

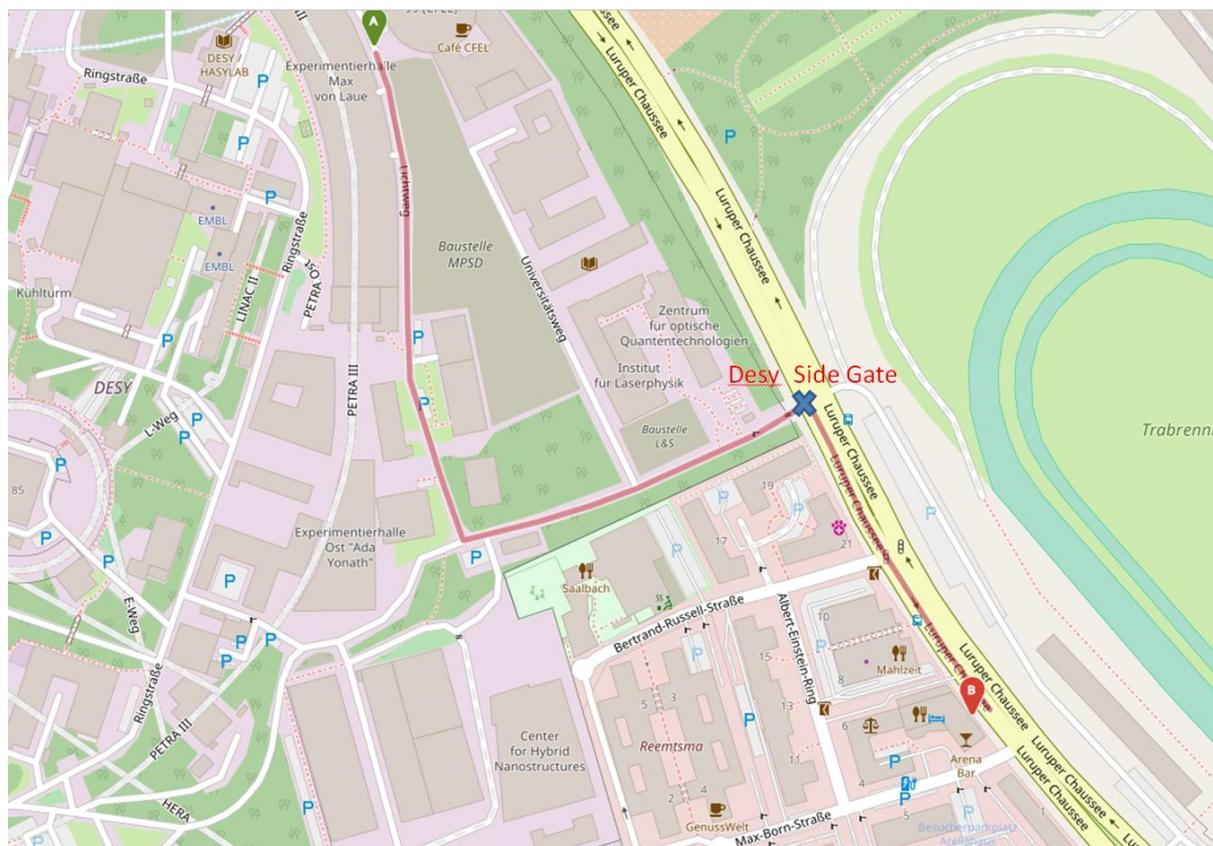
DESY Campus: Note that there are two entrances to the DESY campus: 1) The main entrance via Notkestraße 85, which is close to DESY guest house, and 2) the side entrance via Luruper Chaussee 149, which is close to the CFEL building where the summer school takes place. The main entrance is open 24/7. The same is true for the side entrance for pedestrians and bikers, but for cars it is only open from 6 a.m. to 7 p.m.

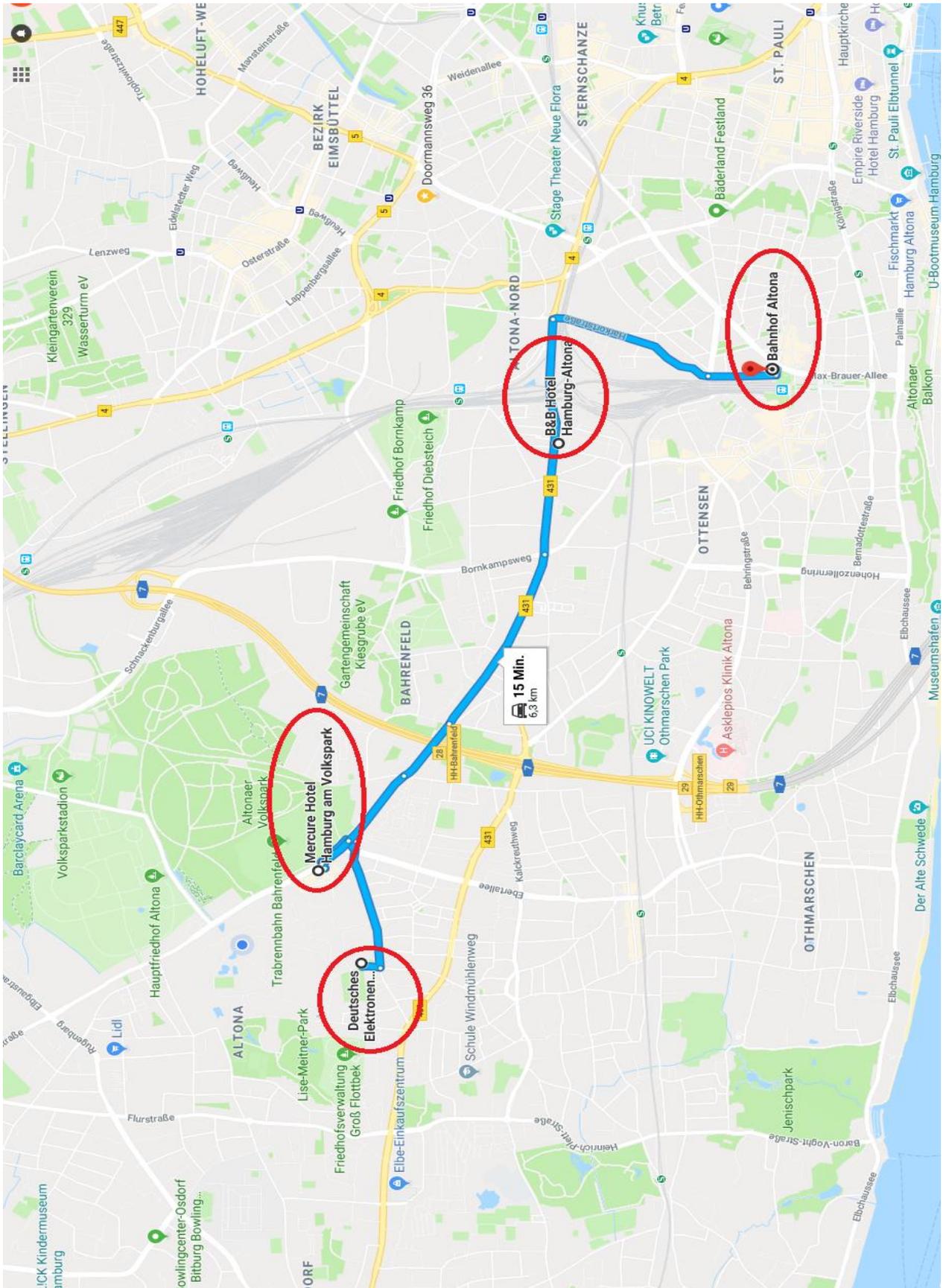
All participants take care of their own accommodation. There are three hotels blocked for the SPP 1807, all of them are marked on the map.

DESY Guest House: The DESY Guest House is located at the DESY main gate. Please remember that the check-in time starts at 14:00 p.m. and check-out time is at 10:30 a.m.

Mercure Hotel: From the Central Station take the S1-Bahn into Wedel or Rissen direction. Continue until Othmarschen Station (it will take you around 20 min from Central Station and 7 min from Altona Station). Once there, you can take the Bus 1 direction “Schenefelder Holt” or “Rissen”. Continue until you reach the bus stop “Trabrennbahn Bahrendfeld” (around 7-8 min). From there is a 5 min walk to the Mercure Hotel.

Mercure Hotel → DESY: The Mercure Hotel is a 10-15 min walk to DESY. Just follow along the Luruper Chaussee as marked on the map below. Mercure Hotel is located at Albert-Einstein-Ring 2, 22761 Hamburg.





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 22nd**. 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, a map of the city. On the campus, there is eduroam (WiFi-Connection/Internet access) as well as the DESY guest WIFI.

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 (coupons for the DESY canteen, including special dietary options).

Child care

If you have any child care needs because of the workshop, please inform Maureen Alfaro (maureen.ayon.alfaro@desy.de) until the 16th of July, 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 22nd, 2018

1st Invited Talk: Theory

Chair: Peter R. Schreiner

16:00-17:45	Arrival / Registration Foyer of the CFEL building (building 99)
17:45-18:00	Peter R. Schreiner / Melanie Schnell Opening remarks
18:00-19:00	Prof. Steven E. Wheeler (University of Georgia, Athens, USA) Toward a More Complete Understanding of Stacking Interactions of Aromatic Molecules
19:00-open end	Welcome Dinner with finger food Foyer of the CFEL building (building 99)

Monday, July 23rd, 2018

1st Session: Spectroscopy I

Chair: Martin Suhm

09:00-09:20	Hannes C. Gottschalk (Georg-August-Universität Göttingen) Tipping the Scales: Using IR Spectroscopic of Intermolecular Energy Balances to Benchmark Quantum Chemical Methods
09:20-09:40	Ginny Karir (Georg-August-Universität Göttingen) Isomer switching in intermolecular balances involving hydrogen bonds
09:40-10:00	Charlotte Zimmermann (Georg-August-Universität Göttingen) Acetophenone derivatives as intermolecular energy balances for dispersion tuned alcohols
10:00-10:30	Coffee Break Foyer of the CFEL building (building 99)

2nd Session: Catalysis I

Chair: Albrecht Berkessel

10:30-10:50	Hauke Engler (Universität zu Köln) Ti-Salalen Complexes: Epoxidation Catalysts Shaped and Driven by Dispersive Interactions
10:50-11:10	Benedikt Sieland (Universität Paderborn) Dispersion Energy Stabilized Lewis Pairs
11:10-11:30	Darius Kootz (Universität zu Köln) Dispersion Interactions in Carbene Catalyzed Umpolung
11:30-11:50	Panyapon Sudkaow (Universität zu Köln) Breslow Intermediates from Aromatic N-Heterocyclic Carbenes (Benzimidazolin-2-ylidenes) and Applications in Catalysis
11:50-14:00	Lunch (incl. conference picture) DESY canteen (building 9)

3rd Session: Structure & Reactivity I

Chair: Peter R. Schreiner

14:00-14:20	Khaleel I. Assaf (Jacobs University, Bremen) Dispersion Interactions in the Gas Phase: Supramolecular Host-Guest Complexation as a Molecular Balance
14:20-14:40	Jan M. Schümann (Justus-Liebig-Universität Gießen) Quantifying London Dispersion with 1,4 Substituted Cyclooctatetraene Based Balances
14:40-15:00	Marcel A. Strauß (Justus-Liebig-Universität Gießen) Tracking the Small Differences - Measuring Dispersion Interactions with Azobenzene Switches in Solution
15:00-15:20	Sören Rösel (Justus-Liebig-Universität Gießen) Hexaphenylethanes - Dispersion Bound Prototype Molecules?
15:20-15:40	Marek Bot (Eidgenössische Hochschule Zürich) Dispersion Interactions in large proton-bound pyridine dimers
15:40-16:10	Coffee Break Foyer of the CFEL building (building 99)

4th Session: Theory I

Chair: Andreas Hansen

16:10-16:30	Oinam Meitei (Friedrich-Alexander-Universität Erlangen-Nürnberg) Molecular properties from the incremental fragmentation method
16:30-16:50	Robert Externbrink (Universität Duisburg-Essen) Theory Dispersion energies and Feynman dipoles for interacting quantum spheres and balls
16:50-17:10	Eike Caldeweyer (Universität Bonn) DFT-D4: An accurate and generally applicable tight-binding based dispersion correction for density functional theory
17:10-18:00	Break Foyer of the CFEL building (building 99)

2nd Invited Talk: Structure & Reactivity

Chair: Frank Biedermann

18:00-19:00	Arthur H. Winter (Iowa State University, Ames, USA) Importance of Dispersion Forces in Radical-Radical Interactions
19:00-open end	Dinner / BBQ In front of the FLASH seminar room (building 28c, organized walk)

Tuesday, July 24th, 2018

5th Session: Theory II

Chair: Giovanni Bistoni

09:00-09:20	Ahmet Altun (MPI für Kohlenforschung, Mülheim an der Ruhr) Applications of the Closed-Shell and Open-Shell Local Energy Decomposition Analysis Method in the Domain Based Local Pair Natural Orbital Coupled Cluster Framework
09:20-09:40	Małgorzata E. Krasowska (MPI für Kohlenforschung, Mülheim an der Ruhr) Heavy main group element - π interactions
09:40-10:00	João Robalo (MPI für Kolloid- und Grenzflächenforschung, Potsdam) Dispersion Interactions in Fluorinated Biopolymers
10:00-10:30	Coffee Break Foyer of the CFEL building (building 99)

6th Session: Spectroscopy II

Chair: Georg Jansen

10:30-10:50	Peter Stange (Universität Rostock) H-bonds and dispersion forces in protic ionic liquids
10:50-11:10	Johannes Gramüller (Universität Regensburg) Dispersive interactions in Brønsted acid catalysis
11:10-11:30	Johnny Hioe (Universität Regensburg) Structural diversity induced by dispersive interaction in Brønsted acid catalysis
11:30-11:50	Lokesh Nanjundappa (Universität Regensburg) Substrate dynamics inside Brønsted catalyst cavity
11:50-12:10	Timo Glodde (Universität Bielefeld) Intramolecular interactions in organochalcogen compounds
12:10-14:00	Lunch DESY canteen (building 9)

7th Session: Structure & Reactivity II

Chair: Ralf Ludwig

14:00-14:20	Laura Grimm (Karlsruher Institut für Technologie) Design and synthesis of a cucurbit [8] uril-based model system for investigating face-to-face π -stacking complexes
14:20-14:40	Ana-Maria Preda (Technische Universität Chemnitz) Bismuth-based dispersion energy donors – Synthesis and structure
14:40-15:00	Sebastian Scholz (Technische Universität Chemnitz) Dispersion type bismuth - π -aryl interactive in substituted biphenyl bismuth compounds
15:00-15:20	Bo Zhang (Technische Universität Dortmund) London Dispersion Interactions in Self-Assembled Host-Guest Systems
15:20-15:40	Fabian Bohle (Universität Bonn) Influence of Dispersion forces on molecular recognition in solution
15:40-16:10	Coffee Break Foyer of the CFEL building (building 99)

8th Session: Spectroscopy III

Chair: Markus Gerhards

16:10-16:30	Dominic Bernhard (Technische Universität Kaiserslautern) IR/UV investigations on a series of dibenzofuran-solvent aggregates
16:30-16:50	Sérgio Domingos (Deutsches Elektronen Synchrotron (DESY) Hamburg) The phenyloxirane dimer topologies and the ruling non-covalent contacts for chiral self-recognition
16:50-17:10	Mallikarjun Karra (Fritz-Haber-Institut der MPG, Berlin) Phthalocyanine, Porphyrin and Phthalocyanine-based complexes in superfluid helium nanodroplets
17:10-17:30	Mariyam Fatima (MPI für Struktur und Dynamik der Materie / DESY Hamburg) Study of dispersion interactions in diphenylether, dibenzofuran and fluorene dimers via broadband rotational spectroscopy
17:30-18:00	Break Foyer of the CFEL building (building 99)

3rd Invited Talk: Spectroscopy

Chair: Melanie Schnell

18:00-19:00	Wolfgang Jäger (University of Alberta, Edmonton, Canada) Spectroscopic Studies of Complexes and Clusters: From Pure Dispersion to Hydrogen-Bond Dominated Interactions
19:00-open end	Dinner DESY canteen (building 9)

Wednesday, July 25th, 2018

9th Session: Theory III

Chair: Andreas Hesselmann

09:00-09:20	Axel Wuttke (Georg-August-Universität Göttingen) Improving the stability of EDA with local orbital spaces
09:20-09:40	Maximilian Rybarczyk (Georg-August-Universität Göttingen) All that bind is not gold
09:40-10:00	Kevin Dzialkowski (Universität Duisburg-Essen) Combined Quantum Chemical and Experimental Study on Metal-Metal Interactions of Heavy Group 15 and Group 16 Compounds
10:00-10:30	Coffee Break Foyer of the CFEL building (building 99)

10th Session: Catalysis II

Chair: Jan Paradies

10:30-10:50	Lijuan Song (Justus-Liebig-Universität Gießen) Quantification of Dispersion-Energy Donors and the Application of Dispersion Effects in Catalysis
10:50-11:10	Joachim Loup (Georg-August-Universität Göttingen) Dispersion Interactions for Selectivity Control in C-H Functionalization
11:10-11:30	Torben Rogge (Georg-August-Universität Göttingen) Ruthenium(II)-catalyzed C-H Alkenylations and Alkylations: Experiment and Computations
11:30-11:45	Peter R. Schreiner / Melanie Schnell Closing Remarks
11:45-13:00	Lunch / Departure DESY canteen (building 9)