Adventures in Polymorphland*
09.45-10.30	**Peter Erk** (BASF, Ludwigshafen, D) *Organic Electronics at BASF*
10.30-11.00	**Coffee break**
11.00-11.45	**Urszula Rychlewska** (Adam Mickiewicz University, Poznań, PL) *Highly Functionalized Molecules - a Challenge for Crystal Engineering*
11.45-12.45	**Dario Braga** (University of Bologna, I) *Making Crystals by Reacting and Transforming Crystals*
12.45	**Lunch**
14.30	**Half-day excursion**
19.30	**Conference Dinner**

Tuesday 21 June

Session IV: Intermolecular Interactions and their Exploitation
Chair: Maria-José Calhorda

09.00-09.45	**Alessia Bacchi** (University of Parma, I) *Engineering of Organic/Inorganic Solids Capable of Reversibly Capturing and Releasing Volatile Guests*
09.45-10.30	**Neil Champness** (University of Nottingham, UK) *The Parallels between Molecular Organisation in Crystals and on Surfaces*
10.30-11.00	**Coffee break**
11.00-11.45	**Janet Scott** (Monash University, AU) *Engineering Intermolecular Interactions in the Solid-state - towards Functional Materials*
11.45-12.45	**Guy Orpen** (University of Bristol, UK) *Crystal Engineering for Synthesis*
13.00	**Lunch**

Chair: Dario Braga

15.30-16.30	**Hubert Schmidbaur** (Technical University of Munich, D) *Gold Compounds as Functional Components in Crystalline Solids*
16.30-17.00	**Coffee break**
17.00-19.00	Poster Session (1 + 2 combined)
19.00	**Dinner**
20.30	**Round Table Discussion** *"Computation of Crystal Properties - when and how?"*

Wednesday 22 June

Session V: Intermolecular Interactions and their Exploitation (continued)
Chair: Kari Rissanen

09.00-09.45	**Andrzej Katrusiak** (Adam Mickiewicz University, Poznań, PL) *Properties of Structures with Designed Networks of Hydrogen Bonds*
	Short talks
09.45-09.55	**Elna Pidcock** (Cambridge Crystallographic Data Centre, UK) *Crystal Packing: Molecular Shape and Intermolecular Interactions*
09.55-10.05	**Fernando S. Delgado** (University of La Laguna, E) *Ammonium Derivative Malonate Complexes:The Important Role of Hydrogen Bonding in the Design of New Metal-Organic Compounds*
10.05-10.15	**Iosif Hafez** (University of Patras, EL) *Nanocrystallic Calcium Phosphate Characterization and Deposition on Grain Surfaces of a Nonconsolidated Porous Medium*
10.15-10.25	**Rupa Hiremath** (Georgetown University, US) *Controlling the Crystal Growth of Polymorphs with 2-Dimensional Templates*
10.25-10.35	**Geoff Cooper** (University of Glasgow, UK) *Engineering a Switch from Antiferromagnetic to Ferromagnetic Exchange by Progressive Substitution of Nickel (II) for Cobalt (II) in a Dodecanuclear Cluster*
10.35-11.00	**Coffee break**
11.00-12.00	**Jerry Atwood** (University of Missouri, US) *Porosity of 'Non-Porous' Solids: Origins and Applications*
12.00-12.30	Concluding Remarks **Guy Orpen**
13.00	**Lunch and departure**