



Agenda: First Annual Meeting of the DFG Research Training Group GRK-2376

GRK-2376 „Confinement-controlled Chemistry“

Date: 09/09/2018 – 15/09/2018

Venue: Landhotel Klaukenhof
Hammecketal 4
57368 Lennestadt-Burbecke

Participants:

PhD and M.Sc. students Kevin Artmann, Niclas Blanc, Kristina Ebbert, Sarah Funke, Maximilian Jaugstetter, Anna Juber, Saskia Körning, Inga Langguth, Patricia Palitza, André Platzek, Julien Rowen, Kevin Scholten, Luisa Weirich, Kevin Wonner

PIs and Research Associates Sergi Ruiz Barragán, Guido Clever, Dominic Marx, Christian Merten, Karina Morgenstern, Patrick Nürnberger, Axel Rosenhahn, Wolfram Sander, Lars Schäfer, Gerhard Schwaab, Federico Sebastiani, Kristina Tschulik

RUB Research School Sarah Gemicioglu, Ursula Justus

Coordinator Sandra Jendrzej

	Sun, 09/09/18	Mon, 10/09/18	Tue, 11/09/18	Wed, 12/09/18	Thu, 13/09/18	Fri, 14/09/18	Sat, 15/09/18					
08.00 – 08.30		Breakfast	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast					
08.30 – 09.00		Breakfast	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast					
09.00 – 09.30		Introduction of the Research Training Group	Workshop by Prof. Morgenstern, Prof. Nürnberger, Dr. Sebastiani, Dr. Schwaab	Workshop by Prof. Marx, Prof. Schäfer, Dr. Barragán	Workshop by Prof. Rosenhahn, Prof. Tschulik	Workshop by Prof. Clever, Prof. Merten	Check-out					
09.30 – 10.00							Networking					
10.00 – 10.30												
10.30 – 11.00												
11.00 – 11.30												
11.30 – 12.00												
12.00 – 12.30		Lunch	Lunch	Lunch	Lunch	Lunch						
12.30 – 13.00												
13.00 – 13.30		Project presentation by PhD and master students	Lunch	Lunch	Lunch	Lunch	Departure					
13.30 – 14.00												
14.00 – 14.30								Workshop by Prof. Sander	Workshop by Prof. Morgenstern, Prof. Nürnberger, Dr. Sebastiani, Dr. Schwaab	Workshop by Prof. Marx, Prof. Schäfer, Dr. Barragán	Workshop by Prof. Rosenhahn, Prof. Tschulik	Workshop by Prof. Clever, Prof. Merten
14.30 – 15.00												
15.00 – 15.30												
15.30 – 16.00												
16.00 – 16.30	Arrival and Check-in											
16.30 – 17.00												
17.00 – 17.30	Group picture, individual pictures	Networking	Dinner	Dinner	Dinner							
17.30 – 18.00						Feedback session						
18.00 – 18.30	Dinner	Dinner	Dinner	Dinner	Dinner							
18.30 – 19.00												
19.00 – 19.30		Gender equality measures (opt.)	Dinner									
19.30 – 20.00												

Monday, 10/09/2018

Introduction

- 09.00 – 09.30: Introduction of participants (*all participants*)
- 09.30 – 09.45: Program of the summer school 2018 (*Dr. Jendrzej*)
- 09.45 – 10.15: Research training group “Confinement-controlled Chemistry” (*Prof. Morgenstern*)
- 10.15 – 10.35: Coffee break
- 10.35 – 11.00: Qualification Schedule for PhD students (*Dr. Jendrzej*)
- 11.00 – 12.00: RUB Research School (*Dr. Justus, Dr. Gemicioglu*)
- 12.00 – 12.30: Distribution of tasks (*Dr. Jendrzej*)
- Organization of RTG seminar for one year
 - Organization of RTG colloquium and methodology seminar for one year
 - Organization of lecture series with a Mercator fellow
 - Organization of three-day-symposium within an organizing committee
 - PhD representative and deputy

Project presentation

- 13.30 – 13.45: Project presentation and introduction of Prof. Martin-Head Gordon from Berkeley (*Kristina Ebbert*)
- 13.45 – 14.00: Project presentation (*André Platzek*)
- 14.00 – 14.15: Project presentation (*Julien Rowen*)

Workshop: From Reactive Intermediates to Reactions in Confined Space (*Prof. Sander*)

- 14.00 – 15.30: Everything you Always Wanted to Know about Chemical Reactions but Were Afraid to Ask – the Basics
- 15.30 – 16.00: Coffee break
- 16.00 – 17.00: How Do We Know What We Know About Chemical Reactions? Methods and Spectroscopy

Tuesday, 11/09/2018

Workshop

- 09.00 – 09.45: Lecture: THz spectroscopy (*Dr. Schwaab, Dr. Sebastiani*)
- 09.45 – 10.30: Seminar: THz spectroscopy (*Dr. Schwaab, Dr. Sebastiani*)
- 10.30 – 11.00: Coffee break
- 11.00 – 11.45: Lecture: Observing a photochemical reaction in real time: experimental approaches and possible implications of confinement (*Prof. Nürnberger*)
- 11.45 – 12.30: Seminar: Observing a photochemical reaction in real time: examples of how absorption changes disclose the course of a reaction (*Prof. Nürnberger*)

Project presentation

- 13.30 – 13.45: Project presentation (*Luisa Weirich*)
- 13.45 – 14.00: Project presentation (*Kevin Scholten*)

Workshop

- 14.00 – 14.45: Lecture: Surface science (*Prof. Morgenstern*)
- 14.45 – 15.15: Coffee break
- 15.15 – 16.00: Seminar: Surface science (*Prof. Morgenstern*)

Wednesday, 12/09/2018

Lecture

- 09:00-09:30: Appetizer I: Prebiotic Chemistry in Nanoconfined Water within Layered Minerals (*Prof. Marx*)
- 09:30-10:00: Ab Initio Molecular Dynamics: Why and How? (*Prof. Marx*)
- 10:00-10:30: Coffee Break
- 10:30-11:00: Appetizer II: Confinement in Supramolecular Cages from a Computational Perspective (*Prof. Schaefer*)
- 11:00-11:30: Classical Molecular Dynamics: Why and How? (*Prof. Schaefer*)
- 11:30-12:00: Tackling Confined Water within Graphene Sheets (*Dr. Ruiz*)

Project presentation

- 13.30 – 13.45: Project presentation and introduction of Prof. Teresa-Head Gordon from Berkeley (*Saskia Körning*)
- 13.45 – 14.00: Project presentation (*Anna Selina Juber*)

Seminar and Discussion

- 14.00 – 16.00: Reading and discussion of four research articles in small groups (*PhD students with Lecturers*) with integrated coffee break
- 16:00 – 17:00: Preparation of electronic presentations on research articles (*PhD students*)
- 17:00 – 18.00: Presentation of research results and methods (15 min each) with discussion (*PhD students and all participants of GRK School*)

Thursday, 13/09/2018

Workshop (Prof. Rosenhahn, Prof. Tschulik)

09.00 – 09.45: Nanoparticle synthesis and characterisation

09.45 – 10.30: Exercises

10.30 – 11.00: Coffee break

11.00 – 11.45: Interaction of X-rays with matter

11.45 – 12.30: Exercises

Project presentation

13.30 – 13.45: Project presentation (*Kevin Wonne*)

13.45 – 14.00: Project presentation and introduction of Prof. Miquel Salmeron from Berkeley (*Maximilian Jaugstetter*)

14.00 – 14.15: Project presentation and introduction of Prof. Richard Saykally from Berkeley (*Niclas Blanc*)

Workshop (Prof. Rosenhahn, Prof. Tschulik)

14.00 – 14.45: Small angle X-ray scattering

14.45 – 15.15: Exercises

15.15 – 15.45: Coffee break

15.45 – 16.30: From basic to advanced electrochemical techniques

16.30 – 17.00: Exercises

Friday, 14/09/2018

Workshop: Assembly and Characterization of Nanocages (Prof. Clever, Prof. Merten)

- 09.00 – 10.30: Lecture: Non-covalent Interactions, Self-Assembly, Coordination Cages and Organic Cages, Host-Guest Chemistry, Association Equilibria
- 10.30 – 11.00: Coffee break
- 11.00 – 12.30: Seminar: Quantification of Binding Energies (IR, NMR, ITC)

Project presentation:

- 13.30 – 13.45: Project presentation and introduction of Prof. Evan R. Williams from Berkeley (*Sarah Funke*)
- 13.45 – 14.00: Project presentation and introduction of Prof. Dan Neumark from Berkeley (*Kevin Artmann*)

Workshop: Assembly and Characterization of Nanocages (Prof. Clever, Prof. Merten)

- 14.00 – 15.30: Lecture: Special Characterization Methods: Ion Mobility Mass Spectrometry, CD Spectroscopy
- 15.30 – 16.00: Coffee break
- 16.00 – 17.00: Seminar: Problem Solving and Wrap Up