FC-RELAX Joint Training Courses and Workshop

16-21 March 2026

Monday 16

Department of Chemistry, University of Rostock,

Albert-Einstein-Straße 27, 18059 Rostock, Germany

BR 020

9:00-9:10 Welcome

9:10-10:30 Anne Strate (UROS)

Introduction into CyFi

10:30-11:00 Coffee break

11:00-12:30 Björn Corzilius (UROS)

Solid-state NMR and sensitivity enhancement by dynamic nuclear

polarization

12:30-13:30 Lunch break

13:30-15:30 Anne Strate/Henning Schröder (UROS)

Practical: Using CyFi

15:30-16:00 Coffee break

16:00-18:00 Björn Corzilius (UROS)

Hands-on dynamic nuclear polarization

19:00 Dinner

**NMR relaxometry for
biomedicine and advanced materials**

Tuesday 17

9:00-10:30   Ralf Ludwig (UROS)

Relaxation mechanisms

10:30-11:00 Coffee break

11:00-12:30   Dietmar Paschek (UROS)

MD simulations - General Introduction

12:30-13:30 Lunch break

13:30-15:30   Dietmar Paschek/Jule Philipp (UROS)

Practical on MD simulations - Starting Jobs

15:30-16:00 Coffee break

16:00-18:00   Dietmar Paschek/Jule Philipp (UROS)

Practical on MD simulations - Deriving properties

19:00   Dinner

Wednesday 18

9:00-10:30   Thomas Wiegand (MPI, Mülheim and RWTH Aachen University)

NMR Hamiltonians

10:30-11:00 Coffee break

11:00-12:30   Thomas Wiegand (MPI, Mülheim and RWTH Aachen University)

Solid-State NMR spectroscopy - Introduction

12:30-13:30 Lunch break

14:00-15:30   *COMPLEMENTARY TRAINING COURSE*

Olaf Wolkenhauer (UROS)

How to apply for funding?

15:30-16:00 Coffee break

16:00-18:00   Olaf Wolkenhauer (UROS)

How to apply for funding?

19:00   Dinner

**NMR relaxometry for
biomedicine and advanced materials**

Thursday 19

Uni Hauptgebäude,

Hörsaal 218 Aula

Chair: Ralf Ludwig

9:00-9:30   Thomas Wiegand (MPI, Mülheim and RWTH Aachen University)

Probing molecular-recognition events by solid-state NMR spectroscopy

9:30-10.00   Leonid Grunin (RS)

NMR Relaxation Times as a Measure of Entropy

10:00-10:15   Valeriia Baranauskaite (RS)

Molecular mobility, phase composition and thickness of domains in commodity polymers (Polystyrene, Polypropylene and Polyethylene) studied by TD-NMR

10:15-10:45   Angelo Galante (UNIVAQ)

Field-cycling NMR relaxometry of MRI contrast agents

10:45-11:15   Coffee break

Chair: Pedro Sebastiao

11:15-11:45   Björn Corzilius (UROS)

Site-specific dynamic nuclear polarization in biomolecular MAS NMR

11:45-12:00   Rajka Pejanovic (ENS)

Joint time-frequency WaveNet architecture for signal processing: from the suppression of vibration artifacts to pure-shift spectra in high-resolution relaxometry

12:00-12:30   Fabien Ferrage (ENS)

Revealing the effects of inhibitor binding to motions in a protein kinase by ultrafast high-resolution relaxometry

12:30-13:30   Lunch break

Chair: Erkki Lahderanta

13:30-14:00 Michael Vogel (TU Darmstadt)

NMR relaxometry studies of heterogeneous dynamics - challenges and opportunities

14:00-14:30 Lionel Broche (UNIABDN)

tbc

14:30-14:45 Kahinga Kamau (UWM)

Combining spin–lattice and spin–spin relaxation of cholesterol methyl-β-cyclodextrin dynamics

14:45-15:15 Pedro Sebastiao (IST)

OneFit-Engine: Data Analysis and Parameter Error Estimation in Model Fitting

15:15-15:45 Coffee break

Chair: Fabien Ferrage

15:45-16:15 Christian Schröder (Bielefeld University)

From trajectory to spectrum: Molecular dynamics simulations as a quantitative tool for intermolecular NMR

16:15-16:30 Muhammad Muntazir Medhi (IST)

Standardized Data Handling and Multi-Component Model Fitting for FFC-NMR Relaxometry in a Smectic Ionic Liquid Crystal

16:30-16:45 Adam Kubrak (UNIFI)

fiRelax – Novel fitting platform for relaxivity data of paramagnetic systems

16:45-17:00 Denis Burov (STELAR)

Incremental improvement of FFC relaxometer under industrial constraints

17:30-18:30 **FC-RELAX Supervisory Board meeting**

18:30-19:00 **FC-RELAX Steering Board meeting**

19:00   Dinner

**NMR relaxometry for
biomedicine and advanced materials**

Friday 20

Uni Hauptgebäude,

Hörsaal 218 Aula

Chair: Danuta Kruk

9:00-9:30 Dietmar Paschek (UROS)

Computer Simulation of the Frequency Dependent NMR Relaxation in

Liquid Water: Insights, Pitfalls, and Recent Developments

9:30-10.00 Ralf Ludwig (UROS)

Field-cycling NMR relaxometry of ionic liquids: assumptions and

approximations

10:00-10:15 Angel Mary Chiramel Tony (UROS)

A Bottom-Up Approach for Calculating the Frequency-Dependent

Relaxation Rates

10:15-10:45 Erkki Lähderanta (LUT)

Molecular dynamics simulations of NMR relaxation of dendrimers

10:45-11:15 Coffee break

Chair: Angelo Galante

11:15-11:45 Danuta Kruk (UWM)

What you need to know to analyze NMR relaxometry data: The

minimum package

11:45-12:00 Mamoona Riffat (LUT)

Effect of SDS and PVP on Aggregation and Stability of γ-Al$_2$O$_3$ Colloids

12:00-12:30 Giacomo Parigi (UNIFI)

Boosting Water Proton Relaxivity with Gd-Hydrogels and Bio-

functionalized Agents

12:30-13:30 Lunch break

Chair: Giacomo Parigi

13:30-14:00 Céline Henoumont (UMONS)

Development of micellar MRI contrast agents based on Manganese

14:00-14:30 Zsolt Baranyai (BRACCO)

Digadoglucitol: A New High Relaxivity MRI Contrast Agent Based on the Dimerization of [Gd(HP-DO3A)] and Activated Intramolecular Catalysis of the Prototropic Exchange

14:30-14:45 Guru Kiran Kadanuru Rajashekar (UMONS)

Manganese Complexes: Synthesis, Relaxometric Characterization, and Silica Nanoparticle Encapsulation

14:45-15:00 Madalina Ranga (BRACCO)

NDTA: Novel DiaCEST Agent with Strongly Shifted Exchanging Protons

15:15   Excursion to Warnemünde (beach), local history museum, Dinner

Saturday 21

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BR 020

9:00-10:30 *COMPLEMENTARY TRAINING COURSE*

Zentrum für Entrepreneurship (UROS)

Create Business plans

10:30-11:00 Coffee break

11:00-12:30 Zentrum für Entrepreneurship (UROS)

Create Business plans

12:30-14:00 Lunch