

General Information: 2nd Workshop of the SPP 1807

“Control of London Dispersion Interactions in Molecular Chemistry”

10th-11th of October 2016 @ “Universität zu Köln”

Venue location / Travel details

The Workshop will take place on ground level of the COPT-Building at the University of Cologne, Luxemburger Straße 90, 50939 Köln.

Map with interactive function: <http://www.chemie.uni-koeln.de/kontakt.html>

All hotels are close to the main train station of Cologne. You need to go by Underground to the COPT-building. From the hotel you use Underground-station “Dom / HBF” – what is “main station”. Take line 18, direction “Klettenberg” or “Brühl, Bonn” until “Eifelwall” (5 Stations, now it is street level). The COPT-building is just across the street, driving direction right, when you leave the train. We will also place signposts at the station Eifelwall.

Underground: You need a ticket Preisstufe 1b for 2,80 € one way. It is less expensive to by a strip with 4 Tickets (10,70 €) or – quiet cheap - a group-ticket for 5 people. To use 24 hours for 12,90€ (what is 1,28 € for one way). You can buy it at the automat (in the station or the trains). There are also ticket desks in the U-Bahn-Station at main station with friendly people, always helping to choose a ticket.

Talks / Poster presentations

Each project will receive a 20 min slot (+5 min discussion) for an oral presentation. The program lists each of the slots according to the project title, but the presenter is free to choose another title for the presentation. If the talk is shared, it will still be subject to the 20 minutes' limit. Due to the tight schedule, we also request that all speakers provide the presentation files before the respective session starts in pdf or Power Point format. The files can be sent to Jan.M.Schuemann@org.chemie.uni-giessen.de or handed over to our technical staff during the workshop.

The number of posters is not limited. There are no poster abstracts, and their titles will not be listed. The poster format should be DIN A0 (portrait orientation) but smaller formats are also acceptable.

The poster displays are planned to be spread over several (3) rooms: We have a room for the café break and another room – a bigger one – with tables to sit at for the buffet in the evening. We have also some space in the lecture hall where the workshop presentations will take place. It might be attractive to walk along the posters during the coffee break or in the evening. We have ordered 25 Poster-displays which can be used from both sides. So it is room for 50 posters.

Materials

A printed copy of the program will be provided upon request. We are able to bring some UzK-ball pens and -notepads.

Meals / Breaks

The lunch on both days will take place at the Mensa of the UzK. Every participant will get bons for both days for lunch in the Mensa. The coffee breaks and dinner on Monday will be set up in rooms beside the lecture hall. Catering for Monday evening includes vegetarian food. We will provide Coffee on Monday morning as a starter when everybody arrives as well as two coffee breaks with cake and soft drinks during the day, and water during the workshop.

Child care

If you have any child care needs as a result of the workshop, please inform S. Geuer (susanne.geuer@uni-koeln.de) as soon as possible 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 and accommodation costs for PI's and SPP funded students/postdocs will be reimbursed according to the DFG guidelines. Participants external to the program will not be covered. Please take into account when booking train/plane tickets that first/business class tickets are not reimbursable. Keep a copy of your tickets as well as the receipt from the Hotel. The necessary forms will be provided during the workshop.

Schedule: 2nd Workshop of the SPP 1807

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Monday, October 10th, 2016

08:00 – 09:00 **Arrival & registration @ reception desk / Poster set up**

09:00 - 09:15 **Opening**

Session 1 *Chair: P. R. Schreiner “Catalysis”*

09:15 - 09:40 **A. Berkessel:**
Dispersion Effects in Carbene Catalysis

09:40 - 10:05 **M. Tamm:**
Control of Dispersion Interactions in Complexes with Anionic N-Heterocyclic Carbene Ligands

10:05 - 10:30 **S. Tsogoeva:**
Synthesis of Nitrogen-Containing Versatile Compounds via Organocatalyzed Multi-Step Domino Reactions

10:30 - 10:45 **Coffee break (Coffee and Cake) (15 min)**

Session 2 *Chair: G. Jansen “Theory”*

10:45 - 11:10 **F. Neese:**
A Local Coupled Cluster based Energy Decomposition Scheme. Theory and Applications

11:10 - 11:35 **S. Verevkin:**
Quantifying Dispersion Forces by means of Thermodynamic Methods

11:35 - 12:00 **W. M. Klopper:**
Accurate Calculations of Intermolecular Interactions

12:00 - 13:00 **Lunch @ Mensa (1 h)**

Session 3	<i>Chair: A. A. Auer</i>	<i>"Theory and Spectroscopy I"</i>
13:00 - 13:25	S. Leutwyler:	From Methane to Adamantane: Accurate Dissociation Energies of Jet-Cooled 1-Naphthol-(Cyclo)alkane Complexes
13:25- 13:50	R. Ludwig:	Dispersion and Hydrogen Bonding Rule - Why the Vaporization Enthalpies of Aprotic Ionic Liquids Are Significantly Larger than those of Protic Ionic Liquids
13:50 - 14:15	M. Gerhards:	Combined IR/UV Investigations on Isolated Aggregates of Diphenyl Ether with Alcohols or Water
14:15 – 14:25	Short Break (10 min)	
Session 4	<i>Chair: M. Gerhards</i>	<i>"Theory and Spectroscopy II"</i>
14:25 - 14:50	P. Chen:	Bridging gas-phase to solution dispersion effects
14:50 - 15:15	G. Jansen:	Combined Quantum Chemical and Experimental Investigations of Intermolecular Interactions Involving Heavy Group-15 and Group-16 Elements
15:15 - 15:40	A. A. Auer:	Heavy Main Group Elements as Dispersion Energy Donors - Electronic Structure Calculations on Bi Coordination Compounds
15:40 – 15:50	Short Break (10 min)	
Session 5	<i>Chair: A. Berkessel</i>	<i>"Structure & Reactivity I"</i>
15:50 - 16:15	M. Mehring:	Dispersion-type Metal- π Interactions in Bismuth Compounds
16:15 – 16:40	W. Nau:	Dispersion Interactions in Host-Guest Inclusion Complexes
16:40- 17:40	Invited Talk: T. Müller:	Dispersion Energy Effects in the Chemistry of Oligosilanes
17:40 – 18:30	Poster session (25 Poster / 50 min)	
18:30 - 19:30	Dinner buffet (arrives @17:45) (1 h)	

Tuesday, October 11th, 2016

Session 6	<i>Chair: S. Leutwyler</i> <i>“Spectroscopy”</i>
09:30 - 09:55	M. Suhm: Extending the Spectroscopic Data Base for O/ π Docking Preferences of Alcohols
09:55 - 10:20	M. Schnell: Dispersion Interactions in Molecular Systems Studied with Broadband Rotational Spectroscopy
10:30 - 10:45	Coffee break (Coffee and Cake) (15 min)

Session 7	<i>Chair: P. Chen</i> <i>“Structure & Reactivity II”</i>
10:45 - 11:10	P. R. Schreiner: Generalization of Structural Stabilization through London Dispersion
11:10 - 11:35	N. W. Mitzel: Intramolecular Dispersive Interactions in the Gas Phase
11:35 - 12:00	L. Ackermann: Dispersion Interactions for Selectivity Control in C-H Activation
12:00 - 13:00	Lunch @ Mensa (1 h)

Session 8	<i>Chair: N. W. Mitzel</i> <i>“Structure & Reactivity III”</i>
13:00 - 13:25	H. Bettinger: Dimerization of Acenes
13:25 - 13:50	G. Clever / R. Mata: Experimental and Computational Insights into Dispersion Interactions in Self-Assembled Supramolecular Host-Guest Systems
13:50 - 14:50	Invited Talk: S. Shaik: Nature of the Halogen Bond
14:50 - 15:30	Discussion and concluding remarks