

EUROMAR 2012 Report – Ref: 3340

Summary

The EUROMAR 2012 conference and two satellite meetings took place in Dublin (IRELAND) from 27th June – 5th July. The conference was partially supported by the ESF Research Networking Programme EMAR (“multidisciplinary Frontiers of magnetic Resonance”). Funding had been approved by the Program Steering Committee. The total assigned budget was € 5000.

The conference was a scientific success and the contribution of the ESF was used to help the participation of 20 postgraduate students and postdoctoral fellows and partially contribute to cover the expenses of speakers.

With the help of the EMAR program, EUROMAR attendance was increased by attending delegates from throughout the world, in particular 504 from European countries, 76 from America and Canada, 50 from Australasia and 18 from Africa.

EMAR received a large publicity and several non-participating countries have shown their interest to support the EMAR network.

Description of the scientific content of the event

EUROMAR 2012

The EUROMAR 2012 conference was held on July 1-5th 2012 in University College Dublin. Two satellite meetings were held prior to the EUROMAR conference.

1. COST Spin Hyperpolarisation; 29th June – 1st July
2. XeMat 2012; 27-29 June

The RNP “Multidisciplinary Frontiers of Magnetic Resonance” shares the same goals that inspired this series of conferences

- a) Exploring new frontiers.
- b) Bringing together the different specialties within the broad field of magnetic resonance.
- c) Integrating groups from different countries and facilitating new collaborations.
- d) Training of young researchers.

Scientific Program

Scientific program of EUROMAR 2012 was well balanced between different fields of magnetic resonance. Plenary and Keynote lectures were delivered by well-known scientists from different areas of the magnetic resonance field and included Liquid State NMR, Solid State NMR, Metabolomics, EPR, Membrane proteins, Hyperpolarisation, Biological NMR, In Vivo and MRI, Paramagnetic systems and Computation. Among the speakers were leading scientists in Metabolomics (Prof. J Nicholson), Biomolecular solid-state NMR (Prof. R Tycko), NMR crystallography (Prof. L Emsley), Structural Biology (Prof. H Oschkinat), singlet NMR (Prof. M Levitt), EPR (Prof. S Van Doorslaer) and Protein complexes (Prof. G Wagner). Geographically speakers represent all the continents; Europe, America and Canada, Africa and Australasia.

Parallel sessions were arranged thematically as follows:

Solid State Methods

Metabolism & In-cell NMR

Biosolids NMR

Liquid State Methods

Nuclei and Electrons

In vivo and MRI

Emerging Areas

Bioliqids NMR

EPR

Computational

Materials

Hyperpolarisation

Biomacromolecular Assemblies

In each of the sessions a broad definition of the subject was discussed, so that specialists in different areas may be exposed to input their knowledge to different fields. New methodological approaches in application to current problems and recent developments were also demonstrated in each of the sessions. Due to popular demand of the subject areas, two

extended sessions were held for EPR, Bioliquids NMR and Biosolids NMR. This allowed expanding the knowledge of the rapidly developing new technologies.

In addition to the Keynote speech by Prof. R. Tycko, there were 12 plenary speaker sessions that covered every angle of the magnetic resonance research. In particular Prof. J. Nicholson explained how simple NMR spectroscopic methods can be used for systems medicine in the real world. Further he explained the development of new powerful tool to identify important biomarkers which would help to study personal and public healthcare models. Under the new methods in solids and oriented media, Prof. M Ernst discussed the phase-altering pulse sequences for decoupling and recoupling which opens new experimental possibilities in solid state NMR. In the same session, Prof. C Nielsen, presented a lecture on the systematic design of improved homo- and heteronuclear coherence transfer elements for biological solid-state NMR with improved resolution and sensitivity.

Metabolism and In-cell NMR session was very popular among all the participants. Prof. J Griffin presented NMR data fusion to improve the sensitivity of proton HR-MAS NMR spectroscopic techniques in Breast Cancer. Prof. G Pielak's presentation covered the macromolecular crowding and protein chemistry from inside and outside cells. For example this session covered the recent scientific developments in In-Cell NMR with clear developments related to medical applications.

Bioliquids NMR has always been a very popular session with recent scientific developments, in academia and industry. Prof. M Sattler gave an excellent presentation in molecular recognition and dynamics of large protein complexes in solution. He developed an efficient protocol for determining the quaternary structure of multi-domain proteins and protein complexes using solution NMR techniques, small angle X-ray and Neutron scattering. Prof. J Feigon presented the combined used of spectroscopic techniques to determine the large molecular structures of ribonucleoprotein complexes.

Well-known EPR specialists have presented their current work and recent results in application to biological systems. Prof. M Bennati presented the distance measurements and dynamic nuclear polarization at different EPR frequencies which would help to develop new applications in NMR spectroscopy of biological samples. The connection between EPR, NMR and other spectroscopic techniques was further discussed by other speakers in this session.

Computational aspects and molecular dynamics session was devoted to various investigations of protein dynamics by NMR and quantum mechanics. World leader in this field, Prof. P Guntert discussed the development of reliable and flexible automated assignment methods of NMR spectra for generating quality molecular structures of proteins. Prof. M Nilges gave a lecture on molecular structures of large complexes from heterogeneous data and Bayesian data analysis.

Overall 64 speaker presentations covered every aspects of the magnetic resonance research. Among speakers were the three MRC Young Scientist award winners, Till Biskup, Jean-Nicolas Dumez and Katja Petzold, who gave excellent presentations in three different sessions related to magnetic resonance. During the conference, over 375 posters were presented continuously during the individual sessions. Dedicated time was allocated for poster sessions to individually discuss the scientific content.

Satellite meetings

Two satellite meetings took place just prior to the EUROMAR 2012 conference in the same venue. These satellite meetings played a very important role that could be considered as a powerful scientific support and strength to begin the main meeting.

The COST Action Spin Hyperpolarisation meeting, 29th June to 1st July, was very well attended with 150 participants. This was a two-day meeting with world leading scientists participated mainly from Europe. Members of the European Science Foundation were also present at the meeting and the Board meeting was held on 1st July at the same venue.

XeMat 2012 meeting was held on 27-29 June at the same venue with over 70 participants. Number of common interests in the DNP, para-hydrogen and hyperpolarized noble gas communities were covered during this meeting.

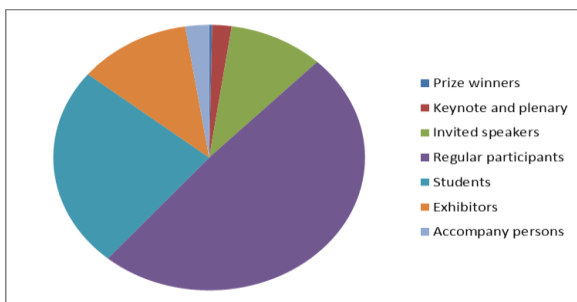
These two satellite meetings increased the active participation of over 50 invited speakers that gave various presentations related to DNP and other related areas. Several small group workshops were also held during the meeting for further developments of magnetic resonance research and networking. These two satellite meetings in association with the EUROMAR helped to strengthen the Magnetic Resonance Community in Europe.

Assessment of the results and impact of the meeting

Statistics of attendance

The total number of participants was 648 divided into

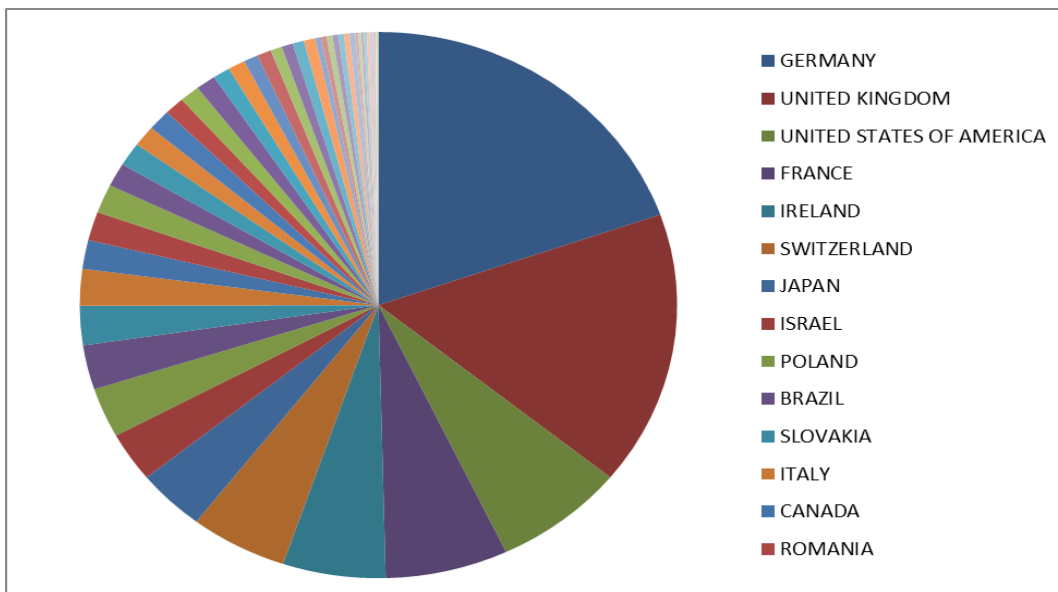
- 2 prize winner speakers
- 13 keynote and plenary speakers
- 64 speakers in parallel sessions (includes 3 MRC prize winners)
- 318 regular participants
- 159 students
- 76 exhibitors
- 16 accompany persons



The participants came from 46 different countries with the following distribution per areas:

- 504 Europe
- 76 America and Canada
- 50 Australasia
- 18 Africa

The distribution of participation from major countries is shown below.



TOTAL DISTRIBUTION OF PARTICIPANTS

GERMANY	127
UNITED KINGDOM	105
UNITED STATES OF AMERICA	46
FRANCE	43
IRELAND	37
SWITZERLAND	34
JAPAN	24
ISRAEL	19
POLAND	19
BRAZIL	17
SLOVAKIA	15
ITALY	14
CANADA	11
ROMANIA	11
THE NETHERLANDS	11
BELGIUM	9
CZECH REPUBLIC	9
RUSSIA	8
SPAIN	8
AUSTRIA	7
GREECE	7
HUNGARY	7
INDIA	6
SWEDEN	6
FINLAND	5
PORTUGAL	5
AUSTRALIA	4
CROATIA	4
DENMARK	4
TAIWAN	4
BULGARIA	2
ESTONIA	2
LATVIA	2
NEW ZEALAND	2
SINGAPORE	2
TURKEY	2
UNITED ARAB EMIRATES	2
SOUTH KOREA	2
CHINA	1
ICELAND	1
ARGENTINA	1
PAKISTAN	1
SOUTH AFRICA	1
SRI LANKA	1
TOTAL	648

The participation for the EUROMAR 2012 was lower than the two previous meetings in 2011 and 2010 which had several extended sessions and also combined with other chemistry related meetings but much higher than usual EUROMAR meetings. Increase in participation shows the popularity of the conference among other NMR conferences. The European participants (77.7%) came from 27 different countries. More than 22% participants came from other parts of the world shows that delegate participation for the European NMR gathering is increasing.

An increase in participant number to the EUROMAR meetings is one of the keystones for the EMAR programme that started in 2007. Extending the EMAR network to other European countries was one of the milestones of the EMAR programme.

The participation of postgraduate students and young postdoctoral fellows is essential for the training objectives of the EMAR programme. The EMAR programme has helped to cover part of the cost of attendance of 20 students and young postdoctoral fellows. Postgraduate students and postdoctoral fellows clearly gained the valuable experience by attending the EUROMAR 2012 that is necessary for their career developments.

In summary: With the help of the European Science Foundation, the EUROMAR conference has reached several objectives:

It has increased the participation of non-European scientists to the EUROMAR.

It has shown to be a networking place for the various European efforts to articulate the further developments of the magnetic resonance community and its related activities.

It has brought together participants from 46 different countries clearly enlarging the base of the EMAR network.

It has presented a quality scientific program that has been rated superior to the many of the most prestigious magnetic resonance conferences in the world.

EUROMAR 2012 Program

	Sunday 1st July
10.00-16.30	Registration
	Health Sciences Building
	Tutorial Lectures
	Chair: Thomas Meersman
14.00-14.45	Lorraine Brennan Current Trends in Metabolomics
14.45-15.30	Philip Grandinetti Quadrupolar NMR in Solids
15.30-16.15	Kurt Zilm The Inner Workings of NMR Probes – How to Get More from CPMAS
	O'Reilly Hall
16.30-16.45	Welcome Remarks Chandralal Hewage Lucio Frydman Beat Meier
16.45-17.00	Remembrance Robert Blinc by Beat Meier Paul Callaghan by Andrew Coy
17.00-18.30	Chair: Hans-Wolfgang Spiess The Raymond Andrew Prize Galia Debelouchina Amyloid Fibril Structure of Peptides and Proteins by Magic Angle Spinning NMR Spectroscopy and Dynamic Nuclear Polarization
	The AMPERE Prize Lyndon Emsley NMR Crystallography
18.30-19.15	Chair: Lucio Frydman Keynote Lecture Robert Tycko Biomolecular Solid State NMR: Getting Better All the Time
19.15-22.15	WELCOME MIXER

Monday 2nd July	
Chair: Lyndon Emsley	
8.30-9.15	Jeremy Nicholson Spectroscopy and systems medicine in the real world
9.15-10.00	Hartmut Oschkinat Structural Biology by DNP MAS NMR and Investigations on the Transport Cycle of an ABC Transporter
10.00-10.45 Coffee	
Chair: PK Madhu	
Chair: L Brennan / P Crowley	
New Methods in Solids and Oriented Media	
Metabolism & In-cell NMR	
10.45-11.20	Matthias Ernst Decoupling and Recoupling Using Phase-Alternating Pulse Sequences
11.20-11.45	Julian Griffin Greater than the sum of the parts : Using Data fusion to improve the sensitivity of ¹ H HR-MAS NMR spectroscopy in Breast Cancer
11.20-11.45	Mika Ala-Korpela High-Throughput Serum NMR – The New Era in Epidemiology & Genetics
11.45-12.10	Yusuke Nishiyama ¹ H ¹⁴ N HMQC above 110 kHz MAS
11.45-12.10	Christina Thiele Fast access to Residual Dipolar Couplings by single-scan 2D NMR in oriented media
11.45-12.10	Philipp Selenko In-cell NMR in Mammalian Cells
12.10-12.45	Niels Nielsen In situ solid-state NMR study of the baseplate antenna complex of Chlorobaculum tepidum located in the lipid envelope
12.10-12.45	Gary Pielak Macromolecular Crowding & Protein Chemistry: Views from Inside & Outside Cells
12.45-13.45 Lunch	
13.45-15.45 Poster Presentation and Tea	
Chair: Paul Malthouse	
Chair: Daniella Goldfarb	
Bioliquids NMR I	
EPR I	
15.45-16.20	Michael Sattler NMR studies of molecular recognition and dynamics of (large) protein complexes in solution
15.45-16.20	Christopher Kay From Solid State Physics to Structural Biology: Putting a Spin on it with EPR Spectroscopy
16.20-16.45	Michael Overduin Structural Mechanism of Calmodulin Activation and Autoinhibition of CaMK1 Kinase
16.20-16.45	Peter Roberts Investigation of Electron Spin Relaxation and Spectral Diffusion using Two-Dimensional Inverse Laplace Transforms
16.45-17.10	Shin-ichi Tate Functionally detuning motion for the hydride transfer step, which is intrinsically encoded in the active loop dynamics of dihydrofolate reductase, DHFR
16.45-17.10	Till Biskup Cryptochromes; Potential compass molecules with an unexpected variety of electron transfer pathways
17.10-17.45	Juli Feigon The Architecture of Telomerase
17.10-17.45	Marina Bennati Distance Measurements and Dynamic Nuclear Polarization at 9 and 94 GHz EPR Frequencies
Chair: Göran Karlsson	
17.55-18.40	Gerhard Wagner New NMR Approaches for Challenging Proteins

Tuesday 3rd July	
Chair: Miquel Pons	
8.30-9.15	Malcolm Levitt Singlet NMR
9.15-10.00	Sabine Van Doorslaer Gaining insight in (bio)inorganic chemistry using EPR and DFT
10.00-10.45	Coffee
	Chair: Anja Böckmann
	Chair: Kenneth Mok
	Biosolids NMR I
	Liquid State Methods
10.45-11.20	Melinda Duer Heavy mice and lighter things: using NMR to elucidate molecular structures in tissues
	Hanudatta Atreya Novel NMR Methods with High Resolution and Sensitivity: from Protein Structures to Nanotubes
11.20-11.45	Shenlin Wang High-resolution structure of a seven-helical membrane protein determined by solid-state NMR
	Warren Warren Revisiting Decades-Old Spin Physics to Improve Modern Magnetic Resonance Imaging
11.45-12.10	Jean-Philippe Demers Solid-state NMR reveals the structural architecture of Shigella flexneri Type-III Secretion Needles
	Hans Kalbitzer Detection of excited states of proteins by high pressure NMR spectroscopy - a new strategy for rational drug design
12.10-12.45	Francesco Ravotti Pushing for resolution in ¹³ C spectra of uniformly labelled proteins
	Gareth Morris Controlling J modulation: new spin echo and pure shift NMR techniques
12.45-13.45	Lunch
13.45-15.45	Poster Presentation and Tea
	Chair: Michael Williamson
	Chair: Janez Dolinšek
	Computational
	Materials
15.45-16.20	Peter Güntert Reliable and flexible automated assignment of NMR spectra
	Denis Arčon Superconductivity competing with an antiferromagnetic Mott-insulating state in alkali-doped fullerides
16.20-16.45	Jochen Balbach Dynamic Inter-Domain Crosstalk Determines Enzyme Activity
	Stephen Cottrell Kinetics of Hydrogen Abstraction in Propane studied by Muon Spin Resonance (μ SR)
16.45-17.10	Patrick Giraudeau Fast 2D and 3D NMR tools for metabolic flux analysis in complex biological mixtures
	Marianne Giesecke Electrokinetic NMR (eNMR) as a tool to study new energetic materials
17.10-17.45	Michael Nilges Structures of large complexes from heterogeneous data and Bayesian data analysis
	Michael Deschamps Supercapacitor electrodes and solid-state electrolytes studied by NMR
	Chair: Muriel Delepierre
17.55-18.40	Michele Vendruscolo Characterization of free energy landscapes of proteins using NMR spectroscopy

Wednesday 4th July	
Chair: Beat Meier	
8.30-9.15	Anne Lesage Dynamic Nuclear Polarization Surface Enhanced NMR Spectroscopy
9.15-10.00	Martin Blackledge Towards an atomic resolution description of functionally important motions in folded and unfolded proteins using high resolution NMR spectroscopy
10.00-10.45	Coffee
	Chair: Clare Grey
	Chair: Gil Navon
	Nuclei and Electrons
	In vivo and MRI
10.45-11.20	Christopher Jaroniec Protein fold determined by paramagnetic magic-angle spinning solid-state NMR spectroscopy
	Yoram Cohen Single and Double-PFG NMR and MRI: From Model Systems to Imaging of the CNS
11.20-11.45	Bela Bode PELDOR distance measurements in homo-oligomeric systems
	Jean-Nicolas Dumez Multidimensional pulses and spatially encoded magnetic resonance
11.45-12.10	Thorsten Maly An Integrated Terahertz Gyrotron for DNP-NMR Spectroscopy
	Alexej Jerschow Long Lived Coherent Response Signal in Bone
12.10-12.45	Dany Carlier NMR spectroscopy combined with DFT calculations to study paramagnetic materials for Li-ion batteries
	Klaas Nicolay Multi-parametric MR imaging and spectroscopy of cardiovascular disease in small animals
12.45-13.45	Lunch
13.45-15.45	Poster Presentation and Tea
	Chair: Christian Griesinger
	Chair: Walter Köckenberger
	Bioliquids NMR II
	Hyperpolarisation
15.45-16.20	Ramakrishna Hosur Protein NMR - Stretching the Limits
	Nicholas Kuzma Dynamic nuclear polarization of frozen gases
16.20-16.45	Jordan Chill NMR Study of Structure and Dynamics in the Intrinsically Disordered C-terminal Domain of WASp-Interacting Protein
	Kent Thurber Dynamic Nuclear Polarization (DNP) with MAS at low temperature (25 K)
16.45-17.10	Dominique Frueh Transient Substrate and Domain Interactions in Non-Ribosomal Peptide Synthetases
	Christian Hilty Investigation of Protein Folding using Dissolution DNP
17.10-17.45	Joshua Wand Unraveling Protein Motion and Hydration
	Simon Duckett Signal amplification via reversible interaction with parahydrogen: Opportunities for NMR
	Chair: Gunnar Jeschke
17.55-18.40	Jörg Wrachtrup Seeing spins at the nanoscale

Thursday 5th July	
Chair: Geoffrey Bodenhausen	
8.30-9.15	Harald Schwalbe RNA regulation elements studied by NMR spectroscopy
9.15-10.00	Kevin Brindle Imaging metabolism – Watching tumours gasp and die with hyperpolarized MRI
10.00-10.45	Coffee
	Chair: Bernhard Blümich
	Chair: Alexej Jerschow
	Emerging Areas
	Biosolids NMR II
10.45-11.20	Jamie Walls Improving resolution in NMR using pathway selective pulses
11.20-11.45	Daniel Huster Solid-State NMR Studies of A β Protofibrils and Mature Fibrils
11.20-11.45	Vikram Bajaj NMR and MRI at the Microscale
11.20-11.45	Henrik Müller Towards structural comparison of spontaneously formed and prion-seeded full-length recombinant PrP-fibrils by solid-state NMR
11.45-12.10	Vasiliki Demas Magnetic Resonance for in vitro diagnostics: from detecting pathogens to characterizing and monitoring the blood physiology
11.45-12.10	Umit Akbey Solid-State NMR Studies of Deuterated Proteins: Higher Resolution and Better Sensitivity
12.10-12.45	Stephan Appelt The physics of PHIP hyperpolarized low field NMR
12.10-12.45	Chad Rienstra Solid State NMR of Fibrils and Membrane Proteins
12.45-13.45	Lunch
13.45-15.45	Poster Presentation and Tea
	Chair: Ad Bax
	Chair: Sabine Van Doorslaer
	Biomacromolecular Assemblies
	EPR II
15.45-16.20	Stanley Opella Structure Determination of Membrane Proteins in Phospholipid Bilayers
15.45-16.20	Aharon Blank Nonlinear Induction Detection of Electron Spin Resonance
16.20-16.45	Katja Petzold Excited States in RNA Using Relaxation Dispersion NMR – a General Behaviour?
16.20-16.45	Gunnar Jeschke Fitting of protein structural transitions with EPR distance constraints: Optimization of algorithms
16.45-17.10	Jason Schnell Structural Studies of Oligomeric TatA, the Pore Component of the Twin Arginine Translocase
16.45-17.10	Christopher Wedge Chemical Engineering of Molecular Qubits
17.10-17.45	Philipp Neudecker NMR Solution Structure of an Invisible Protein State at the Edge between Folding and Aggregation into Amyloid Fibrils
17.10-17.45	Vladimir Dyakonov Application of Electron Paramagnetic Resonance to Study Fundamentals Processes in Organic Photovoltaic Materials and Devices
	Chair: Georgios Papavassiliou
17.55-18.40	Thomas Prisner New methods for EPR and NMR

ESF COST Action – Spin Hyperpolarisation Meeting Program 29th June – 1st July 2012

	Friday 29th June	Saturday 30th June	Sunday 1st July
08:00		Breakfast	Breakfast
08:30		Breakfast	Breakfast
09:00		Y. Crémillieux (Bordeaux)	R.G. Griffin (Boston)
09:30		J. Van Bentum (Nijmegen)	P.J. Nacher WG1 (Paris)
10:00	XeMAT 2012	G. de Paepe (Grenoble)	L. Frydman WG4 (Rehovot)
10:30		Coffee & Tea	Coffee & Tea
11:00		W.S. Warren (Durham)	P. Berthault WG5 (Saclay)
11:30		C. Glaubitz (Frankfurt)	S. Vega WG2 (Rehovot)
12:00	Registration COST	P. Tordo (Marseille)	
12:30		K. Ivanov (Novosibirsk)	J.H. Ardenkjaer-Larsen (Kopenh)
13:00		Lunch	Lunch
13:30		Lunch	Closed Management Committee Meeting
14:00	Welcome to COST	parallel meetings of working groups	
14:30	G. Bodenhausen (Lausanne)		
15:00	E. Chekmenev (Vanderbilt)		
15:30	R. Green (York)		
16:00	J. Matysik (Leiden)		
16:30	Coffee & Tea		
17:00	J. Wild (Sheffield)		EUROMAR 2012
17:30	S. Appelt (Aachen)		
18:00	K. Mok (Dublin)		
18:30	B. Corzilius (Boston)		
19:00	Supper	Supper	
19:30			
20:00	Irish music & drinks		
23:00	Sponsored by Bruker		

XeMat 2012 Program - Wednesday - 27th June

9:00-9:50 Registration / COFFEE

9:50-10:00 Opening remarks

Chair Eike Brunner

10:00-10:35 Patrick Berthault

10:35-11:00 Juan Parra-Robles

COFFEE

Chair Eike Brunner

11:30-12:05 Russ Bowers

12:05-12:30 Wolfgang Kilian

LUNCH

Chair Russ Bowers

14:00-14:35 Brian Saam

14:35-15:05 Mitch Albert

15:05-15:25 Christian Mrozik

15:25-15:45 Maricel Repetto

15:45-16:00 Peggy Xu

COFFEE

Chair Brian Saam

16:30-17:00 Heinz Jänsch

17:00-17:25 Ivan Dmochowski

17:25-17:45 Perttu Lantto

17:45-18:05 Joseph Six

18:05-18:20 Graham Norquay

18:20-19:00 Evening break

19:00-19:30 Transportation to social event

19:30-23:30 River Cruise (buffet dinner)

XeMat 2012 Program - Thursday 28th June

Chair Galina Pavlovskaya

9:00-9:35 Bastiaan Driehuys
9:35-10:05 Juha Vaara
10:05-10:30 Karl Stupic
10:30-11:00 Jacques Fraissard

COFFEE

Chair Heinz Jansch

11:30-12:05 Rachim Rizi
12:05-12:30 Christopher Bidinosti

LUNCH

Chair Jacques Fraissard

14:00-14:35 Igor Mourdrakovski
14:35-14:55 Céline Boutin
14:55-15:15 Caroline Keenan
15:15-15:30 General Lueng

POSTER / COFFEE

Chair Bastiaan Driehuys

17:00-17:35 Giles Santyr
17:35-17:55 Christopher Witte
17:55-18:10 Theodore Hughes-Riley

19:00-19:30 Transportation to social event
19:30-23:30 Guinness Storehouse (food & drinks)

XeMat 2012 Program - Friday 29th June

Chair Igor Mourdrakovski

9:00-9:35 William Hersman
9:35-9:55 Vikram Bajaj
9:55-10:25 Jukka Jokisarri
10:25-11:00 Eike Brunner

COFFEE

Chair Thomas Meersmann

11:30-11:45 Hayley Newton
11:45-12:20 Hans Spiess

12:20-12:35 XeMat Organizational
12:35-12:45 Closing remarks