

General Information and Schedule: 3rd Workshop of the SPP 1807

“Control of London Dispersion Interactions in Molecular Chemistry”

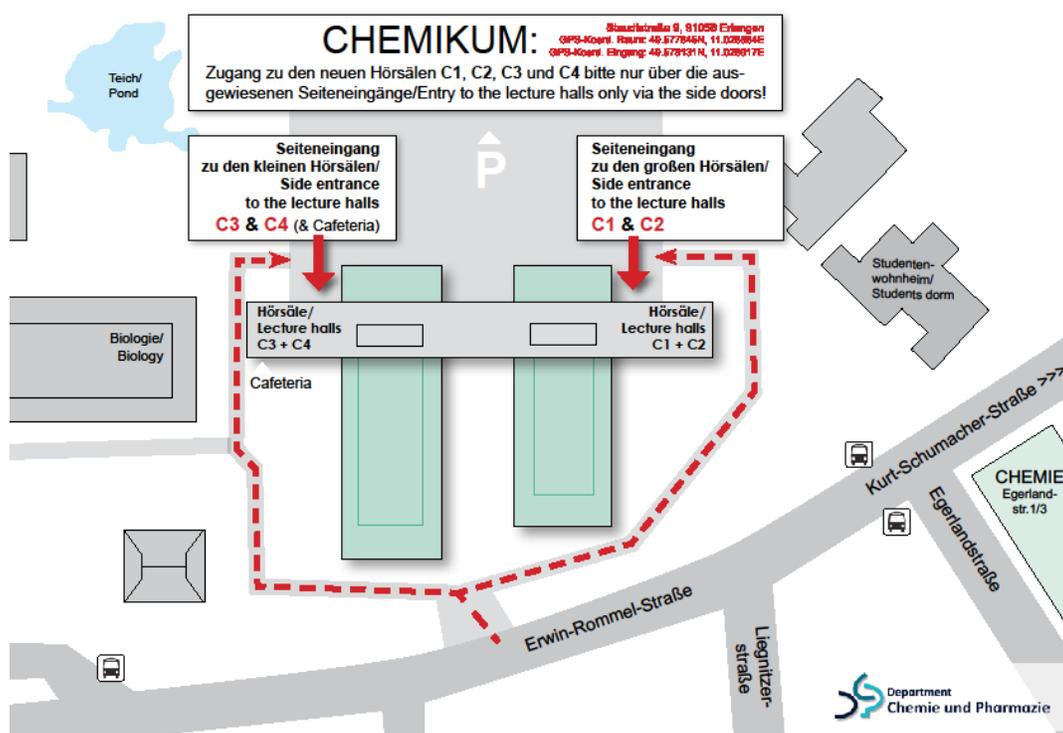
February 25th-26th, 2019

Friedrich-Alexander Universität – Erlangen-Nürnberg

Venue Location / Travel Details

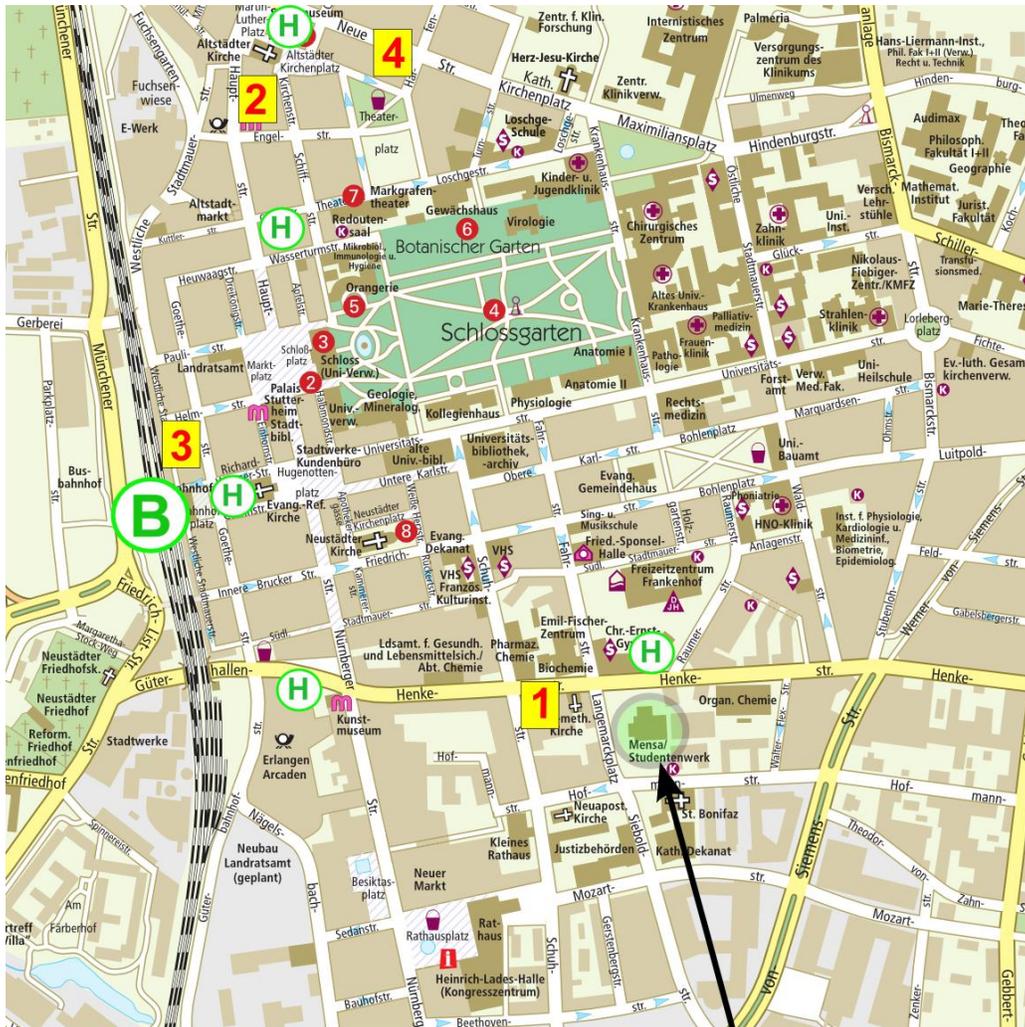
The workshop will take place in the C3 lecture hall in the *Chemikum* building of the University, Nikolaus-Fiebiger-Straße 10, 91058 Erlangen. The *Chemikum* is located in the south of Erlangen, about 3 - 4 km away from the city center. Bus lines **287** and **293** take you from the city center (e.g., the main train station) to the *Chemikum*. Here is a map of all bus lines and stations in Erlangen: www.vgn.de/liniennetze/stadtverkehr_erlangen_stilisiert

Map with locations of the lecture halls in the *Chemikum*:



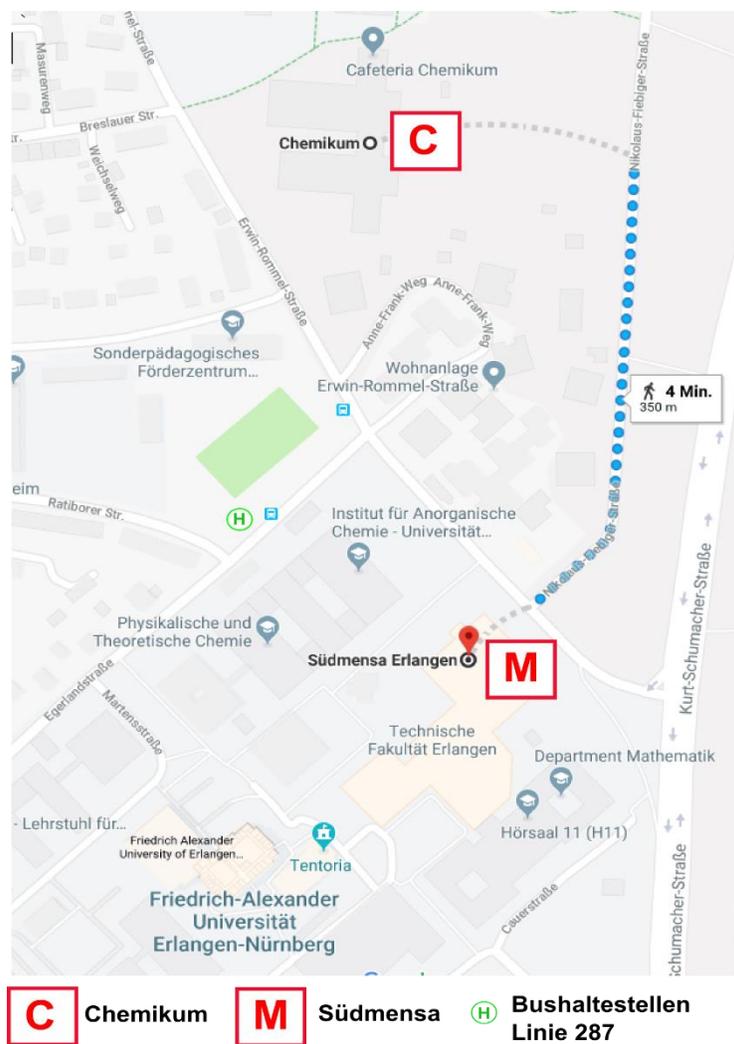
All hotels are located in the city center and are within walking distance from the main train station (the farthest being the AB hotel with a distance of 900 m from the HBF). There are bus stations of line **287** close to each of the hotels and the main train station. A map showing the different sites is given below.

For those who plan to travel by car: it is advisable to ask the hotel in advance for parking. General information about parking areas in the city center can be found under: www.erlangen.de/desktopdefault.aspx/tabid-1275/944_read-12474



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|----------|------------------------------|---------------------------------|
| 1 | Hotel König Humbert | Mensa Langemarckplatz |
| 2 | Hotel Grauer Wolf | H Bushaltestellen |
| 3 | Hotel Fränkischer Hof | Linie 287 |
| 4 | A.B. Hotel | B Hauptbahnhof |

Lunch will be served in the *Südmena* which lies about 350 meters away from the *Chemikum* in the south campus of the university, see the map below.



Dinner on Monday will be served in the *Mensa am Langemarckplatz* in the city center and close to the (old) Organic Chemistry building (see previous map above).

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 walls for the poster presentations are located in the foyer of the *Chemikum*. Depending on the actual number of posters, some poster walls may have to be supplied in other locations of the *Chemikum*.

Materials & Internet Connection

A printed copy of the program will be provided upon request. *Eduroam* can be used in all buildings of the university. For those participants who do not have access to the *eduroam*, a temporary guest account will be arranged for the duration of the workshop.

Meals / Breaks

Lunch on both days will take place at the *Südmensa* located on the south campus of the university, see map above. It is within walking distance of about 3-5 min from the *Chemikum*. A separate room (ground floor, next to the cafeteria) will be provided for the workshop participants by the "Studentenwerk". Every participant will get vouchers for both days for lunch in the Mensa.

The coffee breaks will be in the Foyer and Cafeteria in the *Chemikum*, located in the same wing of the building as the C3 lecture hall on the ground level.

Dinner on Monday will be in the *Mensa am Langemarckplatz* in the city center. Bus **287** from either station Erlangen/Technische Fakultät or station Erlangen/Sebaldussiedlung next to the *Chemikum* building will take you to Langemarckplatz.

Child Care

If you have child care needs, please inform A. Heßelmann (andreas.hesselmann@fau.de) as soon as possible so that we can provide some support. Also, if there are 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.

Monday, February 25th, 2019

08:00 – 09:00 **Arrival & registration / Poster set up @ Foyer Chemikum**

09:00 – 09:15 **Opening**

Session 1 *Chair: Kevin Dzialkowski* “Theory/ Structure & Reactivity”

09:15 – 09:40 **A. Heßelmann**

Study of a molecular torsion balance in solution

09:40 – 10:05 **P. Imhof / A. Vila Verde**

Dispersion interactions in fluorinated biopolymers

10:05 – 10:30 **G. Jansen / S. Schulz**

Combined Quantum Chemical and Experimental Study on Metal-Metal Interactions in Heavy Group15 and Group16 Compounds

10:30 – 10:55 **Coffee break @ cafeteria Chemikum / Poster Session @ Foyer (25 min)**

Session 2 *Chair: Wacharee Harnying* “Catalysis”

10:55 – 11:20 **J. Paradies**

DED-stabilized Frustrated Lewis Pairs

11:20 – 11:45 **A. Berkessel**

Dispersion Effects in Homogeneous Catalysis

11:45 – 12:10 **L. Ackermann**

Dispersion for Selectivity Control in C-H Activation

12:10 – 13:40 **Lunch @ Südmensa (90 min)**

Session 3	<i>Chair: Jan Schümann "Structure & Reactivity"</i>
13:40 – 14:05	P. R. Schreiner Probing the Delicate Balance between Pauli Repulsion and London Dispersion with Triphenylmethyl Derivatives
14:05 – 14:30	F. Biedermann Design and synthesis of a cucurbit[8]uril-based model system for investigating face-to-face π -stacking complexes
14:30 – 14:55	W. Nau Using Macrocycles to Dissect Dispersion Interactions from the Others
14:55 – 15:20	Coffee break @ cafeteria Chemikum / Poster Session @ Foyer (25 min)

Session 4	<i>Chair: Mariyam Fatima "Spectroscopy"</i>
15:20 – 15:45	M. Schnell Understanding complex formation and aggregation using a bottom-up approach
15:45 – 16:10	M. Suhm Intermolecular energy balances in the gas phase: focusing on subtle electronic energy differences
16:10 – 16:35	M. Gerhards Stimulated Raman spectroscopy as a powerful tool for elucidating the structure of dispersion-bound molecular aggregates in the gas phase
16:35 – 17:00	Coffee break @ cafeteria Chemikum / Poster Session @ Foyer (25 min)

Session 5	<i>Chair: Federica Ferraro "Theory"</i>
17:00 – 18:00	Invited Talk: Timothy Clark It need not be London
18:30 – open end	Dinner @ Mensa am Langemarckplatz

Tuesday, February 26th, 2019

Session 6 *Chair: Sebastian Scholz "Theory/Structure & Reactivity/ Spectroscopy"*

09:15 – 09:40

R. Mata / G. Clever

Reviewing the structural impact of London dispersion interactions

09:40 – 10:05

A. A. Auer / M. Mehring

Heavy Main Group Metal - π Interactions, Theory and Experiment

10:05 – 10:30

C. Hättig

Dispersion interactions in excited states

10:30 – 10:55

Coffee break @ cafeteria Chemikum / Poster Session @ Foyer (25 min)

Session 7 *Chair: Robert Pollice "Spectroscopy"*

10:55 – 11:20

R. Gschwind

Dispersion Effects in Ion Pair Catalysis

11:20 – 11:45

P. Chen

Onium ions and their dimers as probes for dispersion

11:45 – 12:10

B. Friedrich / A. Slenczka

Molecular complexes formed and probed in superfluid He droplets

12:10 – 13:40

Lunch @ Südmensa (90 min)

Session 8	<i>Chair: Timo Glodde "Structure & Reactivity"</i>
13:40 – 14:05	S. P. Verevkin / R. Ludwig Quantification of dispersion interactions in protic and aprotic ionic liquids
14:05 – 14:30	H. A. Wegner Azobenzene switches as tool to investigate London dispersion interactions
14:30 – 14:55	R. Berger/ N. Mitzel Cuprophilic interactions in the gas phase
14:55 – 15:20	Coffee break @ cafeteria Chemikum / Poster Session @ Foyer (25 min)

Session 9	<i>Chair: Ahmet Altun "Theory"</i>
15:20 – 15:45	G. Bistoni / F. Neese Quantifying London dispersion effects through novel local correlation techniques.
15:45 – 16:10	W. Klopper GW-SAPT analysis of classically and non-classically hydrogen-bonded complexes
16:10 – 16:35	S. Grimme New Low-Cost Quantum Chemistry Methods
16:35 – 17:00	Coffee break @ cafeteria Chemikum / Poster Session @ Foyer (25 min)

Session 10	<i>Chair: Benedikt Sieland "Catalysis"</i>
17:00 – 18:00	Invited Talk: Masaya Sawamura Non-covalent interactions in our studies on asymmetric transition metal catalysis
18:00 – 18:15	Discussion and concluding Remarks
