

**International Symposium**

**Connecting EPR, ssNMR and DNP for the**

**Study of complex Biomolecules**

Schloss Ringberg, Schlossstraße 20, 83708 Kreuth, Germany,  
Tagungsstätte der Max-Planck-Gesellschaft (<http://www.schloss-ringberg.de>),  
December 14<sup>th</sup>-17<sup>th</sup> 2016

**Organizers**

Clemens Glaubitz, Goethe University Frankfurt

Wolfgang Lubitz, MPI for Chemical Energy Conversion, Mülheim an der Ruhr

Heinz-Jürgen Steinhoff, Osnabrueck University

Fraser MacMillan, University of East Anglia

**Conference Administration**

Simone Kobyłka, Goethe University Frankfurt  
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## Program Overview

<b>Time</b>	<b>Wed. 14.12.2016</b>	<b>Thu. 15.12.2016</b>	<b>Fri. 16.12.2016</b>	<b>Sat. 17.12.2016</b>	
08:00		<b>Breakfast</b>	<b>Breakfast</b>	<b>Breakfast</b>	
08:30					
09:00		Goldfarb	Linser	Departure	
09:30		Jeschke	Lewandowski		
10:00		Bordignon	Heise		
10:30		<b>Coffee</b>	<b>Coffee</b>		
11:00		Polenova	Reif		
11:30		Kaupp	Carlomagno		
12:00		Kuprov	Buntkowsky		
12:30					
13:00		<b>Lunch</b>	<b>Lunch</b>		
13:30					
14:00		Watts	Baldus		
14:30		Mao	Joseph		
15:00		<b>Arrival</b>	Poster Flash		Etzkorn
15:30		<b>Coffee</b>	Talks		Yang (*)
16:00	Opening	<b>Coffee</b>	<b>Coffee</b>		
16:30	Prisner	Poster	Weber		
17:00	Lelli		Klose		
17:30	<b>Guided</b>		Savitsky		
18:00	<b>Tour</b>		Blank		
18:30	<b>Dinner</b>	<b>Dinner</b>	<b>Bavarian Evening</b>		
19:00					
19:30	Corzilius				
20:00	Kaushik (*)	Kaur (*)	Matysik		
20:30	Griffin	Grubmüller	van Doorslaer		
21:00		Get-together	Conclusions		
21:30	Get-together	Career panel	Get-together		

(\*) Promoted talks

**Wednesday, 14.12.2016**

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<b>15:00-16:00</b>	<b>Arrival + Coffee</b>
<b>16:15-16:30</b>	<b>Opening</b>
<b>16:30-18:30</b>	<b>Session 1 (Chair Wolfgang Lubitz)</b>
16:30-17:00	Thomas Prisner, Goethe University Frankfurt High field dynamic nuclear polarization in the liquid state
17:00-17:30	Moreno Lelli, CERM Florence Dynamic nuclear polarization with high-fields, fast-MAS and high temperatures
<b>17:30-18:30</b>	<b>Guided Castle Tour</b>
<b>18:30-19:30</b>	<b>Dinner</b>
19:30-20:00	Björn Corzilius, Goethe University Frankfurt Dynamic nuclear polarization using endogenous metal ions for sensitivity-enhances NMR of biomolecules
20:00-20:25	Monu Kaushik (promoted talk), Goethe University Frankfurt Dynamic nuclear polarization enhanced solid state NMR using bis-Gd <sup>3+</sup> complexes as polarizing agents
<b>20:25-21:10</b>	<b>Keynote Lecture (Chair Wolfgang Lubitz)</b>
	Robert G. Griffin, MIT USA Amyloid, the magic angle, and microwaves
21:10	Get together

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**Thursday, 15.12.2016**

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**08:00-09:00**

**Breakfast**

**09:00-10:30**

**Session 2 (Chair Heinz-Jürgen Steinhoff)**

09:00-09:30

Daniella Goldfarb, Weizmann Institute Israel

ATPase activity of the DEAD box RNA helicase YxIN studied by EPR spectroscopy

9:30-10:00

Gunnar Jeschke, ETH Zürich

EPR restraints for hybrid structure determination

10:00-10:30

Enrica Bordignon, Ruhr University Bochum

Exploring conformational equilibria of a heterodimeric ABC transporter

**10:30-11:00**

**Coffee**

**11:00-12:30**

**Session 3 (Chair Rasmus Linser)**

11:00-11:30

Tatyana Polenova, University of Delaware

Structure and dynamics of HIV-1 capsid assemblies: Insights from an integrated MAS NMR, DNP, MD simulations, and density functional theory approach

11:30-12:00

Martin Kaupp, TU Berlin

The quantum-chemistry/NMR/EPR link to biomolecular structure

12:00-12:30

Ilya Kuprov, University of Southampton

Fokker-Planck equation as a unifying formalism for the simulation of NMR, EPR, DNP and MRI experiments

**12:30-14:00**

**Lunch**

<b>14:00-15:00</b>	<b>Session 4 (Chair Björn Corzilius)</b>
14:00-14:30	Antony Watts, University of Oxford The challenges of membrane proteins
14:30-15:00	Jiafei Mao, Goethe University Frankfurt Membrane protein safari by DNP-enhanced MAS ssNMR
<b>15:00-15:45</b>	<b>Poster Flash Talks (Chair Clemens Glaubitz)</b>
<b>15:45-16:15</b>	<b>Coffee</b>
<b>16:15-18:30</b>	<b>Poster Session</b>
<b>18:30-19:30</b>	<b>Dinner</b>
<b>19:45-21:00</b>	<b>Session 5 (Chair Heinz-Jürgen Steinhoff)</b>
19:45-20:10	Hundeep Kaur (promoted talk), Goethe University Frankfurt Extending the paradigm: ATP consumption and generation by ABC transporters
20:10-20:55	<b>Keynote Lecture:</b> Helmut Grubmüller, MPI Göttingen Single molecule scattering experiments and atomistic simulations of molecular machines
21:00	Get-together & Career advice panel session

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## Friday, 16.12.2016

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<b>08:00-09:00</b>	<b>Breakfast</b>
<b>09:00-10:30</b>	<b>Session 6 (Chair Jiafei Mao)</b>
09:00-09:30	Rasmus Linser, Ludwig-Maximilians University Munich Protons as a tool to elucidate protein structure and dynamics in solid-state NMR spectroscopy

- 09:30-10:00 Josef Lewandowski, University of Warwick  
Structure and dynamics of protein complexes by solid-state NMR
- 10:00-10:30 Henrike Heise, FZ Jülich/University Düsseldorf  
Conformational ensembles of (disordered) proteins with DNP-NMR
- 10:30-11:00 Coffee**
- 11:00-12:30 Session 7 (Chair Moreno Lelli)**
- 11:00-11:30 Bernd Reif, TU Munich  
Soluble protein complexes investigated by MAS solid-state NMR
- 11:30-12:00 Teresa Carlomagno, Leibniz University Hannover  
Combining solution-/solid-state NMR, DNP and EPR to study the Box C/D sRNP complex
- 12:00-12:30 Gerd Buntkowsky, TU Darmstadt  
Applications of solid-state NMR spectroscopy and DNP in heterogeneous catalysis
- 12:30-14:00 Lunch**
- 14:00-16:00 Session 8 (Chair Clemens Glaubitz)**
- 14:00 -14:30 Marc Baldus, Utrecht University  
Cellular solid-state NMR supported by dynamic nuclear polarization at high magnetic field
- 14:30-15:00 Benesh Joseph, Goethe University Frankfurt  
Spinning on the cells: In situ dipolar spectroscopy on a membrane transporter
- 15:00-15:30 Manuel Etzkorn, FZ Jülich/University Düsseldorf  
Selective protein hyperpolarization using targeted DNP
- 15:30-15:55 Yin Yang, (promoted talk), Weizmann Institute Israel  
New Gd(III) tags via C-S conjugation for DEER distance measurements in-vitro and in-cell
- 16:00-16:30 Coffee**

<b>16:30-18:30</b>	<b>Session 9 (Chair Fraser MacMillan)</b>
16:30-17:00	Stefan Weber, University Freiburg Hyperpolarization of electrons and nuclei as a tool to study electron transfer in DNA-repair and magnetoreceptor proteins
17:00-17:30	Daniel Klose, ETH Zürich Cu(II) binding of a self-assembling cyclic D,L- $\alpha$ -peptide studied by EPR spectroscopy
17:30-18:00	Anton Savitsky, MPI Mülheim ELDOR-detected NMR: a powerful EPR technique for hyperfine and polarization transfer studies
18:00-18:30	Aharon Blank, Israel Institute of Technology Haifa Microresonators for ESR spectroscopy of microcrystals
<b>18:30-20:00</b>	<b>Bavarian Evening</b>
<b>20:00-21:00</b>	<b>Session 10 (Chair Heinz-Jürgen Steinhoff)</b>
20:00-20:30	Jörg Matysik, University Leipzig Collective events in biomolecular machines
20:30-21:00	Sabine von Doorslaer, University Antwerpen EPR analysis of heme proteins of the CDE superfamily
21:00	Conclusions
21:10	Get-together

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## Saturday, 17.12.2016

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08:00-09:00      Breakfast & Departure