



1st Workshop on Nuclear Magnetic Resonance Relaxometry

13/02/2017 - 15/02/2017

Olsztyn (Poland)

Monday, 13th February

- 8⁰⁰ – 9⁰⁰ - **Registration**
- 9⁰⁰ – 9³⁰ - **Opening**
- 9³⁰ – 10⁰⁰ - **Administrative information**

Overviews of background and current status of NMR relaxometry

- 10⁰⁰ – 10⁴⁵ - lecture: *Applications of NMR relaxometry*
Moreno Pasin
Stelar s.r.l. (Mede, Italy)
- 10⁴⁵ – 11³⁰ - lecture: *NMR relaxometry hardware*
Dominique Petit
CNRS & Université de Montpellier (Montpellier Cedex 5, France)
- 11³⁰ – 12⁰⁰ - break
- 12⁰⁰ – 13⁰⁰ - **tutorial**: *How to analyze NMR relaxometry data:*
How to analyze relaxometry data of paramagnetic molecules
Giacomo Parigi
University of Florence (Sesto Fiorentino, Italy)
Consorzio Interuniversitario Risonanze Magnetiche Metallo Proteine (CIRMMMP)
(Sesto Fiorentino, Italy)
- 13⁰⁰ – 14³⁰ - lunch



COST is supported by
the EU Framework Programme
Horizon 2020

Parallel sessions:

1. NMR relaxometry for material science – I

- 14³⁰ – 15⁰⁰ - *The solvent dynamics at pore surfaces in molecular gels studied by field-cycling magnetic resonance relaxometry*
Jadwiga Tritt-Goc
Institute of Molecular Physics (Poznań, Poland)
- 15⁰⁰ – 15³⁰ - *NMR relaxometry and microimaging of starchy products*
Corinne Rondeau-Mouro
IRSTEA UR OPAALE (Optimization of processes for agriculture, agri-food industries and environment) IRMFood team (France)
- 15³⁰ – 16⁰⁰ - *NMR study of the molecular dynamics in magnetic and non-magnetic ionic liquids*
Maria Beira
Instituto Superior Técnico, University of Lisbon (Lisbon, Portugal)
- 16⁰⁰ – 16³⁰ - *Fast Field Cycling NMR relaxometry as a method to investigate protein dynamics and study aggregation*
Enrico Ravera
Magnetic Resonance Center, Consorzio Interuniversitario Risonanze Magnetiche di Metallo Proteine (Sesto Fiorentino, Italy)
- 16³⁰ – 17⁰⁰ - *Cation-gelator interaction at the liquid-solid interface in low molecular weight ionogel*
Michał Bielejewski
Institute of Molecular Physics, Polish Academy of Sciences (Poznań, Poland)

2. NMR relaxometry for biomedical applications

- 14³⁰ – 15⁰⁰ - *The influence of therapeutic components on relaxivity of theranostic paramagnetic liposomes*
Beata Wereszczyńska
Department of Macromolecular Physics, Faculty of Physics AMU (Poznań, Poland)
NanoBioMedical Centre AMU (Poznań, Poland)
- 15⁰⁰ – 15³⁰ - *Rotating frame relaxation techniques as MRI contrast in brain*
Olli Gröhn
University of Eastern Finland (Kuopio, Finland)
- 15³⁰ – 16⁰⁰ - *FFC-NMRD profiles of tumour cells as a diagnostic tool for biomedical applications*
Maria Rosaria Ruggiero
University of Turin (Turin, Italy)

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- 16⁰⁰ – 16³⁰ - *Synthesis and characterization of monophosphinic acid DOTA derivatives: A smart tool with functionalities for multimodal imaging*
Satya Chilla
Department of General organic and biomedical science, NMR and molecular imaging lab,
University of Mons (Mons, Belgium)
- 16³⁰ – 17⁰⁰ - *d-element relaxation agents for ¹⁹F-MRI: chemistry and physics toward in vivo applications*
Jan Blahut
Department of Inorganic Chemistry, Faculty of Science, Charles University
(Prague 2, Czech Republic)
- 17⁰⁰ – 17³⁰ - break
- 17³⁰ – 18³⁰ - **Round –Table Discussion:** *Applications of NMR relaxometry*
- 18³⁰ – 20⁰⁰ - **Poster session** and dinner

Tuesday, 14th February

- 9⁰⁰ – 10⁰⁰ - lecture: *Principles of NMR relaxation theory*
Danuta Kruk
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)

Parallel sessions:

1. NMR relaxometry for food and environmental applications

- 10⁰⁰ – 10³⁰ - *Application of field-cycling NMR relaxometry to determination of molecular dynamic processes in vegetable oils and oil seeds*
Adam Rachocki
Institute of Molecular Physics, Polish Academy of Science (Poznań, Poland)
- 10³⁰ – 11⁰⁰ - *Field-Cycling NMR Relaxometry Measurements of Hydrocolloidal Systems*
Małgorzata Florek-Wojciechowska
Faculty of Mathematics and Computer Sciences, University of Warmia & Mazury (Olsztyn, Poland)
- 11⁰⁰ – 11³⁰ - *Real-Time dynamical monitoring plants status in normal and stress conditions: from Low Fields NMR in laboratory to compact NMR in planta*
Rahima Sidi-Boulenouar
BioNanoNMRI group, University of Montpellier (Montpellier, France)

2. Exotic applications of NMR relaxometry

- 10⁰⁰ – 10³⁰ - *"Other" Applications of Magnetic Field Cycling*
Tomaž Apih
J. Stefan Institute (Ljubljana, Slovenia)
- 10³⁰ – 11⁰⁰ - *Evanescent Waves Nuclear Magnetic Resonance: an experimental approach, Potential Applications to Relaxometry*
Christophe Goze-Bac
BioNanoNMRI group, University of Montpellier (Montpellier, France)
- 11⁰⁰ – 11³⁰ - *The use of relaxometry in the study of dosage forms of drugs*
Sławomir Wilczyński
Department of Basic Biomedical Science, School of Pharmacy, Medical University of Silesia in Katowice (Katowice, Poland)
- 11³⁰ – 12⁰⁰ - break
- 12⁰⁰ – 13⁰⁰ - **tutorial:** *How to analyze NMR relaxometry data – continuation Medical data fitting*
Lionel Broche
University of Aberdeen, Biomedical Engineering Building (Aberdeen, United Kingdom)

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13⁰⁰ – 14³⁰ - lunch

Session: Experimental aspects of NMR relaxometry

14³⁰ – 15⁰⁰ - *Exploring the conformational space with a sample shuttle*
Fabien Ferrage
ENS/CNRS (Paris Cedex 05, France)

15⁰⁰ – 15³⁰ - *Instrumental development of FFC-MRI for in vivo applications*
Ludovic de Rochefort
Aix-Marseille Université (Marseille, France)
CNRS (Marseille, France)

15³⁰ – 16⁰⁰ - *Fast-Field-Cycling Relaxometry with T₂-Encoding*
Carlos Mattea
Technische Universität Ilmenau, Institut für Physik, Fachgebiet Technische Physik II /
Polymerphysik (Ilmenau, Germany)

Session: Paramagnetic Systems and Nanoparticles

16⁰⁰ – 16²⁰ - *Relaxometry and Overhauser Dynamic Nuclear Polarisation*
Giacomo Parigi
University of Florence (Sesto Fiorentino, Italy)
Consorzio Interuniversitario Risonanze Magnetiche Metallo Proteine (CIRMMMP)
(Sesto Fiorentino, Italy)

16²⁰ – 16⁴⁰ - *Unrevealing the effect of Size, Shape and Dispersant on the Local Spin Dynamics of Iron Oxide Magnetic Nanoparticles*
Martina Basini
Dipartimento di Fisica, Università degli studi di Milano (Milano, Italy)

16⁴⁰ – 17⁰⁰ - *Nuclear Magnetic Resonance relaxometry of water molecules at different depths in hydrating cement pastes with SiO₂ nanoparticles*
Andrea Bede
Technische Universität Ilmenau, Institute of Physics (Ilmenau, Germany)
Technical University of Cluj-Napoca, Faculty of Materials and Environmental Engineering
(Cluj-Napoca, Romania)

17⁰⁰ – 17³⁰ - break

17³⁰ – 18³⁰ - **Round –Table Discussion:** *Collaboration possibilities*

18³⁰ – 20⁰⁰ - **Software presentation** and dinner

Wednesday, 15th February

- 9⁰⁰ – 10⁰⁰ - lecture: *Advances in NMR relaxometry
Fast Field Cycling Magnetic Resonance Imaging*
David Lurie
University of Aberdeen (Aberdeen, United Kingdom)
- 10⁰⁰ – 10⁴⁵ - *Contrast by quadrupole enhanced relaxation (CONQUER): A
concept for novel smart MRI contrast agents*
Hermann Scharfetter
Graz University of Technology (Graz, Austria)
- 10⁴⁵ – 11³⁰ - *Correlated Brownian interface and translational dynamics
simulation for nuclear spin relaxation in fluid membrane phases*
Pär Håkansson
University of Oulu (Oulu, Finland)
- 11³⁰ – 12⁰⁰ - break
- 12⁰⁰ – 12³⁰ - **tutorial**: *How to set up NMR relaxometry experiments*
Evrin Umut
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)
- 12³⁰ – 13⁰⁰ - **tutorial**: *How to extract translational diffusion coefficient from
NMR relaxometry experiments*
Danuta Kruk
University of Warmia and Mazury in Olsztyn (Olsztyn, Poland)
- 13⁰⁰ – 14³⁰ - lunch

Parallel sessions:

1. NMR relaxometry for material science – II

- 14³⁰ – 15⁰⁰ - *Proton relaxometry in a wide frequency range to study protein
rotational diffusion under crowding conditions*
Alexey Krushelnitsky
Institute of Physics - NMR Group, Faculty of Natural Sciences II, Martin-Luther-University
Halle-Wittenberg (Halle, Germany)
- 15⁰⁰ – 15³⁰ - *NMR Relaxometry studies of the molecular dynamics and self-
organized materials*
Pedro Sebastião
Instituto Superior Técnico (Lisboa, Portugal)

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- 15³⁰ – 16⁰⁰ - *NMR Relaxation of Liquid Crystal Dendrimers*
Carlos Cruz
Instituto Superior Técnico, University of Lisbon (Lisbon, Portugal)
Center of Physics and Engineering of Advanced Materials, Instituto Superior Técnico, University of Lisbon (Lisbon, Portugal)
- 16⁰⁰ – 16²⁰ - *Structure and dynamics of monolayer-protected nanoparticles: from NMR relaxation to molecular recognition*
Federico Rastrelli
Department of Chemical Sciences, Università degli Studi di Padova (Padova, Italy)
- 16²⁰ – 16⁴⁰ - *NMR Investigation of Cellular Uptake of Nanoparticles*
Manuel Mariani
Università degli Studi di Pavia, Dipartimento di Fisica (Pavia, Italia)
- 16⁴⁰ – 17⁰⁰ - *Insight into collagen structure from ¹⁵N-labelled synthetic model peptides and mouse bone*
Ieva Goldberga
Department of Chemistry, University of Cambridge (Cambridge, United Kingdom)

2. Varia

- 14³⁰ – 15⁰⁰ - *Relaxation measurements using Nuclear Quadrupole Resonance Spectroscopy on Bi-aryl compounds*
Christian Gösweiner
Institute of Medical Engineering, Graz University of Technology (Graz, Austria)
- 15⁰⁰ – 15³⁰ - *Liquid-state paramagnetic relaxation from first principles*
Jyrki Rantaharju
NMR Research Unit, University of Oulu (Oulu, Finland)
- 15³⁰ – 16⁰⁰ - *High Field FFC-MRI - A System for 3T*
Markus Bödenler
Graz University of Technology (Graz, Austria)
- 16⁰⁰ – 16²⁰ - *Dynamics of CO₂ adsorbed in an anisotropic metal-organic framework*
Jan Lang
Charles University in Prague (Prague 8, Czech Republic)
- 16²⁰ – 16⁴⁰ - *Deuteron FC NMR relaxometry in simple liquids and polymers*
Max Flämig
Universität Bayreuth, Experimentalphysik II (Bayreuth, Germany)
- 16⁴⁰ – 17⁰⁰ - *Toward a Better Understanding of Dielectric Responses of van der Waals Liquids: The Role of Chemical Structures*
Agnieszka Jędrzejowska
Institute of Physics, University of Silesia (Katowice, Poland)
Silesian Center for Education and Interdisciplinary Research (Chorzów, Poland)

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- 17⁰⁰ – 17³⁰ - break
- 17³⁰ – 18³⁰ - **Round – Table Discussion:** *Needs for training*
- 18³⁰ – 20⁰⁰ - **Summary of the workshop** and dinner