

## Program

### 4<sup>th</sup> SPP 1807 Summer School

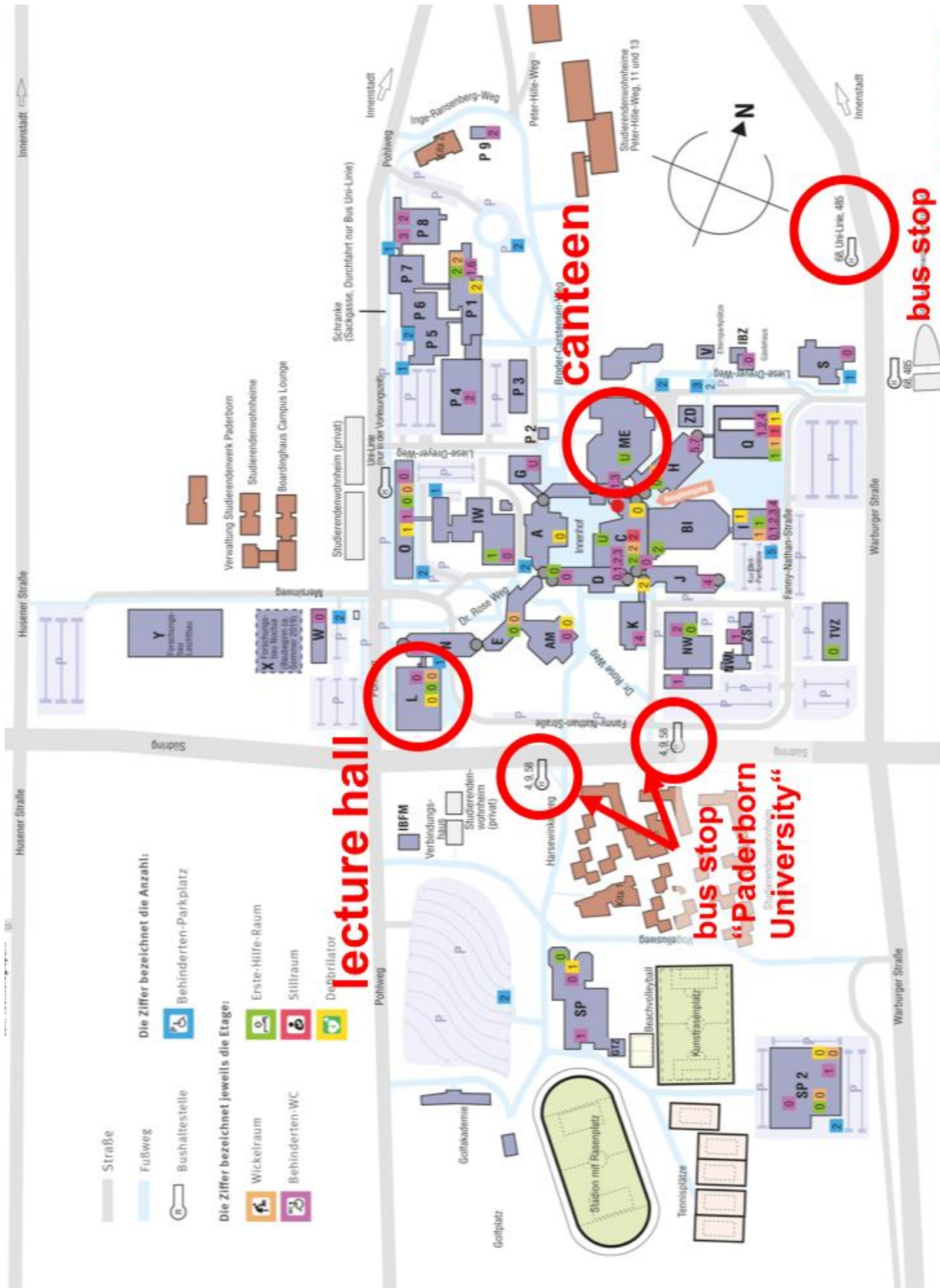
### *Control of London Dispersion Interactions in Molecular Chemistry*

**Date:** July 16<sup>th</sup> – July 19<sup>th</sup>  
**Location:** Universität Paderborn  
**Lecture hall (L), Hörsaal L1**  
**Warburger Str. 100, 33098 Paderborn**

#### Venue location / Travel details / Accommodation

The **fourth summer school** of the SPP 1807 “Dispersion” will take place at the **Universität Paderborn in Paderborn**. The registration as well as all talks will take place in the lecture hall L1 in the L building (marked on the map). Lunch will be served in the canteen (**ME**). The **conference dinner** will be held on **Thursday** evening at the **Brauhaus “Zum Goldenen Handwerk”** in the city center (address: Kamp 31, 33098 Paderborn).





**Paderborn main train station → Lecture hall (L)**

From Paderborn main train station take any of the following buses to the university: Line 4 direction "Dahl", Line 9 direction "Kaukenberg", Line 68 direction "Schöne Aussicht", Line "UNI" during the semester. For the campus "Fürstenallee/Zukunftsmühle", take bus number 11. Further Information and schedules: [www.padersprinter.de](http://www.padersprinter.de)

**About the city of Paderborn (Sightseeing and Food)**

If you would like to take part in the City Tour on Wednesday, July 17<sup>th</sup>, please register via Email to Daniela Kästing ([daniela.kaesting@uni-paderborn.de](mailto:daniela.kaesting@uni-paderborn.de)) by July 1.

For a walk through the city please look at:

[https://www.paderborn.de/tourismus-kultur/download/V1\\_Willkommen\\_komplett\\_online.pdf](https://www.paderborn.de/tourismus-kultur/download/V1_Willkommen_komplett_online.pdf)

City map:

<https://www.unser-stadtplan.de/Stadtplan/Paderborn/map/Stadtplan-Paderborn.map>

Restaurants:

[https://www.paderborn.de/tourismus-kultur/download/Restaurants\\_Gruppen.pdf](https://www.paderborn.de/tourismus-kultur/download/Restaurants_Gruppen.pdf)

**Accommodation**

We have organized your accommodation in Paderborn. In the following hotels rooms are on hold until about one month before the start of the summer school. To book the rooms please write an e-mail mentioning the code word "spp1807" for your booking, indicate your billing address, your name and mobile number, and if you wish to have breakfast at the hotel.

Hotel Aspethera: Am Busdorf 7, 33098 Paderborn; [Info@hotel-aspethera.de](mailto:Info@hotel-aspethera.de)

B&B Hotel Paderborn; Bahnhofstraße 31, 33098 Paderborn; [paderborn@hotelbb.com](mailto:paderborn@hotelbb.com)

Welcome Hotel Paderborn; Fürstenweg 13; [info.pad@welcome-hotel.com](mailto:info.pad@welcome-hotel.com)

### Talks

Each participant (PhD student or postdoc) will receive a 15 minutes time slot (+ 5 minutes discussion) for an oral presentation. Due to the tight schedule, we request the speakers to provide their presentation files **before** the respective session starts as pdf or ppt-file. The files should be sent to [Jan.M.Schuemann@org.chemie.uni-giessen.de](mailto:Jan.M.Schuemann@org.chemie.uni-giessen.de) until **July 10** the latest. Invited speakers will have 45 min for their talk and 15 minutes for discussions.

### Materials

Upon registration, you will receive a printed copy of the program, a notepad (DIN A4), a pen and a city map. There is eduroam on campus (WiFi-Connection/Internet access). For installation support please visit:

[https://hilfe.uni-paderborn.de/Netzzugang\\_f%C3%BCr\\_Besucher#Zugriff\\_.C3.BCber\\_eduroam.2FDfNRoaming](https://hilfe.uni-paderborn.de/Netzzugang_f%C3%BCr_Besucher#Zugriff_.C3.BCber_eduroam.2FDfNRoaming)

### Meals/Breaks

Lunch from Tuesday to Thursday will be served in the Canteen on the University Campus. **Please bring your Student ID, so that you will not be charged as “guest”.**

There will be some finger food and beverages on Tuesday evening at the foyer of the lecture hall. The conference dinner will be held on Thursday evening at the Brauhaus “Zum Goldenen Handwerk” in the city center (address: Kamp 31, 33098 Paderborn). Wednesday evening is at your own disposal and dinner needs to be organized individually.

### Child care

If you have any child care needs because of the workshop, you can use the short-time child care from the University of Paderborn. You find more Information:

<https://www.uni-paderborn.de/universitaet/familiengerechte-hochschule/kinderbetreuungsangebote-der-universitaet-paderborn/kinderkurzzeitbetreuung/>

If you have any further questions please inform Daniela Kästing ([daniela.kaesting@uni-paderborn.de](mailto:daniela.kaesting@uni-paderborn.de)) until **July 1**, so that we can provide some support. Also, if there are any child care related expenses back home, please inform P. R. Schreiner ([prs@uni-giessen.de](mailto:prs@uni-giessen.de)) beforehand, including a cost estimate.

### Reimbursement

All travel costs for PI's and SPP funded students / postdocs will be reimbursed according to the DFG guidelines. Please note when booking train / plane tickets that first and business class tickets are not reimbursable. Please keep your original tickets! The necessary forms will be provided during the registration at the workshop. Travel costs of participants external to the program will **not** be covered (with the exception of the invited speakers, of course).

## Tuesday, July 16<sup>th</sup>, 2019

### 1<sup>st</sup> / 2<sup>nd</sup> Invited Talk: Theory/ Catalysis

*Chair: Peter R. Schreiner*

|                |                                                                                                                                                                             |
|----------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 15:00-16:30    | <b>Arrival / Registration</b><br>Foyer of the lecture hall (L1)                                                                                                             |
| 16:30-16:45    | <b>Peter R. Schreiner / Jan Paradies</b><br>Opening remarks                                                                                                                 |
| 16:45-17:45    | <b>Prof. Daniel S. Lambrecht</b> (University of Pittsburgh, Pittsburgh, Pennsylvania, USA)<br>Identifying the Impact of Intermolecular Forces on Catalysis from Computation |
| 17:45-18:00    | <b>Short break</b>                                                                                                                                                          |
| 18:00-19:00    | <b>Prof. Matthew S. Sigman</b> (University of Utah, Salt Lake City, Utah, USA)<br>Developing Modern Data Analysis Tools for Synthesis & Catalysis                           |
| 19:00-open end | <b>Welcome dinner with finger food</b><br>Lecture hall (L1)                                                                                                                 |

## Wednesday, July 17<sup>th</sup>, 2019

### 1<sup>st</sup> Session: Spectroscopy I

*Chair: Martin Suhm*

|             |                                                                                                                                                      |
|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| 09:00-09:20 | <b>Hannes C. Gottschalk</b> (Georg-August-Universität Göttingen)<br>Introducing the "Gratin Jet": A Sustainable Setup for FTIR Jet Spectroscopy      |
| 09:20-09:40 | <b>Manuel Lange</b> (Georg-August-Universität Göttingen)<br>Dispersion Interactions for the Chirality Induction by Methyl Lactate                    |
| 09:40-10:00 | <b>Charlotte Zimmermann</b> (Georg-August-Universität Göttingen)<br>Tilting and Tipping the Ketone-Alcohol Gas-phase Solvation Balance by Alkylation |
| 10:00-10:30 | <b>Coffee Break</b><br>Foyer of the lecture hall (L1)                                                                                                |

### 2<sup>nd</sup> Session: Theory I

*Chair: Ana Vila Verde*

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|-------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 10:30-10:50 | <b>João Robalo</b> (MPI für Kolloid- und Grenzflächenforschung, Potsdam)<br>Defects in the Hydration Shell of Hydrophobic Molecules                                                                                    |
| 10:50-11:10 | <b>Federica Ferraro</b> (Friedrich-Alexander-Universität Erlangen-Nürnberg)<br>Intra- versus Intermolecular Forces: the Influence of Solute-Solvent Interactions on the Structure and Properties of Extended Molecules |
| 11:10-11:30 | <b>Fabian Bohle</b> (Universität Bonn)<br>Accurate Conformer Ensembles in Solution                                                                                                                                     |
| 11:30-13:00 | <b>Lunch</b><br>Canteen (ME)                                                                                                                                                                                           |

### 3<sup>rd</sup> Session: Structure & Reactivity I

*Chair: Peter R. Schreiner*

**13:00-13:20** **Finn M. Wilming** (Justus-Liebig-Universität Gießen)  
 Synthesis of 2,2'-Substituted 9,9'-Bifluorenylidenes as Hydrocarbon-based Dispersion Balances

**13:20-13:40** **Jan M. Schümann** (Justus-Liebig-Universität Gießen)  
 Quantifying London Dispersion with 1,4 Substituted Cyclooctatetraene Based Balances

**13:40-14:00** **Marcel A. Strauß** (Justus-Liebig-Universität Gießen)  
 Exploring Subtleties in Alkyl-Alkyl Interactions Using Azobenzene Switches

**14:00-14:30** **Coffee Break**  
 Foyer of the lecture hall (L1)

### 4<sup>th</sup> Session: Spectroscopy II

*Chair: Martin Suhm*

**14:30-14:50** **Johannes Fischer** (Universität Regensburg)  
 Stark-Spectroscopic Investigations of Organic Molecules in Superfluid Helium Nanodroplets

**14:50-15:10** **Florian Schlaghauser** (Universität Regensburg)  
 Rotational Envelopes of Electronic Transitions of Phthalocyanines in the Gas Phase

**15:10-15:30** **Mallikarjun Karra** (Fritz-Haber-Institut der MPG, Berlin)  
 Anomalous Rotational Behaviour of "Large" Rotors Solvated in Helium Nanodroplets

**15:30-16:00** **Coffee Break**  
 Foyer of the lecture hall (L1)

### 5<sup>th</sup> Session: Spectroscopy III

*Chair: Norbert Mitzel*

**16:00-16:20** **Anja Poblitzki** (Georg-August-Universität Göttingen)  
 Moving to the  $\pi$  site: Complexation of Furan Derivatives with Alkyl Alcohols

**16:20-16:40** **Vladimir Gorbachev** (ETH Zürich)  
 Using IRPD-Spectroscopy for Onium Ions Serving as a Molecular Balance for the Estimation of Non-covalent Interactions

**16:40-17:00** **Timo Glodde** (Universität Bielefeld)  
 Non-covalent Interactions in Organotellurium Systems

**17:00-17:30** **Break and conference picture**

### 3<sup>rd</sup> Invited Talk: Structure & Reactivity

*Chair: Jan Paradies*

**17:30-18:30** **Prof. Ayan Datta** (School of Chemical Sciences in Jadavpur, Kolkata, Republic of India)  
 Symmetry Breaking in Low-Dimensional Systems - Why Heavier Analogues of Graphene are Buckled?

**19:00** **City tour, alternatively free evening**  
 Meeting point: old town hall in Paderborn City

**Thursday, July 18<sup>th</sup>, 2019**

**6<sup>th</sup> Session: Theory II**

**Chair: Giovanni Bistoni**

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|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>09:00-09:20</b> | <b>Ahmet Altun</b> (MPI für Kohlenforschung, Mülheim an der Ruhr)<br>Local Energy Decomposition Studies of Non-covalent Interactions within the DLPNO-CCSD(T) Framework |
| <b>09:20-09:40</b> | <b>Felix van der Vight</b> (Universität Duisburg-Essen)<br>Structural Consequences of d-Shell Dispersion Contributions in Heavy Group 15 Compounds                      |
| <b>09:40-10:00</b> | <b>Patrick Strebert</b> (Technische Universität Kaiserslautern)<br>Computational Studies of Dispersion Interaction in Ketone-Alcohol Aggregates                         |
| <b>10:00-10:30</b> | <b>Coffee break</b><br>Foyer of the lecture hall (L1)                                                                                                                   |

**7<sup>th</sup> Session: Theory & Catalysis**

**Chair: Lutz Ackermann**

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|--------------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>10:30-10:50</b> | <b>Lijuan Song</b> (Justus-Liebig-Universität Gießen)<br>The Role of London Dispersion in CBS Reduction - a Computational Study              |
| <b>10:50-11:10</b> | <b>Zheng-Wang Qu</b> (Universität Bonn)<br>Reduction of Phosphine Oxide Using Chlorination Reagents and Dihydrogen: DFT Mechanistic Insights |
| <b>11:10-11:30</b> | <b>Torben Rogge</b> (Georg-August-Universität Göttingen)<br>Experimental and Computational Studies on Ruthenium-Catalyzed C-H Activation     |
| <b>11:30-13:00</b> | <b>Lunch</b><br>Canteen (ME)                                                                                                                 |

**8<sup>th</sup> Session: Catalysis**

**Chair: Albrecht Berkessel**

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|--------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>13:00-13:20</b> | <b>Christian Eschmann</b> (Justus-Liebig-Universität Gießen)<br>Reconsidering Steric Effects in the CBS-Reduction                                            |
| <b>13:20-13:40</b> | <b>Benedikt Sieland</b> (Universität Paderborn)<br>Stabilization of Encounter Complexes of Intermolecular Frustrated Lewis Pairs by Dispersion Energy Donors |
| <b>13:40-14:00</b> | <b>Wacharee Harnying</b> (Universität zu Köln)<br>Dispersion Effects in NHC Catalysis: Synthesis of Nepetalactone                                            |
| <b>14:00-14:30</b> | <b>Coffee break</b><br>Foyer of the lecture hall (L1)                                                                                                        |

**9<sup>th</sup> Session: Spectroscopy IV**

**Chair: Markus Gerhards**

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|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>14:30-14:50</b> | <b>Dominique Maué</b> (Technische Universität Kaiserslautern)<br>Elucidating Dispersion Interaction by Ionization Gain and Loss Stimulated Raman Spectroscopy                       |
| <b>14:50-15:10</b> | <b>Daniel Obenchain</b> (Deutsches Elektronen Synchrotron (DESY) Hamburg)<br>Seeing Dispersion Interactions from the Point of View of a Quadrupolar Nucleus                         |
| <b>15:10-15:30</b> | <b>Pablo Pinacho Morante</b> (Deutsches Elektronen Synchrotron (DESY) Hamburg)<br>The Interplay Between Hydrogen Bond and Dispersive Interactions in Complexes of Diadamantyl Ether |
| <b>15:30-16:00</b> | <b>Coffee break</b><br>Foyer of the lecture hall (L1)                                                                                                                               |

### 10<sup>th</sup> Session: Structure & Reactivity II

*Chair: Lutz Ackermann*

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|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 16:00-16:20 | <b>Laura Grimm</b> (Karlsruher Institut für Technologie)<br>Design and Synthesis of a Cucurbit[8]uril-based Model System for Investigating Face-to-Face $\pi$ -Stacking Complexes |
| 16:20-16:40 | <b>Lars Rummel</b> (Justus-Liebig-Universität Gießen)<br>Towards Stable Gomberg Systems <i>via</i> Tetrel Variation                                                               |
| 16:40-17:00 | <b>Sebastian Scholz</b> (Technische Universität Chemnitz)<br>Heavy Main Group Element as Dispersion Energy Donors – Experimental Studies                                          |
| 17:00-17:30 | <b>Break</b><br>Foyer of the lecture hall (L1)                                                                                                                                    |

### 4<sup>th</sup> Invited Talk: Structure & Reactivity

*Chair: Albrecht Berkessel*

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|----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 17:30-18:30    | <b>Prof. Markus Albrecht</b> (RWTH Aachen, North Rhine-Westphalia, Germany)<br>How Strong is Weak? Hierarchical Helicates - From Weak Interactions to Supramolecular Devices |
| 18:30-open end | <b>Conference dinner</b><br>“Brauhaus: Zum Goldenen Handwerk” (Kamp 31, 33098 Paderborn)                                                                                     |

## Friday, July 19<sup>th</sup>, 2019

### 11<sup>th</sup> Session: Structure & Reactivity III

*Chair: Stephan Schulz*

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|-------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| 09:00-09:20 | <b>Bo Zhang</b> (Technische Universität Dortmund)<br>Dispersion Interactions in Self-Assembled Supramolecular Host-Guest Systems                 |
| 09:20-09:40 | <b>André Platzek</b> (Technische Universität Dortmund)<br>Dispersion-driven Binding of Neutral Guests in Interpenetrated Double Cages            |
| 09:40-10:00 | <b>Alexander Gehlhaar</b> (Universität Duisburg-Essen)<br>Dispersion Interactions in Bridged Bimetallic Complexes of the Heavy Group 15 Elements |
| 10:00-10:30 | <b>Coffee Break</b><br>Foyer of the lecture hall (L1)                                                                                            |

### 12<sup>th</sup> Session: Spectroscopy V

*Chair: Markus Gerhards*

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|-------------|----------------------------------------------------------------------------------------------------------|
| 10:30-10:50 | <b>Johannes Gramüller</b> (Universität Regensburg)<br>Dispersion Interactions in Brønsted Acid Catalysis |
| 10:50-11:10 | <b>Adélaïde Savoy</b> (ETH Zürich)<br>NMR Study of Intramolecular H-Bonds in Bipyridines                 |
| 11:10-11:30 | <b>Short break</b><br>Foyer of the lecture hall (L1)                                                     |

### 5<sup>th</sup> Invited Talk: Structure & Reactivity

*Chair: Peter R. Schreiner*

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|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 11:30-12:30 | <b>Prof. Jay S. Siegel</b> (Tianjin University, Tianjin, PRC)<br>Dispersion, Repulsion, Binding, Bonding: Rationalizing Polynuclear Aromatic Hydrocarbon Interactions |
| 12:30-12:45 | <b>Peter R. Schreiner / Jan Paradies</b><br>Closing remarks / Departure                                                                                               |