

Program

2nd SPP 1807 Summer School

Control of London dispersion interactions in molecular chemistry

Date: July 9th – July 12th

Location: Universität Rostock “Forschungsbau der Interdisziplinären Fakultät“

Albert-Einstein-Str. 25

Venue location / Travel details / Accommodation

The **second summer school** of the SPP 1807 “Dispersion” will take place at the **Universität Rostock** in the “Forschungsbau der Interdisziplinären Fakultät - Department Leben, Licht und Materie” (research building LL&M on the map). The Registration will take place in the Foyer of the research building. An informational Office is located in R 0.02. The talks will be held in the first floor in room 1.09/1.10. All participants take care of their own accommodation. There are three hotels blocked for the SPP 1807, all of them are marked on the map. If you booked the Hotel “Motel-One” or “Hotel Greifennest”, you can easily access Tram 4 at the stop “Schröderplatz” in the direction “Mensa”. If you are staying at the “Hotel Kleine Sonne” you need to go to the stop “Neuer Markt”, there you can choose between Tram 6 (via main station) or Tram 4 (via Schröderplatz) in the direction “Mensa”. If you are at the stop “Mensa” it is just a short walk to the research building.

Overview map of Rostock – 2nd Summer School of the SPP 1807



If you are attending the summer school by car, there are parking lots beyond the Forschungsbau LL&M. To reach them coming from the direction of “Motel-One” you need to take the Erich-Schlesinger-Straße until you reach a roundabout traffic. There you take the third exit into Albert-Einstein-Straße, you follow this street until the next crossing. Turn right in direction to „Leibniz-Institut für Katalyse e.V.“, beyond the building site you will find the parking lot (Barriers are opened).

[Google/maps](#)

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 until **July 1**. 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 A5), a pen, a map of the city centre and an information flyer concerning the Chemical Department of the University of Rostock. If you don't have access to eduroam (WiFi-Connection/Internet access), you will receive a temporary code.

Meals/Breaks

All meals, except breakfast, during the summer school will be organized, including lunch from Monday to Wednesday and finger food / dinner / BBQ from Sunday to Tuesday (all in buffet format, including special dietary options).

Child care

If you have any child care needs because of the workshop, please inform A. Wilhelms (anika.wilhelms@uni-rostock.de) until the 30th of June, 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) 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.

Sunday, July 9th, 2017

1st Invited Talk: Theory Chair: *Ralf Ludwig*

15:00-17:00	Arrival / Registration Foyer of the Forschungsbau LL&M @ Albert-Einstein-Str. 25
17:00-17:15	Peter R. Schreiner / Ralf Ludwig Opening remarks
17:15-18:15	Prof. Stefan Scheel Macroscopic Quantum Electrodynamics and Dispersion Forces
18:15-open end	Welcome Dinner with finger food Foyer of the Forschungsbau LL&M

Monday, July 10th, 2017

1st Session: Spectroscopy Chair: *Andreas Hesselmann*

09:00-09:20	Fabian Menges (Spectroscopy) Disentangling the Spectral Signatures of Distinct Cation-Cation Binding Motifs in Hydroxyl-Functionalized IIs Using IR-IR Double Resonance Spectroscopy of the Isolated (M ⁺) ₂ (A ⁻) Complexes
09:20-09:40	Helen Zeng (Spectroscopy) Characterization of Local Interactions in Hydroxyl-Functionalized Ionic Liquid Cationic Constituents with Cryogenic Ion Vibrational Pre-Dissociation Spectroscopy of Compositions-Selected Cluster Ions
09:40-10:00	Dr. Richard Knochenmuss (Spectroscopy) Spectroscopic Measurement of 1-naphthol-X Dissociation Energies: From Pure Dispersion to Hydrogen Bonding
10:00-10:30	Coffee Break Foyer of the Forschungsbau LL&M

2nd Session: Spectroscopy II Chair: *Martin Suhm*

10:30-10:50	Mariyam Fatima (Spectroscopy) Study of Intermolecular Interactions using Broadband Rotational Spectroscopy
10:50-11:10	Anja Poblitzki (Spectroscopy) Multi-spectroscopic Approaches to Benchmark Dispersion Interactions
11:10-11:30	Peter Stange (Spectroscopy) Dispersion Forces in Ionic Liquids - Infrared Spectroscopy and Thermodynamics
11:30-11:50	Dominic Bernhard (Spectroscopy / Structure and Reactivity / Theory) Multi-spectroscopic and Theoretical Investigations on the Isolated Di-phenyl-ether - tert.-butyl Alcohol Complex
11:50-14:00	Lunch Foyer of the Forschungsbau LL&M

3rd Session: Theory Chair: *Ricardo Mata*

14:00-14:20	Robert Externbrink (Theory) Dispersion Wavefunctions and Dispersion-induced Density Changes for Simple Model Systems
14:20-14:40	Christof Holzer (Theory) GW Methods in Molecular Quantum Chemistry
14:40-15:00	Axel Wuttke (Theory) Computational Insights into Dispersion Interactions in Self-Assembled Supramolecular Host-Guest Systems
15:20-15:40	Oinam Meitei (Theory) Efficient Geometry Optimizations of Extended Molecules Using an Incremental Fragmentation Method
15:40-16:10	Coffee Break Foyer of the Forschungsbau LL&M

4th Session: Theory / Structure & Reactivity Chair: *Stefan Grimme*

16:10-16:30	Dr. Malgorzata E. Krasowska (Structure & Reactivity / Theory) Heavy Main Group Element π Interaction
16:30-16:50	Dr. Lijuan Song (Catalysis / Theory) Quantification of Dispersion-Energy Donors and the Role of Dispersion Effects in Catalysis
16:50-17:10	Dr. Giovanni Bistoni (Structure & Reactivity / Theory) Weak Interactions in Organocatalysis: New Insights from Local Coupled Cluster Calculations
17:10-17:15	Short Break

2nd Invited Talk: Theory Chair: *Ricardo Mata*

17:15-18:15	Prof. Martin Head-Gordon Advances in Quantum Chemistry for Describing Dispersion Effects on Intermolecular Interactions: Computations and Analysis Hörsaalgebäude Physik Albert-Einstein-Str. 24 HS I
18:15-19:00	Dinner Foyer of the Forschungsbau LL&M
20:00-open end	Trip to Warnemünde

Tuesday, July 11th, 2017

5th Session: Theory / Spectroscopy Chair: Lutz Ackermann

09:00-09:20	Dr. Jens Anthony (Theory) Rotational Constants and Vibrational Spectra of Acenaphthene Water Complexes
09:20-09:40	Hannes C. Gottschalk (Theory / Spectroscopy) Benchmarking Quantum Chemical Methods Using IR Spectroscopy
09:40-10:00	Mallikarjun Karra (Theory / Spectroscopy) The Pc-H ₂ O Complex in Superfluid He Nanodroplets
10:00-10:30	Coffee Break Foyer of the Forschungsbau LL&M

6th Session: Organocatalysis Chair: Svetlana Tsogoeva

10:30-10:50	Dominik Grau (Catalysis) Novel Organocatalyzed Multi-step Domino Reactions: Role of London Dispersion Interactions
10:50-11:10	Simon Bönisch (Catalysis) DFT Studies on the Influence of Dispersion Interactions on Novel Organocatalyzed Domino Reactions
11:10-11:30	Darius Kootz (Catalysis) Dispersion Interactions in Carbene Catalyzed Umpolung
11:30-11:50	Animesh Biswas (Catalysis) New Aspects in Carbene Chemistry: Reactivity, Structure and Application
11:50-12:00	Group Photo Atrium (Green Area on the left-hand side of the Forschungsbau LL&M)
12:00-14:00	Lunch Foyer of the Forschungsbau LL&M

7th Session: Structure & Reactivity I Chair: Markus Gerhards

14:00-14:20	Luong Phong Ho (Structure & Reactivity) London Dispersion Effects in Dipnictenes Bearing Anionic N-heterocyclic Carbenes
14:20-14:40	Dr. Dzmitry Zaitsau (Structure & Reactivity) Direct Thermochemical Determination of the Dispersion Interaction of Alkyl Groups
14:40-15:00	Thomas Geiger (Structure & Reactivity) Investigation on Anthracene Dimers
15:20-15:40	Sören Rösel (Structure & Reactivity) London Dispersion Enables the Shortest Intermolecular Hydrocarbon H•••H Contact
15:40-16:10	Coffee Break Foyer of the Forschungsbau LL&M

8th Session: Dispersion in Solution *Chair: Peter R. Schreiner*

16:10-16:30	Marcel A. Strauß (Structure & Reactivity) Sensing Odd-Even Effect in n-Alkanes in Solution by Meta Substituted Azobenzene Probes
16:30-16:50	Jan M. Schümann (Structure & Reactivity) To What Degree is London Dispersion Solvent Dependent?
16:50-17:10	Robert Pollice (Structure & Reactivity) London Dispersion in Bond Dissociation Reactions in the Gas Phase and in Solution
17:10-17:15	Short Break

3rd Invited Talk: Structure & Reactivity *Chair: Peter R. Schreiner*

17:15-18:15	Prof. Ken D. Shimizu Solution Studies of Dispersion Interactions Hörsaalgebäude Physik Albert-Einstein-Str. 24 HS I
18:15-open end	BBQ Atrium (Green Area on the left-hand side of the Forschungsbau LL&M)

Wednesday, July 12th, 2017

9th Session: Structure & Reactivity II *Chair: Jan Schümann*

09:00-09:20	Timo Glodde (Structure & Reactivity) Molecular London Dispersion Interactions in Bifunctional Molecules
09:20-09:40	Dr. Ana-Maria Preda (Structure & Reactivity) Dispersion Type Metal- π Interactions in Bismuth Compounds
09:40-10:00	Bo Zhang (Structure & Reactivity) London Dispersion Interactions in Self-Assembled Host-Guest Systems
10:00-10:30	Coffee Break Foyer of the Forschungsbau LL&M

10th Session: C-H Activation *Chair: Ralf Ludwig*

10:30-10:50	Torben Rogge (Catalysis) DFT-Studies on Dispersion Control in Ruthenium-catalyzed C-H Activation of Benzoic Acids
10:50-11:10	Joachim Loup (Catalysis) Dispersion Interactions for Selectivity Control In C-H Activation
11:10-11:30	Daniel Zell (Catalysis) Full Regiocontrol in Cobalt(III)-Catalyzed C-H Alkylation's
11:30-11:45	Peter R. Schreiner / Ralf Ludwig Closing Remarks
11:45-13:00	Lunch / Departure Foyer of the Forschungsbau LL&M