

# 1<sup>st</sup> Summer School of the SPP 1807 "Control of London dispersion interactions in molecular chemistry"



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**Date:** May 29 – June 01, 2016  
**Location:** Jacobs University Bremen

## Venue location/Travel details/Accommodation

The Summer School will take place at the Jacobs University Bremen (Campus Ring 1, 28759 Bremen). Information about how getting to Jacobs you'll find here: <http://www.jacobs-university.de/campus-map-directions>. If you are travelling by car, there are sufficient free parking locations directly on Campus. The university has a train station (Bremen-Schönebeck) in 5-min walking distance. The talks will be held in the Lecture Hall of Research III. All participants will have a single room directly on Campus in the College Nordmetall, A-Block, or in the Guesthouse. You will receive the keys upon arrival at the porter's office, which is located right at the entry gate.

## Talks

Each participant (PhD student or postdoc) will receive a 13 min time slot (+ 5 min 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.P.Wagner@chemie.uni-giessen.de](mailto:Jan.P.Wagner@chemie.uni-giessen.de) until May 27. Invited speakers will have 45 min for their talk and 15 minutes for discussions.

## Materials

A printed copy of the program will be provided.

## Meals/Breaks

All meals during the summer school will be organized, including breakfast and lunch from Monday to Wednesday and dinner from Sunday to Tuesday (all in buffet format, including special dietary options). Additional meal and restaurant options are available, but will need to be paid for directly.

## Reimbursement

All travel costs for PI's and SPP funded students/postdocs will be reimbursed according to the DFG guidelines. Please take into account 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 workshop. Travel costs of participants external to the program will not be covered.

The college and guesthouse accommodation costs will be settled directly through the SPP. Costs for the accommodation of external participants will be invoiced to them.

# Program for the Summer School of the SPP 1807



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## Sunday, May 29, 2016

<b>15:00-17:00</b>	<b>Registration</b> in front of the lecture hall of Research III
<b>17:00-17:15</b>	<b>Prof. Peter R. Schreiner</b> Opening remarks
	<b>Invited Talk:</b>
<b>17:15-18:15</b>	<b>Prof. Clémence Corminboeuf</b> On the Many Facets of Analyzing and Quantifying (Non)-Covalent Interactions
<b>18:15-open end</b>	<b>Dinner / Welcome with Finger food</b> University Club on campus

## Monday, May 30, 2016

<b>7:30 – 8:30</b>	<b>Breakfast</b> Servery of College Nordmetall (probably)
<b>9:00-10:36</b>	<b>1<sup>st</sup> Session: Theory I, Chair: Georg Jansen</b>
	<b>Invited Talk:</b>
<b>9:00-10:00</b>	<b>Prof. Wesley Allen</b> Struggling with Intramolecular Dispersion
<b>10:00-10:18</b>	<b>Alberto Fabrizio</b> Balancing London dispersion and the delocalization error with DFT functionals
<b>10:18-10:36</b>	<b>Johannes Hoja</b> The Role of Collective Electronic and Thermal Fluctuations in Molecular Crystals
<b>10:36-11:00</b>	<b>Coffee break</b> Seminar room in Research III (in front of the lecture hall)
<b>11:00-12:36</b>	<b>2<sup>nd</sup> Session: Dispersion Interactions in Solution I, Chair: Werner Nau</b>
	<b>Invited Talk:</b>
<b>11:00-12:00</b>	<b>Prof. Hans-Jörg Schneider</b> Dispersion Interactions in Supramolecular Complexes in Solution – Experimental Insights
<b>12:00-12:18</b>	<b>Dr. Khaleel Assaf</b> Cucurbiturils: Rigid Hosts for Studying the Interplay of Dispersion and Hydrophobic Interactions
<b>12:18-12:36</b>	<b>Dr. Jens Antony</b> Prediction of affinities to cucurbiturils using electronic structure theory methods
<b>12:36-14:00</b>	<b>Lunch break</b> Servery of College Nordmetall

**14:00-15:30** **3<sup>rd</sup> Session: Catalysis I, Chair: Albrecht Berkessel**

**Christina Bock**

**14:00-14:18** Synthesis of N-containing versatile compounds through organocatalytic multi-step domino reactions

**14:18-14:36** **Felix Held**

Multi-Step Branched Domino Reactions towards New Fluorophores

**14:36-14:54** **Darius Kootz**

Dispersion Interaction in Carbene Catalyzed Umpolung

**14:54-15:12** **Joachim Loup**

Dispersion Interactions in Iron-Catalyzed C-H Activation

**15:12-15:30** **Daniel Zell**

Dispersion Interactions in Cobalt(III)-Catalyzed C-H Activation

**Coffee break**

**15:30-16:00** Seminar room in Research III (in front of the lecture hall)

**16:00-17:30** **4<sup>th</sup> Session: Spectroscopy I, Chair: Markus Gerhards**

**16:00-16:18** **Anja Poblitzki**

Competition for methanol solvation between the pi cloud and the oxygen atom in aromatic heterocycles

**16:18-16:36** **Fabian Dietrich**

Investigation of aromatic ether-alcohol clusters by application of quantum chemical methods with regard to different hydrogen bonding motifs

**16:36-16:54** **Mariyam Fatima**

Broadband Microwave Spectroscopy as a Tool to Study Dispersion Interactions in Camphor-Alcohol Systems

**16:54-17:12** **Mallikarjun Karra**

Stark Spectroscopy of van der Waals Complexes controlled via London dispersion forces in He-nanodroplets: Theory and Simulation

**17:12-17:30** **Surajit Maity**

Accurate binding energies of 1-naphthol-alkane dispersive complexes

**Dinner**

**18:00-19:00** Servery of College Nordmetall

**Clinic**

**19:00-open end** University Club on campus

**Tuesday, May 31, 2016**

**7:30 – 8:30** **Breakfast**  
Servery of College Nordmetall

**9:00-10:30** **5<sup>th</sup> Session: Theory II, Chair: Andreas Hesselmann**

**Christof Holzer**

**9:00-9:18** Explicitly correlated wave function methods to describe Van-der-Waals interactions

**9:18-9:36** **Oinam Meitei**

9:36-9:54	On the stability of cyclophane derivatives using molecular fragmentation method <b>Majid Mortazavi</b> First-principles investigation of molecular crystal inclusion complexes
9:54-10:12	<b>Robert Stadler</b> Second- and third-order dispersion coefficients from a linear rigid rotor model
10:12-10:30	<b>Axel Wuttke</b> TBA
10:30-11:00	<b>Coffee break</b> In front of the lecture hall
11:00-12:36	<b>6<sup>th</sup> Session: Structure &amp; Reactivity I, Chair: Peter Chen</b>
11:00-12:00	<b>Invited Talk:</b> <b>Dr. David Liptrot</b> Dispersion Force Effects in Organometallic Chemistry
12:00-12:18	<b>Dr. Ana-Maria Preda</b> Heavy main group elements as dispersion energy donors - Experimental studies of bismuth compounds with bismuth- $\pi$ -interactions as structure determining component
12:18-12:36	<b>Dr. Kai Brandhorst</b> Control of Dispersion Interactions in Complexes with Anionic N-Heterocyclic Carbene Ligands
12:36-14:00	<b>Lunch break</b> Servery of College Nordmetall
14:00-15:30	<b>7<sup>th</sup> Session: Theory III, Chair: Philipp Wagner &amp; Christof Holzer</b>
14:00-14:18	<b>Mirko Bauer</b> The structural manifold of large <i>n</i> -alkanes
14:18-14:36	<b>Dr. Giovanni Bistoni</b> Local Energy Decomposition analysis for intermolecular interactions at the DLPNO-CCSD(T) level: insights into Frustrated Lewis Pair Chemistry
14:36-14:54	<b>Fabian Bohle</b> Investigation of noncovalent interactions on a Blindtest-System
14:54-15:12	<b>Marek Bot</b> Experimental and Theoretical Investigations of Dispersion Interactions in Tetraalkylammonium Ions
15:12-15:30	<b>Thomas Geiger</b> Investigation of anthracene dimers
15:30-16:00	<b>Coffee break</b> In front of the lecture hall
16:00-17:30	<b>8<sup>th</sup> Session: Dispersion Interactions in Solution II, Chair: Guido Clever</b>
16:00-16:18	<b>Philipp Wagner</b> Do London Dispersion Interactions Cancel in Solution?
16:18-16:36	<b>Robert Pollice</b> London Dispersion in Bond Dissociation Reactions of Proton-bound Dimers in the Gas-Phase and in Solution
16:36-16:54	<b>Jan Michael Schümann</b>

	To what degree is London dispersion solvent dependent? Re-vitalizing an old molecular balance
<b>16:54-17:12</b>	<b>Marcel Strauß</b> Attraction or Repulsion? London Dispersion Forces Control Azobenzene Switches
<b>17:12-17:30</b>	<b>Yanan Miao</b> Towards Reversal of Stereoselectivity in Jacobsen-Katsuki Epoxidation Reaction by Manipulating Dispersion Effects
<b>18:00</b>	BBQ for all in the University Club on campus
<b>- open end</b>	

## Wednesday, June 01, 2016

<b>7:30 – 8:30</b>	<b>Breakfast</b> Serving of College Nordmetall
<b>9:00-10:30</b>	<b>9<sup>th</sup> Session: Structure &amp; Reactivity II, Chair: Norbert Mitzel</b>
<b>9:00-9:18</b>	<b>Sebastian Blomeyer</b> Dispersive interactions in the gas-phase
<b>9:18-9:36</b>	<b>Marvin Linnemannstöns</b> Synthesis of compounds for intramolecular $\pi$ - $\pi$ -interactions in acetylenes
<b>9:36-9:54</b>	<b>Sören Rösel</b> Hexaphenylethanes as model compounds to gauge dispersion energy donor abilities of alkyl substituents
<b>9:54-10:12</b>	<b>Jutta Tumpach</b> Intramolecular pi-pi interaction energies - the influence of different phenyl-to-phenyl bridging units
<b>10:12-10:30</b>	<b>Bo Zhang</b> Dispersion in Self-Assembled Host-Guest System
<b>10:30-11:00</b>	<b>Coffee Break</b> Seminar Room in Research III - in front of the lecture hall
<b>11:00-12:05</b>	<b>10<sup>th</sup> Session: Spectroscopy II, Chair: Martin Suhm</b>
<b>11:00-11:18</b>	<b>Dominic Bernhard</b> The bonus of dispersion – the diphenyl ether-methanol complex investigated using a multi-spectroscopic and theoretical approach
<b>11:18-11:36</b>	<b>Peter Stange</b> Quantifying Dispersion Interactions In Ionic Liquids Using Far-Infrared Spectroscopy
<b>11:36-11:54</b>	<b>Dr. Oleg Pimenov</b> Experimental determination of cuprophilic distances in the gas phase
<b>11:54-12:05</b>	<b>Prof. Peter R. Schreiner</b> Closing Remarks
<b>12:30-13:30</b>	<b>Coffee Break with Light Lunch</b> Departure