

organised by



Quantitative NMR Methods for Reaction and Process Monitoring

Venue

University of Kaiserslautern
Rotunde (Building 57)
Gottlieb-Daimler-Straße 57
67663 Kaiserslautern

Conference Dinner

21 Cafe - Bar - Lounge
Willy-Brandt-Platz 1
67655 Kaiserslautern
www.21-lounge.de

Network Access

WLAN-SSID: TU-KL_guest
username: nmrpm
password: B4S3L1N3



Contact

Jun. Prof. Dr.-Ing. Erik von Harbou
University of Kaiserslautern
Laboratory of Engineering
Thermodynamics (LTD)
Erwin-Schrödinger-Str., Building 44
67663 Kaiserslautern

Tel: +49 (0)162 232-4438
Fax: +49 (0)631 205-3835

www.uni-kl.de/nmrpm

Symposium

January 15th-16th, 2015
Kaiserslautern, Germany



Thursday, January 15th, 2015

- 08:30 **Registration**
- 09:00 **Welcome**
Erik von Harbou, University of Kaiserslautern, GER
- 09:15 **Compact NMR Relaxometry and NMR Spectroscopy for Reaction Monitoring**
Bernhard Blümich, RWTH Aachen, GER
- 09:45 **Nanolitre ¹H NMR and MRI Detectors for Applications**
Jan Korvink, University of Freiburg, IMTEK, GER
- 10:15 **Desktop High Resolution NMR Spectroscopy**
John Paul Cerroti, Magritek, GER
- 10:45 *Coffee break*
- 11:15 **Towards Fully Automated and Intelligent Processing for Time Sliced NMR Reaction Monitoring Data**
Michael Bernstein, Mestrelab, UK
- 11:45 **Quantification of Chemical Composition at Low Signal-to-Noise Ratio Using Bayesian Analysis**
Dan Holland, University of Cambridge, UK
- 12:15 **Introducing Indirect Hard Modeling to Process NMR**
Dirk Engel, S-Pact Aachen, GER
- 12:45 *Lunch*
- 13:45 **NMR Process Understanding & Dissolution Monitoring in Pharmaceutical Development**
Steven Coombes, AstraZeneca, UK
- 14:15 **Mechanistic Investigation of an Active Pharmaceutical Ingredient Utilizing Online NMR Spectroscopy**
Brian Marquez, Bruker BioSpin, GER
- 14:45 **Catalysis Research in the NMR Tube: Reactions with Gases under Realistic Conditions**
Wolfgang Baumann, LIKAT Rostock, GER
- 15:15 *Coffee break*
- 15:45 **Online Measurements in MR-NMR in a Bypass - Challenges and Possibilities**
Gisela Guthausen, KIT, GER

- 16:15 **Poster Presentation**
- 16:45 **Poster Session**
- 19:30 **Conference Dinner at 21 Cafe - Bar - Lounge**

Friday, January 16th, 2015

- 09:00 **NMR Besides Spectroscopy - Options and Obstacles to Quantification**
Nikolaus Nestle, BASF SE, GER
- 09:30 **Hyperpolarization Methods for NMR and MRI Sensitivity Enhancement**
Kerstin Münnemann, MPI Polymer Research, GER
- 10:00 **Quantitative - Online - NMR Spectroscopy: Three Good Arguments for a Comprehensive Process Understanding**
Michael Maiwald, BAM Federal Institute for Materials Research and Testing, GER
- 10:30 **Open Space Discussion - NMRPM: the road ahead**
- 11:30 **Resumée**
- 12:00 *Lunch*

Poster Program

- 01 **NMR Spectroscopic Study of Chemical Equilibria and Reaction Kinetics in Complex Reacting Mixtures of Formaldehyde, Water, and Butynediol**
J. Berje et al., University of Kaiserslautern, GER
- 02 **Multiple Applications of a Micro-Mixer Based Online NMR Probe**
A. Brächer et al., University of Kaiserslautern, GER

- 03 **Investigation of Physico-Chemical Properties of a Complex Multi-Component System from Biobased Synthesis Using Quantitative NMR Spectroscopy**
A. Fröscher et al., University of Kaiserslautern, GER
- 04 **Continuous NMR for Reaction Monitoring of Small Molecule Reactions**
J. Kind, C.M. Thiele, TU Darmstadt, GER
- 05 **Application of Low-Field NMR for the Determination of Proton-Deuteron Exchange Kinetics in Mixtures of EMIMAc and D₂O**
C. Marks et al., RWTH Aachen University, GER
- 06 **A Robust Method for Process Monitoring of Reactive Absorption of CO₂ in Industrial Gas Streams Based on Online-NMR and -Raman Spectroscopy**
K. Meyer et al., BAM Federal Institute for Materials Research and Testing, GER
- 07 **Real Time Study of Kinetic Isotope Effect with Compact NMR**
K. Singh et al., RWTH Aachen University, GER
- 08 **Design and Modeling of a Micro-Mixer NMR Probe**
R. Behrens et al., University of Kaiserslautern, GER
- 09 **Single Step Mould and Metal Patterning for Electrodeposition Enables Rapid and Low-Cost Fabrication of NMR Field Coils**
M. Meissner et al., University of Freiburg, GER
- 10 **Quantitative Metabolomics of the Nematode C. Elegans in a Microfluidic NMR Chip Device**
C. Trautwein et al., University of Freiburg, GER
- 11 **Automated Data Evaluation and Modeling of Simultaneous ¹⁹F-¹H Medium Resolution NMR Spectra for Online Reaction Monitoring**
N. Zientek et al., BAM Federal Institute for Materials Research and Testing, GER