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AMPERE

SE CONNAÎTRE, S'ENTENDRE, S'ENTRAIDER

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Contents

Editorial	1
Minutes of the Meeting of the AMPERE Bureau	2
Welcome to Euromar 2013	7
Specialized Colloque AMPERE Meeting 2013	12
AMPERE NMR School	13
NMRCM second announcement	15
SRMR division report	23
ICMRM 12	25
Executive Officers and Honorary Members of the AMPERE Bureau	27
Future conferences and AMPERE events	33

If you would like to become a member of the AMPERE Group, you can register online under: **www.ampere.ethz.ch**

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Editorial

Dear AMPERE colleagues,
an important subject coming up in the Bureau Meeting on March 23rd 2013 in Zurich was the visibility of Groupement AMPERE. Our President, Bernhard Blümich, has suggested to introduce an AMPERE logo and to publish a flyer that explains our mission and activities. The new logo and flyer will be introduced at EUROMAR 2013. For the welcome address and list of speakers at this annual conference (<http://www.euromar2013.org/>), see pages 7-11.

The Minutes of the Bureau meeting are published at pages 2-6. As you can see on page 6 the AMPERE finances are in a healthy state, so that we can again fund student grants for the EUROMAR conference and for the AMPERE NMR school (<http://www.staff.amu.edu.pl/~school/>), see also pages 13-14.

At EUROMAR 2013 the tradition of Specialized Colloques AMPERE is continued with a Colloquium on Advances in Solid State Broadband Magnetic Resonance (page 12). Bureau AMPERE generally welcomes initiatives for such Specialized Colloquia as well as for summer schools.

To strengthen our activities in the field of EPR spectroscopy we have agreed with the Zavoisky Physical-Technical Institute of the Russian Academy of Sciences, to put the annual International Conference "Modern Development of Magnetic Resonance" in Kazan, which is accompanied by the Zavoisky Award ceremony, under the auspices of Groupement AMPERE.

I wish all of you a beautiful summer and great scientific inspiration from the upcoming conferences.



Gunnar Jeschke
Secretary General of Groupement AMPERE

Minutes of the Meeting of the AMPERE Bureau

in Zurich, on March 22, 2013

Members Present:

B. Blümich, A. Böckmann, B. Meier, G. Jeschke, J. Dolinšek, M. Pons (via Skype), L. Frydman (via Skype), F. Stallmach, J. van Duynhoven (via Skype), M. Ernst

Excused:

C. Hewage, B. Balcom, S. Jurga, H.-W. Spiess

Agenda:

1. Approval of the minutes of the AMPERE Bureau meeting in Dublin July 3rd, 2012
2. Report on the state of the AMPERE Society (B. Blümich)
3. Financial Report (G. Jeschke)
4. EUROMAR Division (L. Frydman via Skype)
5. Financial report EUROMAR division (M. Pons via Skype)
6. Report on the Andrew Prize (B. H. Meier)
7. Final reports past meetings
 - EUROMAR 2012 Dublin (Ireland) (L. Frydman via Skype)
 - MRPM11, Guildford, Surrey (United Kingdom) (F. Stallmach)
 - MRFOOD 2012 (J. van Duynhoven, via Skype)
8. Future meetings 2013-2015:
 - EUROMAR 2013, Hersonissos, Crete, Greece June 30-July 5 (L. Frydman via Skype)
 - Summer School on Cultural Heritage and Portable Magnetic Resonance, Volterra, Italy June 12-15 (B. Blümich)
 - ICMRM12, Cambridge, UK August 22-25 (B. Balcom)
 - EUROMAR 2014, Zürich, Switzerland June 29 - July 3 (G. Jeschke)
 - EUROMAR 2015, Prague, Czech Republic (L. Frydman via Skype)
9. Student grants: Allocation of funds and selection procedure
10. Visibility and AMPERE logo (B. Blümich)
11. Varia
12. Date of the next meeting

At 11:50 hours G. Jeschke opened the meeting. The agenda was approved unanimously

Ad 1.

The minutes of the AMPERE Bureau meeting in Dublin, July 3, 2012, published in the AMPERE Bulletin 247/248, were approved unanimously.

Ad 2.

B. Blümich delivered his report on the state of the Groupement AMPERE. After taking office last summer, he tried to assess the current state of the Groupement AMPERE. There are many AMPERE events organized by one of the five divisions or by individuals. However, the visibility of the Groupement AMPERE is sometimes very low and there is a need to discuss how this could be improved.

Ad 3.

G. Jeschke distributed a short overview (see Appendix) over the finances of the Groupement AMPERE. The finances are solid and have increased slightly. The main income is the membership fees while the main expense in the last year was the student grants for conferences. It should be noted that of the full amount only CHF 60'000 are freely available. The remaining funds belong either to one of the divisions or to the funds for the Andrew prize.

Ad 4.

L. Frydman reported about the EUROMAR division. Last years' EUROMAR in Dublin was very successful with about 800 participants (only 25 from Ireland!). It was an excellent meeting and the satellite meetings worked out very well. There is a final report available and L. Frydman thanked C. Hewage for the excellent organization. This year the EUROMAR will be held on Crete and is organized by Georgios Papavassiliou. The program is complete and two satellite meetings (Marie Curie workshop and COST Hyperpolarization) will be held before it. The EUROMAR 2014 will be in Zürich and the 2015 EUROMAR will be in Prague organized by Vladimír Sklenář. There is already a proposal for EUROMAR 2017 (Lille) which could be combined with ISMAR. This proposal will be discussed at the EUROMAR board meeting in Crete. To increase the visibility of the Groupement AMPERE, it is important that the president of AMPERE is part of the opening ceremony.

Ad 5.

M. Pons reported about the finances of the EUROMAR division. The finances are very good (current balance Euro 78'000.-) but this is only a fraction of what organizing a conference actually costs (Euro 300000.-).

The EUROMAR 2012 in Dublin had a financial support of Euro 25'000 (student stipend) and a surplus from Euro 11'000 which will be given to this year's EUROMAR organizers.

Ad 6.

B. Meier reported that there were many proposals of high quality for the Andrew prize and that the final decision will be made soon. After that the prize winner should be added to the EUROMAR and AMPERE web sites.

Ad 7.

The reports for the past meetings were accepted. The AMPERE Bureau thanks all the scientific and local organizers for their time and effort.

- EUROMAR 2012 in Dublin, Ireland: see point 4.

- MRPM11 in Guildford, UK (F. Stallmach): The conference was very successful with about 200 participants and the final report was in the AMPERE Bulletin 249. The financial report is still missing because the proceedings are not yet published.

- NMRFOOD 2012 in Wageningen, the Netherlands (J. van Duynhoven): The conference was a success with significantly increased attendance (120 people). There were new groups participating and the support from vendors was very good. It was decided that there will be future conferences in this series. The division will try to give itself official statutes and had a surplus of Euro 5'000.- which will be deposited in the AMPERE account of the division.

Ad 8.

Planned meetings for 2013-2015

- EUROMAR 2013 Crete, Greece (L. Frydman): see point 4

- Summer School on Cultural Heritage and Portable Magnetic Resonance, Volterra, Italy (B. Blümich): This is a special event to train art conservators in NMR. It is jointly organized by the RWTH Aachen University and the Pratt Institute with 25 participants. The emphasis is on practical training in NMR. It is not yet clear whether this will be a one-time school or whether it might be repeated.

- ICMRM12, Cambridge, UK (B. Blümich for B. Balcom): The program was a bit slow in advertising but now the web page is up and the 1st circular has been sent out. The speakers list can be found on the web page. The ICMRM13 will be in Munich in 2015 organized by Axel Haase.

- EUROMAR 2014, Zürich, Switzerland (G. Jeschke): The organization is well underway and a budget has been decided. The conference fees will be around Euro 500/250 for full participants/students, respectively. There will be a flyer ready for distribution at the EUROMAR 2013 and the web pages will be set up. Planning for speakers will start at the EUROMAR 2013 in Crete.
- MRPM12 Wellington, New Zealand (F. Stallmach): The web page is set up and the organization is well underway. There have been decisions for the next two conferences: MRPM13 will be in Bologna, Italy in 2016 and MRPM14 will be in Gainsville, Florida in 2018.
- EUROMAR 2015, Prague, Czech Republic: see point 4.

Ad 9.

The AMPERE Bureau decided to give again 10 student grants of Euro 500 each for the EUROMAR 2013 and for the AMPERE Summer School in Zakopane.

Ad 10.

B. Blümich raised the question of the poor visibility of the Groupement AMPERE at many AMPERE events. He suggested three things to change this: (i) insist on better visibility of AMPERE at sponsored conferences, (ii) distribute a flyer which explains what AMPERE is, and (iii) make a logo for AMPERE that could be put on the web page of the conferences. He distributed a draft for a flyer and the logo. There was a lively discussion with suggestions for additions and changes. He will try to incorporate them and circulate a second draft of the logo and flyer among the members of the AMPERE Bureau.

Ad 11.

Varia: It was suggested by B. Meier to make sure that the AMPERE web page does not use JAVA for the navigation buttons.

Ad 12.

The next annual meeting of the AMPERE Bureau will be on March 14, 2014 in Zurich.

At 14:10 hours G. Jeschke closed the meeting and thanked all the present members for their time and effort.

Zürich, 22.3.2013

Matthias Ernst

Financial Situation of the Groupement AMPERE

Fortune of the Society per March 20th 2013

AMPERE Accounts (CHF)

Savings Account	30'815.05
Current Account	25'890.45
Security Depot	0.00
Savings Account Andrew	34'744.00
Security Depot Andrew	90'795.57

Total **182'245.07**

Accounts of subdivisions (CHF)

NMR school (AMPERE)	8'616.86	€ 7'067.31
MRPM	35'600.45	
Savings Account SMRM	27'831.70	
Savings Account EUROMAR	61'411.65	
Current Account EUROMAR	33'917.65	€ 27'818.32
DNP	0.00	
EPR	7'399.40	
FOOD NMR	0.00	

Total **174,777.71**

Grand Total **CHF 357,022.78**

1 Euro = 1.219256 CHF



Welcome to EUROMAR 2013

EUROMAR is the main annual meeting of the European magnetic resonance community covering all aspects of magnetic resonance including NMR, EPR and MRI.

EUROMAR 2013 will be held in Hersonissos, situated in the beautiful island of Crete, Greece.

The aim of the conference is to provide an educational and stimulating forum where participants can exchange ideas on the latest scientific breakthroughs in a unique Mediterranean location.

On behalf of the organizing committee and the EUROMAR board, it is my pleasure to cordially invite you to join us in making EUROMAR 2013 a memorable scientific and personal experience.

Georgios Papavassiliou
Chairman
Euromar 2013 Conference

Plenary Speakers

Anja Boeckmann	Institute of Biology&Chemistry of Proteins, France
Dmitri Budker	University of California Berkeley, U.S.A.
Isabella Felli	University of Florence, Italy
Daniella Goldfarb	Weizmann Institute of Science, Israel
Stephen Hill	NHMFL/Florida State University, U.S.A.
Charalampos Kalodimos	Rutgers University, U.S.A.
Arno Kentgens	Randboud University, The Netherlands
Dominique Massiot	CEMHTI-CNRS, France
Alex Pines	University of California Berkeley, U.S.A.
Graham Smith	University of St Andrews, United Kingdom
Yi-Qiao Song	Schlumberger-Doll Research, U.S.A
Shimon Vega	Weizmann Institute of Science, Israel
Daniel B. Vigneron	MRI Technology Resource Center, U.S.A.
Peter van Zijl	Kennedy Krieger Institute, U.S.A.

Invited Speakers

Jerome L. Ackerman	Harvard Medical School, U.S.A.
Mikael Akke	Lund University, Sweden
David Awschalom	University of California Santa Barbara, U.S.A.
Marc Baldus	Bijvoet Center for Biomolecular Research, The Netherlands
Lucia Banci	CERM-University of Florence, Italy
Aharon Blank	Technion-Israel Institute of Technology, Israel
Bela Bode	University of St Andrews, United Kingdom
Alexandre Bonvin	Utrecht University, The Netherlands
Donatella Capitani	CNR Rome, Italy
John Christodoulou	University College London, United Kingdom
Hadassa Degani	Weizmann Institute of Science, Israel
Volker Dötsch	University of Frankfurt, Germany
Matvey Fedin	International Tomography Center, Russia
Lynn Gladden	University of Cambridge, United Kingdom
Angela M. Gronenborn	Institute for Advanced Studies Berlin, Germany
Christian Hilty	Texas A&M University, U.S.A.
Sami Jannin	Laboratory of Biomolecular Magnetic Resonance (LRMB), Switzerland
Marc-Henri Julien	Grenoble High Magnetic Field Laboratory, France
Hae Jin Kim	Korea Basic Science Institute, Korea
Martin Klanjšek	Jožef Stefan Institute, Slovenia
Igor Koptuyg	International Tomography Center, Russia
Cynthia K. Larive	University of California - Riverside, U.S.A.
Mathilde LercheAlbeda	Research Aps, Denmark
Perunthiruthy Madhu	Tata Institute of Fundamental Research, India
Ann McDermott	Columbia University, U.S.A.
Eva Meirovitch	Bar-Ilan University, Israel
John Morton	London Centre for Nanotechnology, UK
Frank Neese	Max-Planck Mülheim an der Ruhr, Germany
Vasilis Petrouleas	NCSR Demokritos, Greece
Tatyana Polenova	University of Delaware, U.S.A.
James Prestegard	University of Georgia, U.S.A.
Bernd Reif	Helmholtz Center München, Germany
Jeffrey Reimer	University of California Berkeley, U.S.A.
Dimitrios Sakellariou	CEA in Saclay, France
Ago Samoson	University of Warwick, United Kingdom
Rob Schurko	University of Windsor, Canada
Vladimir Sklenar	Masaryk University, Czech Republic
Leo Spyrapoulos	University of Alberta, Canada
Janez Stepisnik	University of Ljubljana, Slovenia
Kiyonori Takegoshi	Kyoto University, Japan
Alexander Tartakovskii	University of Sheffield, United Kingdom
Nico Tjandra	NHLBI, U.S.A.
Daniel Topgaard	Lund University, Sweden

Joris Van Slageren	University of Stuttgart, Germany
Gianluigi Veglia	University of Minnesota, U.S.A.
Nicolas Wolff	Institut Pasteur, France
Xianyu Xue	Okayama University, Japan
Sergei Zvyagin	Helmholtz-Zentrum Dresden-Rossendorf, D

Tutorial Speakers

Geoffrey Bodenhausen	ENS, France
Gunnar Jeschke	ETH Zurich, Switzerland
Beat Meier	ETH Zurich, Switzerland

Committees

Program Committee

Claude Berthier	Lucio Frydman
Ivano Bertini †	Ioannis Gerothanassis
Bernhard Blümich	Malcolm Levitt
Geoffrey Bodenhausen	Beat Meier
Muriel Delepierre	Gil Navon
Janez Dolinsek	Georgios Papavassiliou
Sabine Van Doorslaer	Thomas Prisner

Local Organizing Committee

Georgios Papavassiliou (Chairman)	Georgios Mitrikas
Yiannis Deligiannakis	Maria Pelecanou
Emmanuel Mikros	Yiannis Sanakis
Thomas Maris	Georgios Spyroulias
Fany Milia (Honorary Member)	Konstantina Yannakopoulou

		Sunday 30th June	Time	Monday 1st July	Tuesday 2nd July				
			Chair						
			8:30-9:15	PL 1	PL 4				
			9:15-10:00	PL 2	PL 5				
10:00 - 17:00 Registration	10:00-14:00	IDPbyNMR Workshop	10:00-10:40	Coffee		Coffee			
			Chair						
			10:40-11:10	PS 1	PS 2	PS 3	PS 7	PS 8	PS 9
			11:10-11:30						
			11:30-11:50						
			11:50-12:10						
			12:10-12:40	Lunch		Lunch			
			12:40-14:30	Lunch		Lunch			
			14:00-16:15	Tutorial Lectures	14:30-16:00	POSTER SESSION ONE		POSTER SESSION TWO	
	Chair								
	16:00-16:30	PS 4			PS 5	PS 6	PS 10	PS 11	PS 12
	16:30-16:50								
	16:50-17:10								
	17:10-17:30								
	16:30-19:15	Opening and Prize Session	17:30-18:00	Chair					
			18:15-19:00	PL 3		PL 6			
			19:30	Welcome party		Bruker Hospitality Suite			
			19:00-22:00	Bruker Hospitality Suite					

 **PL: Plenary lecture**
 **PS: Parallel Session**
 **Colloque AMPERE Session**

Wednesday 3rd July			Thursday 4th July			Friday 5th July		
PL 7			PL 9			PL 13		
PL 8			PL 10			PL 14		
Coffee			Coffee			Coffee		
PS 13	PS 14	PS 15	PS 16	PS 17	PS 18	PS 22	PS 23	PS 24
Lunch			Lunch			CLOSING		
POSTER SESSION THREE			POSTER SESSION FOUR					
Excursion			PS 19	PS 20	PS 21			
			PL 11					
			PL 12 (19:00-19:45)					
			20:30 Dinner					

Specialized Colloque AMPERE Meeting 2013

EUROMAR 2013 is hosting a Specialized Colloque AMPERE entitled;
„Advances in Solid State Broadband Magnetic Resonance“

The event will run jointly with „EUROMAR 2013“ during the period of Sunday June 30th until Friday July 5th, 2013 in Hersonissos, Crete, Greece.

The aim of the Colloque AMPERE is to bring together scientists that are actively involved in the application of Magnetic Resonance techniques on:

1. Magnetism and Superconductivity
2. Materials and Methods in the Nanoscale
3. Intermetallic and Composite Materials
4. Spatially Resolved NMR and EPR of solids

The topics will be discussed in four sessions following the same schedule with the other EUROMAR 2013 sessions (EUROMAR 2013 includes 20 sessions), each session including two invited lectures (25+5 min), three oral presentations selected from the submitted abstracts (15+5 min), and poster presentations in the poster sessions.

Registration is common for both EUROMAR 2013 and Colloque AMPERE and participants will have access to all 24 sessions.

Invited Speakers

Jerome L. Ackerman	Harvard Medical School, U.S.A.
David Awschalom	University of California Santa Barbara, U.S.A.
Aharon Blank	Weizmann Institute of Science, Israel
Marc-Henri Julien	Grenoble High Magnetic Field Laboratory, France
Hae Jin Kim	Korea Basic Science Institute, Korea
Martin Klanjšek	Jožef Stefan Institute, Slovenia
Alexander Tartakovskii	University of Sheffield, United Kingdom
Sergei Zvyagin	Helmholtz-Zentrum Dresden-Rossendorf, D

Specialized Colloque AMPERE Organizing Committee

Claude Berthier
Jani Dolinsek
Bernhard Blümich
Georgios Papavassiliou



The AMPERE NMR School, is organized by the Macromolecular Physics Department of Adam Mickiewicz University in Poznań, in collaboration with Centre for European Integration, under the auspices of the Groupement AMPERE.

The School is addressed to young scientists (post graduate students, PhD students and post-doctoral fellows) and is focused on theoretical and experimental aspects of NMR methods, as well as on application of NMR in nanoscience and nanotechnology.

The School covers the following topics:

- solid state and soft matter NMR
- NMR diffusometry and relaxometry
- application of NMR in biology and medicine
- application of NMR material and environmental sciences
- magnetic resonance imaging and spectroscopy
- NMR and quantum information
- theoretical and experimental aspects of dynamic nuclear spin polarization
- advanced NMR techniques

Organizing Committee:

Stefan Jurga - Chair
Agata Zabor - Executive Secretary
Lidia Szutkowska
Eugeniusz Szczesniak
Barbara Peplińska
Maria Dobies
Zbigniew Fojud
Marek Kempka
Monika Makrocka-Rydzik

Mariusz Jancelewicz
Grzegorz Nowaczyk
Magdalena Walawender
Justyna Iżykowska
Jacek Jencyk
Bakyt Orozbaev
Kosma Szutkowski
Marcin Jarek
Zuzanna Pietralik

Scientific Committee:

B. Meier (Zurich), Switzerland	S. Jurga (Poznan), Poland
J. Blicharski (Kraków), Poland	A. MacKay (Vancouver), Canada
B. Blümich (Aachen), Germany	J. Stepišnik (Ljubljana), Slovenia
V. Chizhik (Saint Petersburg), Russia	S. Vega (Rehovot), Israel
J. Dolinšek (Ljubljana), Slovenia	D. Lurie (Aberdeen), UK
F. Fajara (Darmstadt), Germany	

Preliminary Programme

23.06.2013	Opening & Welcome dinner (late afternoon)
24.06 - 28.06.2013	Lectures, poster sessions
27.06.2013	Lectures, Excursion (after lunch)
28.06.2013	Lectures, Closing Dinner
29.06.2013	Departure Day

For actual information please go to:

<http://www.staff.amu.edu.pl/~school/index.html>

Saint Petersburg State University
Physical Faculty
Department of Quantum Magnetic Phenomena

Nuclear Magnetic Resonance in Condensed Matter

**10th meeting: "NMR in Life Science"
8 – 12 July 2013**

Second Announcement and Call for Papers

an AMPERE event

Saint Petersburg, Russia
2013

Nuclear Magnetic Resonance in Condensed Matter

10th International Symposium and Summer School

„NMR in Life Sciences“

St. Petersburg July 8 - 12, 2013

Preliminary list of speakers:

CHARNAYA Elena (Saint Petersburg, Russia)

NMR studies of nanostructured sodium and sodium-potassium alloys. Experimental data of NMR studies on metallic sodium and sodium-potassium alloy embedded into nanoporous matrices are presented. Size-effects and influence of nanoconfinement on the Knight shift, melting and freezing phase transitions, and spin relaxation in liquid and solid sodium and its alloy are revealed. Alterations in atomic mobility were evaluated within the framework of theoretical models of spin relaxation in solid and liquid metals.

DVINSKIY Sergey (Stockholm, Sweden)

Surfactant chain dynamics in solid-, meso- and confined phases. Restricted conformational dynamics of surfactant molecules was studied by nuclear magnetic resonance. Nitrogen-14 NMR and ²H NMR of selectively deuterated molecules provided information on head group mobility. Advanced ¹³C-1H solid state NMR techniques were applied to study alkyl chain dynamics. Solid, liquid crystalline, intercalated, confined, and adsorbed states of surfactants were investigated.

FRAISSARD Jaques (Paris, France)

A "pot-pourri" of ¹²⁹Xe NMR technique

The ¹²⁹Xe NMR technique introduced in 1980 allows the determination of pore size, location and charge of compensating cations, structural defects, distribution of adsorbed species, etc. It is applied for the characterization of a lot of solids: mesoporous silica, clays, liquid crystals, metal-organic framework compounds (mainly their elasticity), carbons, polymers, diffusion in porous structures and even in archaeology.

Since 2000, this technique has taken a new turn with the advent of laser-hyperpolarized xenon (HP-Xe) in the characterization of materials and organisms. The use of HP-Xe increases the sensitivity for the detection of xenon by several orders of magnitude. The range of its applications becomes wider each day. Now this monotonic probe allows for remarkable explorations ranging from intricate experiments on single-crystal surfaces to the study of the complex nature of gas exchange in mammalian lungs.

For example, encaged in a cryptophane cage bearing a ligand, xenon is a very sensitive sensor for detecting biomedically relevant protein targets or metal cations involved in many pathological and physiological processes. Medical applications increase each day, such as: xenon dissolved in the blood for the measurement of the rate of blood in arteries and veins, xenon imaging in brain or human lungs collected in vivo.

We will give some applications of this universal probe for material and biological characterizations.

FUENTES Sergio (Ensenada, Mexico)

Inorganic-Fullerenes based on MS_2 dichalcogenides ($M= Mo, W, Ta, Nb$) and TiO_2

Transition metal dichalcogenides MS_2 ($M= Mo, W, Ta, Nb$) have been extensively used as catalysts and lubricants due to their anisotropic behavior related with their layer structure where basal planes are very stable and border planes very reactive. Indeed, MS_2 closed structures have been synthesized as multilayer nanotubes, ribbons and onion-like nanostructures and have named the Inorganic Fullerenes (IF) by Tenne [1,2]. Some of these materials such as the hollow-nanoparticles of WS_2 present entirely new properties for lubrication. On the other hand, titania nanotubes, can be considered other type of inorganic fullerenes which have large potential for applications in environmental protection and health care [3] due to their photocatalytic and nanostructural properties.

In this work, the synthesis methods, the physicochemical properties and the nanostructure characterization of several types of IFs will be presented. The application to areas of catalysis [4], lubrication, health care, impact protection will also be discussed.

References:

[1] Y. Rapoport, Y. Bilik, M. Feldman, S.R. Homyonfer, R. Cohen and R. Tenne, *Nature*, 387, (1997) 791-793.

[2] R. Tenne and G. Seifert, *Annu. Rev. Mater. Res.*, 39 (2009) 387-413.

[3] Batur Ercan, Erik Taylor, Ece Alpaslan, Thomas J Webster, *Nanotechnology*, 29 (2011)22.

[4] A. Olivas, S. Fuentes, A. Camacho and M.J. Yacaman, *J. Materials Research*, vol 19, 2176-2184, (2004).

GREBENKOV Denis (Paris, France)

Theoretical and numerical methods for DWMRI

Diffusion Weighted Magnetic Resonance Imaging is a widespread experimental technique that relies on encoding of the random trajectories of diffusing nuclei by inhomogeneous magnetic fields. The non-invasive character of DWMRI made this technique the gold standard in material sciences, neurosciences and medicine. A geometrical confinement considerably affects the diffusive motion of the nuclei and the consequent signal attenuation under inhomogeneous magnetic fields. In this lecture, we focus on theoretical and numerical aspects of restricted diffusion in NMR.

We will present probabilistic, PDE and spectral approaches to describe restricted diffusion and the consequent signal formation. These approaches provide complementary views onto DWMRI and suggest efficient numerical techniques for simulating DWMRI in artificial or image-reconstructed porous media.

KISELEV Valerij (Freiburg, Germany)

Tracking neuronal fibers using diffusion-weighted MRI

Neuronal fibers forming brain white matter realize connections between different cortical areas and other parts of the brain. In vivo knowledge of the individual-specific configuration of neuronal fibers would be of great value for the diagnostics, for the surgical planning, and for the fundamental neuroscience. There has been a significant progress towards this goal during last decade inspired by the development of diffusion-weighted magnetic resonance imaging (dMRI) of the brain. This technique exploits the fact that diffusion of water molecules is strongly anisotropic within the neuronal fiber bundles.

An inherent problem of dMRI is its relatively coarse resolution of a few millimeters, often resulting in a number of fiber bundles placed within one voxel of an MRI image. This puts more weight on the biophysical modeling of the MRI signal in order to resolve the fiber content of each voxel, and to reconstruct the global fiber connectivity map.

We address this challenge by utilizing the self-consistency conditions resulted from the global nature of neuronal tracts stretching across many voxels. This strategy is pursued in the algorithm which we call "Global fiber tracking", inspired by the parallels with statistical physics of disordered systems. At its core, our algorithm employs the global „energy“ minimization for the interacting segments with a tendency to polymerize into long fibers, placed in an external „field“ locally orienting them in accord with the measured diffusion anisotropy. The resulting fiber configuration is

a „ground state“ into which such interacting segments freeze. This algorithm has been successfully validated by reconstructing fiber configuration in an artificial phantom, and demonstrates good performance on clinical dMRI data.

LAPINA Olga (Novosibirsk, Russia)

Multinuclear SSNMR/DFT GIPAW for molecular structure and reactivity relationships for supported oxide catalysts

In this lecture we are going to present multinuclear SSNMR/DFT GIPAW data on the molecular structure and reactivity/selectivity relationships for supported vanadium oxide catalysts. According to experimental SSNMR data the versatile types of vanadia domains could be formed in supported catalysts. It is impossible to realize experimentally each type of vanadium site separately and to estimate their catalytic characteristics. However, this problem could be solved by quantum chemical calculations. Combining finite cluster and periodic DFT-GIPAW quantum mechanical calculations of structural/spectral properties the adequate structures for the most basic systems were obtained for a number of binary VO_x/MO_x systems and for multilayered VO_x/M1O_x/M2O_x catalysts, where M1, M2 – Si, Al, Ti, Zr, Nb. The main criterion for the choice of adequate structure was the similarity between nmr parameters retrieved from NMR experiments and nmr parameters calculated for theoretically predicted structure.

NOVIKOV Dmitry (New York, USA)

Characterizing tissue microstructure with time-dependent diffusion

Molecular diffusion measurements are widely used to probe microstructure in materials and living organisms noninvasively. The precise relation of diffusion metrics to microstructure remains a major challenge: In complex samples, it is often unclear which structural features are most relevant and can be quantified. Here we classify the structural complexity in terms of the long time tail exponent in the molecular velocity autocorrelation function. The specific values of the dynamical exponent let us identify the relevant tissue microanatomy affecting water diffusion measured with MRI in muscles and in brain, and the microstructural changes in ischemic stroke.

Our framework presents a systematic way to identify the most relevant part of structural complexity using transport measured with a variety of techniques.

NUNES Rita (Lisbon, Portugal)

Diffusion-Weighted Imaging pulse sequences: Echo Planar Imaging and alternative methods

Single-shot echo planar imaging (ssEPI) is the sequence most commonly used to acquire diffusion-weighted images. Unfortunately it is very sensitive to field inhomogeneities and the images suffer from spatial distortions and signal loss particularly at tissue-air interfaces. Additionally, the image resolution attained with single-shot techniques is limited due to relaxation and so multi-shot approaches are needed for high-resolution imaging. Unfortunately, subject motion during the diffusion module results in spatially varying phase patterns; navigators are therefore required to correct for inconsistencies between shots.

In this lecture the advantages and limitations of ssEPI will be discussed and alternative sequences introduced to address some of these limitations will be described, focusing on the use of self-navigated trajectories, Fast Spin Echo methods and Steady-State Free Precession acquisitions.

PRIVALOV Alexei (Darmstadt, Germany)

Recent developments in Field Cycling NMR

The introduction in field cycling NMR for relaxometry and double-resonance NMR-NQR is presented. Experimental mechanical and electronic field-cycling setups and practical applications on various systems are discussed with the focus on the last achievements: the relaxation in polymers in ultra low magnetic fields, MAS and rotational resonance.

SKRIPOV Alexander (Ekaterinburg, Russia)

Nuclear magnetic resonance studies of atomic motion in borohydride-based hydrogen storage materials

Development of new sustainable and environment-friendly energy systems requires safe and efficient ways of energy storage. Renewable energy can be stored directly as electricity in batteries or indirectly as hydrogen in solid-state hydrides. Metal borohydrides have received recent attention as promising hydrogen-storage materials due to their high hydrogen densities. However, practical use of the known metal borohydrides is hindered by their stability with respect to thermal decomposition and the slow hydrogen sorption kinetics. Elucidation of the complex structures and hydrogen dynamics in these materials may give a key to improving their hydrogen-storage properties.

This lecture presents a review of the dynamical properties of borohydrides and the related compounds. It is based mainly on recent experimental results obtained by the NMR group at the Institute of Metal Physics

(Ekaterinburg). We will discuss the relations between the motional parameters derived from NMR experiments and the structural features of the borohydrides. A special emphasis will be made on novel borohydride-based systems showing both fast reorientational motion of BH₄ groups and fast translational diffusion of ions.

SKRYNNIKOV Nikolai (Purdue, USA)

Ensemble-restrained MD simulations: accurate structure leads to accurate dynamics

Currently, the best existing MD force fields cannot correctly reproduce the global free-energy minimum which realizes the experimental protein structure. As a result, long MD trajectories tend to drift away from the starting coordinates (e.g. crystallographic structures). To address this problem, we have devised a new simulation strategy aimed at protein crystals. An MD simulation of protein crystal is essentially an ensemble simulation involving multiple protein molecules in a crystal unit cell (or a block of unit cells). To ensure that mean protein coordinates remain correct during the simulation, we introduced crystallography-based restraints into the MD protocol. Since these restraints relate to the ensemble-average structure, the individual protein molecules in the simulated ensemble largely retain their motional freedom, i.e. their native-like internal dynamics, as dictated by the original force field.

To validate this approach we have used the data from solid-state NMR spectroscopy, which is the orthogonal experimental technique uniquely sensitive to protein local dynamics. The new method has been tested on ubiquitin and SH3 domain from chicken α -spectrin. The ensemble-restrained MD simulations produced lower crystallographic R factors than conventional simulations; they also led to more accurate predictions for solid-state chemical shifts and backbone order parameters. Taken together, these results suggest that our trajectories may be among the most realistic protein MD simulations ever reported. In this context the ensemble restraints based on high-resolution crystallographic data can be viewed as protein-specific empirical corrections to the standard force fields.

TAGIROV Murat (Kazan, Russia)

Fullerene like nanoparticles of PrF₃: from creations to medical applications
Recently, the interest in nanoparticles has been steadily increasing owing to their unique physical and chemical properties. Deposition from colloid solutions is a well elaborated method, which makes it possible to obtain nanosized samples of double and triple rare-earth fluorides [1]. A modification of this technology with the use of microwave radiation is

described in [2], where it was shown that there are internal cavities in the synthesized particles (such nanoparticles are called fullerene like nanoparticles). This technology was used to synthesize a series of crystalline fullerene like PrF₃ nanoparticles [3,4]. Since the hydrothermal synthesis is performed in an aqueous solution, it is possible to suppose that water is located in the internal cavities of such nanoparticles. According our results of experiments this hypothesis was demonstrated by using nuclear magnetic resonance cryoporometry and high-resolution transmission electron microscopy methods [5].

Finally some possible application for medicine will be presented.

References

- [1] X. Wang and Y. D. Li, *Angew. Chem. Int. Ed.* 42, 3497 (2003).
- [2] L. Ma, W. Chen, Y. Zheng, et al., *Mater. Lett.* 61, 2765 (2007).
- [3] M. S. Tagirov, E. M. Alakshin, R. R. Gazizulin, et al., *J. Low Temp. Phys.* 162, 645 (2011)
- [4] M. S. Tagirov, E. M. Alakshin, R. R. Gazizulin, et al., *J. Low Temp. Phys.* 162, 645 (2011).
- [5] E. M. Alakshina, D. S. Blokhina, A. M. Sabitova, et al., *JETP Letters*, 2012, Vol. 96, No. 3, pp. 181–183.

VASILIEV Sergey (Turku, Finland)

Dynamic nuclear polarization at ultralow temperatures

I shall present a short review of our recent experiments with atomic hydrogen in solid H₂ and ³¹P in silica crystals at temperatures below 1K. We use Electron Spin Resonance at 130 GHz and Overhauser effect to manipulate hyperfine level populations. With these techniques we reached nearly 100% nuclear polarization by pumping with low RF powers and in relatively short times. I shall discuss possible applications of high DNP and control of nuclear spin for quantum computing.

Division of Spatially Resolved Magnetic Resonance

The principle activity of the SRMR Division is a biennial international conference. The division is in good health having had a very successful meeting in 2011 in Beijing, with the division looking forward to a similarly successful 2013 meeting in Cambridge UK.

The Beijing 2011 conference final report was presented to the Ampere executive at our last meeting in March 2013. The conference final report lacked a final budget. The conference chair Prof. Lizhi Xiao has recently produced a final budget, which follows this report.

International registrations and sponsorships were received through MIT Conference Services (MITCS). Reimbursement of international invited speaker expenses and student stipends was undertaken through the University of New Brunswick to avoid US taxes.

The Cambridge 2013 meeting has been slow advertising their conference, but they have recently generated a new web site with significant information; www.paceprojects.co.uk/ICMRM.html

The Cambridge local organizing committee generated a first circular. Instead of a formal second circular an e-mail notification was distributed (see page 25). The Cambridge conference has a very impressive list of invited and plenary speakers. They are listed on the conference web site.

The Cambridge local organizing committee has tried hard to match the conference dinner in Beijing. The State Banquet Hall of the Great Hall of the People is hard to beat, but in Cambridge the conference dinner will be held in the Great Hall at Trinity College. Bruce Balcom, SRMR Chair, visited Cambridge in summer 2013 in part to check conference preparations and venues with the local organizers.

The 2015 conference will be held in Munich with Professor Axel Haase named as conference chair.

Bruce J. Balcom
March 19, 2013

ICMCM Beijing 2011 Budget

Income:	
Registration, MITCS, US	59695.00
Sponsorship, MITCS, US	14822.52
Registration, CUP, China	45800.00
Sponsorship, CUP, China	82500.00
Total	202817.52
Expenses:	
US	
MITCS On-Line Form Set Up Fee	350.00
MITCS Registration Services Fee	3960.00
Credit Card Fee	2697.00
Disbursement to UNB	29092.00
Disbursement to Groupment Ampere	2373.77
China	
Tour	6898.00
Shuttle	4428.00
Poster Board Rental	988.00
IT Support	900.00
Food and Bevergaes, at CUP	44682.00
Dinner at the Great Hall	68650.00
Dinner at the Auspicious Hotel	16380.00
Organising Committee Costs	3971.00
Conferece Books + Bags +T-Shits	5869.00
Rooms Charge: Conference, Poster	6820.00
University Services Charge	4682.00
Total	202740.77
Remainder	76.75

ICMRM12: 12th International Conference on Magnetic Resonance Microimaging

25th-29th August 2013, Fitzwilliam College,
University of Cambridge, UK



The chairs and organising committee are pleased to announce the first call for abstracts for ICMRM12, to be held at Fitzwilliam College, Cambridge, UK. Detailed information about the conference and abstract submission can be found at: <http://www.paceprojects.co.uk/ICMRM.html>

Location

The conference will be held in the historic City of Cambridge at Fitzwilliam College, one of the 28 undergraduate colleges of the University of Cambridge. The conference dinner will be held in the Great Hall at Trinity College.

Cambridge is within easy reach of London (<50 min. by train from King's Cross station) and it's major airports and is even closer to Stansted Airport (~30 min. by train)

Provisional Programme

ICMRM12 will open with an education session on Sunday 25th August 2013 at 11:00 am and will close on Thursday 29th August 2013 at 5:00 pm. In addition to the oral and poster sessions, there will be plenary speakers as well as keynote presentations by a number of invited speakers. There will also be a session dedicated to the Colloquium on Mobile NMR (CMMR).

Plenary speakers: Lucio Frydman, Klaas Prüssmann and Warren S. Warren. We are pleased to vonfirm the following invited speakers: Stephen Blackband, Sarah Codd, Simon Duckett, Axel Haase, Jürgen Hennig, Peter Jakob, Katsumi Kose, Malcom Levitt, Ben Newling, John Pauly, Daniel Topgaard.

Abstract Submissions

Submissions for oral and poster presentations at ICMRM12 are now invited. Please access the ICMRM12 website for detailed information about abstract submissions.

Important Dates

25th June 2013: Early bird registration deadline
15th July 2013: Deadline for abstract submission for poster presentations

Sponsors and Exhibitors

Please contact us to discuss opportunities for sponsorship and exhibitions during ICMRM12.

Contact

ICMRM12 Administration: tricia@paceprojects.co.uk

We look forward to welcoming you to ICMRM12 in 2013.

Regards,

Professor Lynn Gladden, Dr. Andy Sederman,
ICMRM12 Chairs

Executive Officers and Honorary Members of the AMPERE Bureau

The AMPERE BUREAU includes the executive officers (which take the responsibility and the representation of the Groupement between the meeting of the committee), the honorary members of the Bureau and the organizers of forthcoming meetings.

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Future conferences

Ampere events 2013

AMPERE NMR School	Zakopane (Poland)	June 23-29 2013
EUROMAR 2013	Hersonissos, Crete (Greece)	June 30-July 5 2013
Specialized Colloque AMPERE „Advances in Solid State Broadband Magnetic Resonance“	Hersonissos, Crete (Greece)	June 30-July 5 2013
NMRCM 2013	St. Petersburg (Russia)	July 8-12 2013
ICMRM 12	Cambridge (UK)	August 25-29 2013
4 th International DNP Symposium	Copenhagen (Denmark)	August 28-31 2013

2014

MRPM 12	Wellington (New Zealand)	February 9-13 2014
EUROMAR 2014	Zurich (Switzerland)	June 29-July 3 2014

Other events 2013

55 th Rocky Mountain Conference on Magnetic Resonance	Denver, CO (USA)	July 28 - August 1 2013
5 th Asia-Pacific NMR Symposi- um (APNMR5) and 9 th ANZMAG Meeting	Brisbane, QLD (Australia)	October 27-30 2013