

# 54<sup>th</sup> Symposium on Theoretical Chemistry

## „Non-Covalent Interactions“

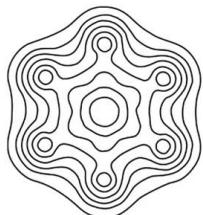
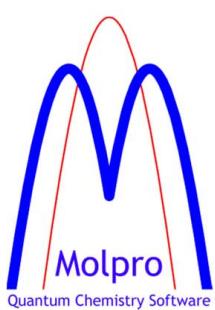
## Conference Program

(no abstracts)



17.–20. September 2018, Halle (Saale)

<https://stc2018.de/>



FCI  
FONDS DER  
CHEMISCHEN  
INDUSTRIE



## **Impressum**

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## **Part I.**

# **Conference Information**



# 1. Information from A to Z

## AGTC Meeting

The meeting of the “Arbeitsgemeinschaft Theoretische Chemie” (AGTC) will take place on Monday evening, 18:10 – 18:50, in the Auditorium Maximum (*Universitätsplatz 1*).

## Airport

The Leipzig–Halle airport (LEJ) is very close to Halle (Saale). It can be reached from Halle main station with the S5 and S5X trains (direction: Zwickau) in 12 minutes. These trains go twice an hour.

## Book of Abstracts

The book of abstract is included in the conference book, but this is the short version without abstracts. Please download the full conference book. As already practiced at the STC conferences of the last years, we do **not** offer printed copies of the conference book. If you would like to have a printed version, we recommend printing it before your travel to Halle.

## Charging Mobile Devices

*see Power*

## Child Care

We offer free child care during the conference (Monday morning until Thursday noon). If you are interested in our child care program, please contact us at your earliest convenience.

## Coffee Breaks

All coffee breaks (*see schedule*) take place in the Auditorium Maximum (*Universitätsplatz 1*), next to the lecture hall. We offer coffee, tea, softdrinks, and a selection of cookies in each of the coffee breaks.

## Conference Desk

The conference desk is located in the Melanchthonianum (*Universitätsplatz 9, room “Medienraum”*), close to the entrance. It will be continuously staffed from 15:00 to 20:00 on Sunday, from 9:00 to 18:00 on Monday till Wednesday, and from 9:00 till 14:00 on Thursday.

## *1. Information from A to Z*

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### **Conference Dinner**

The conference dinner takes place on Wednesday, 19.09.2018, from 19:00 till 23:00 in the “Dormero Hotel Rotes Ross” (*Leipziger Straße 76*). You will require your name badge to enter. The food is for free, and standard drinks (beer, wine, softdrinks) are free until 22:00. Starting from 22:00, all drinks have to be paid.

### **Excursions**

The excursions take place on Wednesday afternoon, starting at 15:00. All excursions are covered by the conference fee (*no additional cost*). Sign-in to the excursions is handled at the conference registration. The number of participants is limited for some excursions. Please pick one single “excursion ticket” at the conference desk. For a list of excursions, please see page 16.

### **Lunch**

In your conference bag, you will receive lunch vouchers for Monday till Wednesday. These are valid in the “Harzmensa” (*Harz 41*) and include one meal (not including drinks/desserts) per day.

### **Medical Service**

In case of medical emergencies, please immediately call phone number 112 for first aid. If you require less urgent medical aid, please contact the conference desk.

### **Participants**

There are 291 participants registered for the STC 2018. You can find a list of participants on page 37.

### **Poster Sessions**

The poster sessions will take place on Monday and Tuesday evening (19:00 – 22:00) in the Melanchthonianum (*Universitätsplatz 9*). We will offer a selection of alcoholic and non-alcoholic drinks as well as snacks (“belegte Brötchen”) during both poster sessions. Posters with odd numbers are scheduled for session A on Monday; posters with even numbers will be presented in session B on Tuesday. Posters should be in A0 portrait format. Please put your poster to the wall during the afternoon before the session in which your poster is scheduled. Please take off your poster **at latest** in the morning after your session. Posters which are left at the wall at lunch time will be disposed without further notice.

### **Poster Slam**

We will have a so-called ”poster slam“ directly before each poster session (*see schedule*), where every presenting author has the chance to advertise his or her poster to the full audience with a few words. This short presentation will have a length of 60 seconds per participant, and uses one single slide, which had to be handed in before the conference. 22 persons registered for the poster slam.

### **Power**

For your convenience, we installed power distributor sockets in many different seat rows within the Audimax, where the lectures take place. Therefore, you will be able to charge your electronic devices during the talks. If you don’t need electricity, please do not occupy the places close to the distributor sockets.

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## **Public Transport**

Halle (Saale) is a relatively small city, and the conference venue is located directly in the city center. Therefore, you will probably not need to use the public transport (e. g., walking from the main station to the conference venue takes around 20 minutes). Otherwise, you should buy an “Einzelfahrkarte” for 2.30€, which is valid for one hour within the whole city of Halle. Please note that there are frequent ticket controls in the trams.

## **Presentations**

*see Talks*

## **Printing**

We do not offer poster printing service for participants of the conference. As the conference center is located directly in the city center, there are several copy shops within a few hundred meters of the venue.

## **Registration**

Registration takes place at the conference desk, which is located in the Melanchthonianum (*Universitätsplatz 9, room “Medienraum”*), close to the entrance. It will be staffed from 15:00 to 20:00 on Sunday, from 9:00 to 18:00 on Monday till Wednesday, and from 9:00 to 14:00 on Thursday.

## **Restaurants**

As the conference center is located directly in the city center, there are plenty of restaurants within a few hundred meters of the venue. Some restaurants and bars which are suitable for larger groups of people are marked in the map on page 8.

## **Schedule**

*see page 9*

## **Talks**

The conference program includes 11 invited talks and 32 contributed talks, which were selected from over 100 applications. Please understand that we had to reject even some very promising talks due to the large interest. All talks take place in the Auditorium Maximum (*Universitätsplatz 1*). Invited talks are scheduled for 30 minutes talk and 10 minutes discussion (40 minutes in total). Contributed talks are scheduled for 15 minutes talk and 5 minutes discussion (20 minutes in total). Please strictly adhere to these maximum times.

Speakers please upload their talks to the presentation computer in the break before their session. Own laptops may be used if really required (connection via **HDMI only**). Audio playback is not possible.

## *1. Information from A to Z*

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### **Taxi Companies**

Below, you find the phone numbers of some local taxi companies (without ranking):

Taxi Halle	+49345 525252
Taxi Wienecke	+49345 5200022
Taxi Kobsch	+49345 5606222
Taxi Peschke	+4934602 20754
Taxi Kremmer	+49345 5323452
Taxi Banse	+49345 5601982

### **Venue**

*see page 7*

### **Weather Forecast**

The 10-day weather forecast for Halle (Saale) indicates temperatures of above 20 °C and a low probability of precipitation during the conference. Sounds good. Consider bringing your swimsuit :-)

### **Welcome Reception**

An informal welcome reception will take place on Sunday evening, 18:00 – 20:00, in the “Stadthaus” (*Marktplatz 2*). There, we offer sparkling wine, orange juice, and pretzels to all participants which already have arrived (*included in the conference fee*).

### **WLAN**

In both the Audimax (*where the lectures and coffee breaks take place*) and the Melanchthonianum (*where the poster sessions are located*) you can use WLAN to access the internet. You can either use Eduroam or our conference network. For the latter, connect to the network “event-net”, open your web browser, and enter user name “stc2018@uni-halle.de” and password “atxt2o3Z”. Please note that the conference network is not encrypted and should not be used for sensitive data.

## 2. Program

### 2.1. Venue

The conference venue of the STC 2018 is located directly in the city center of Halle (Saale):

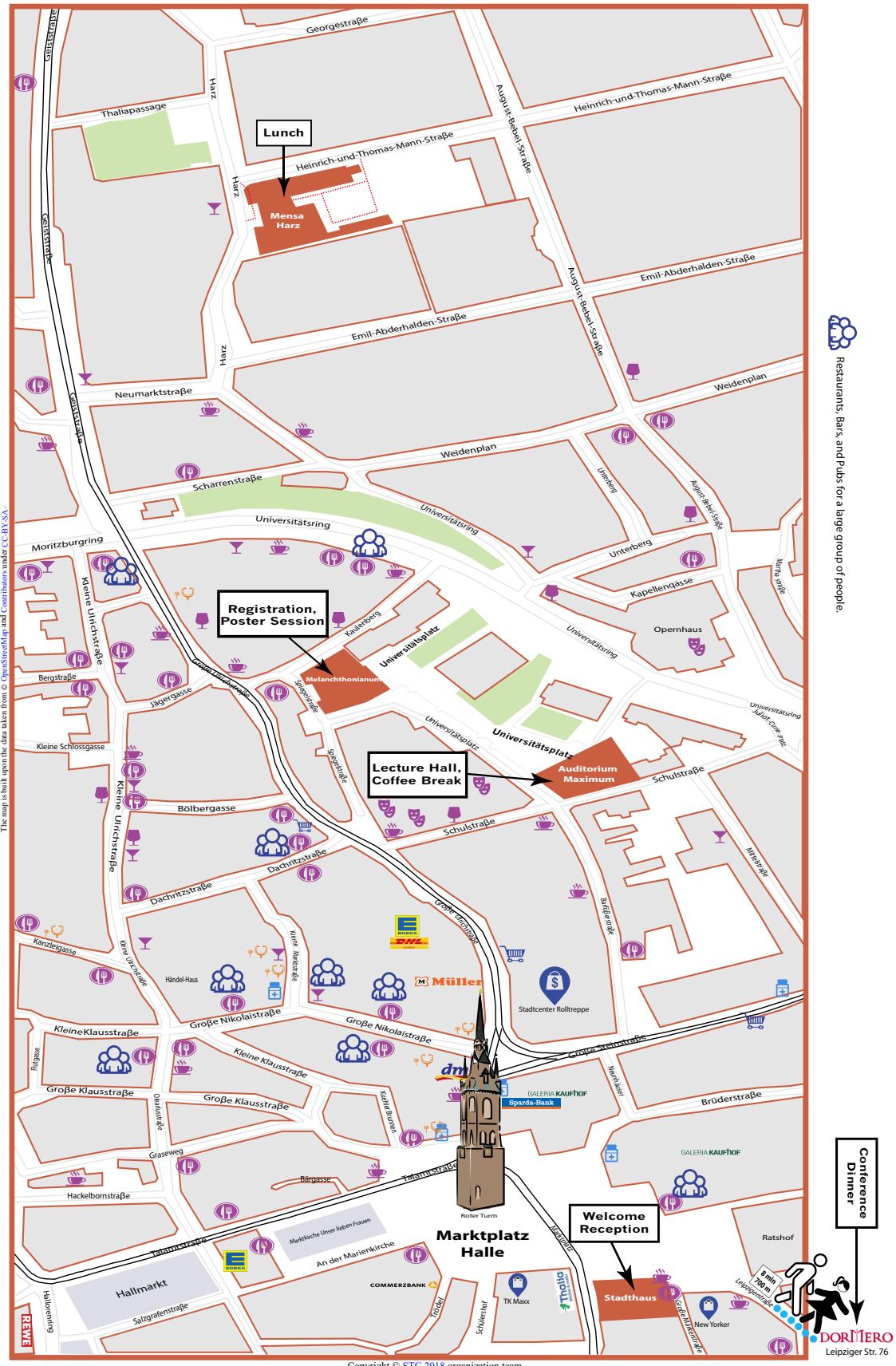
- The **lectures** and **coffee breaks** will take place in the “Auditorium Maximum” (“Audimax”, *Universitätsplatz 1*).
- The **registration** and **poster sessions** will take place in the “Melanchthonianum”, which is directly opposite to the Auditorium Maximum (*Universitätsplatz 9, room „Medienraum“*). There, also the **conference desk** can be found, which is continuously staffed from 15:00 to 20:00 on Sunday, from 9:00 to 18:00 on Monday till Wednesday, and from 9:00 till 14:00 on Thursday.
- The informal **welcome reception** on Sunday evening will take place in the “Stadthaus Halle” (*Marktplatz 2*).
- You will receive **lunch vouchers** for the “Harzmensa”, which is located a few hundred meters north of the conference venue (*Harz 41*).
- The **conference dinner** will be located in the “Dormero Hotel Rotes Ross” (*Leipziger Straße 76*).

The map on the next page shows these places. There, also some restaurants and bars which are suitable for large groups of people are suggested.

You can find an interactive map on our conference homepage (section “Location & Travel”), where the above locations are highlighted by markers.

<https://stc2018.de/>

## 2. Program



## 2.2. Schedule

Time	Sunday 16.9.	Monday 17.9.	Tuesday 18.9.	Wednesday 19.9.	Thursday 20.9.
08:50 - 09:00		Opening			
09:00 - 09:40		I1 P. Jungwirth	Hellmann Award	I7 R. Mata	I10 G. Hummer
09:40 - 10:00		C1 J. P. Götze	Hückel Award	C21 J. M. Westermayr	C27 A. Bande
10:00 - 10:20		C2 M. Wolter		C22 C. Wiebelner	C28 D. Picconi
10:20 - 10:50		Coffee Break	Coffee Break & "Sekt-Empfang"	Coffee Break	Coffee Break
10:50 - 11:10		I2 L. A. Nafie	C10 T. Jagau	I8	C29 F. Pauly
11:10 - 11:30			C11 P. Pinski	R. Vuilleumier	C30 F. A. Bischoff
11:30 - 11:50		C3 D. Sidler	C12 M. Roemelt	C23 I. Barth	C31 D. Golze
11:50 - 12:10		C4 M. Springborg	C13 S. Stopkowicz	C24 H. Elgabarty	C32 D. R. Rehn
12:10 - 12:50		Lunch Break	Lunch Break	Lunch Break	I11 A. Krylov
12:50 - 13:10					Closing / Poster Prize
13:10 - 13:40					
13:40 - 14:20		I3 R. Ludwig	I5 M. Sulpizi	I9 T. Kühne	
14:20 - 14:40		C5 H. Bahmann	C14 G. Gryn'ova	C25 E. Caldeweyher	
14:40 - 15:00		C6 B. Hartke	C15 R. H. Henchman	C26 T. Weymuth	
15:00 - 15:30	Registration	Coffee Break	Coffee Break	Excursions	
15:30 - 15:50		I4 D. Andrienko	I6 M. Thoss		
15:50 - 16:10		C7 M. Hellström	C16 J.-M. Mewes		
16:10 - 16:30		C8 J. George	C17 W. Quapp		
16:30 - 16:50		C9 R. Tonner	Coffee Break		
16:50 - 17:10		Coffee Break	C18 J. Wilhelm		
17:10 - 17:20			C19 G. Berghold		
17:20 - 17:40		Poster Slam A	C20 A. Blume		
17:40 - 18:00	Welcome Reception		Poster Slam B		
18:00 - 18:10	AGTC Meeting		Conference Dinner		
18:10 - 18:20					
18:20 - 18:50	Poster Session A (odd numbers)	Poster Session B (even numbers)			
18:50 - 19:00					
19:00 - 20:00					
20:00 - 22:00					
22:00 - 23:00					

## 2. Program

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The author names are links to the list of participants. The contribution numbers and titles are links to the book of abstracts. Click to jump to the corresponding sections.

### Sunday, 16. September 2018

**15:00 – 20:00** Registration (*Melanchthonianum, Universitätsplatz 9*)

**18:00 – 20:00** Welcome Reception (*Stadthaus, Marktplatz 2*)

### Monday, 17. September 2018

Session Chair: Daniel Sebastiani			
<b>8:50 – 9:00</b> Opening			
<b>9:00 – 9:40</b> I1 Pavel Jungwirth			Exploring Solvated Electrons by Explosive as well as Non-Explosive Experiments and Simulations
<b>9:40 – 10:00</b> C1 Jan Philipp Götze			QM/QM Models of a Molecular Mechanism Controlling Photoprotective Quenching in Higher Plants
<b>10:00 – 10:20</b> C2 Mario Wolter			Improved Partitioning of Biomolecules for Quantum-Chemical Embedding Calculations Based on Graph Theory

**10:20 – 10:50** Coffee Break

Session Chair: Daniel Sebastiani			
<b>10:50 – 11:30</b> I2 Laurence Nafie			Chirality and Electron Transition Current Density in Molecular Vibrations: VCD and ROA
<b>11:30 – 11:50</b> C3 Dominik Sidler			Beyond Rosenfeld Equation: Computation of Vibrational Circular Dichroism Spectra for Anisotropic Solutions
<b>11:50 – 12:10</b> C4 Michael Springborg			On the Theoretical Optimization of Properties

**12:10 – 13:40** Lunch Break

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<b>Session Chair:</b> Pavel Jungwirth			
<b>13:40 – 14:20</b>	<b>I3</b>	<b>Ralf Ludwig</b>	Competing Interactions in Ionic Liquids: When Cooperative Hydrogen Bonding Overcomes Coulomb Repulsion Between Ions of Like Charge
<b>14:20 – 14:40</b>	<b>C5</b>	Hilke Bahmann	Hybrid Exchange Density Functionals within the Local Range Separation Scheme
<b>14:40 – 15:00</b>	<b>C6</b>	Bernd Hartke	Global Geometry Optimization of Molecular Assemblies on Surfaces

**15:00 – 15:30 Coffee Break**

<b>Session Chair:</b> Pavel Jungwirth			
<b>15:30 – 16:10</b>	<b>I4</b>	<b>Denis Andrienko</b>	Molecular Understanding of Organic-organic Interfaces and Mixtures
<b>16:10 – 16:30</b>	<b>C7</b>	Matti Hellström	Proton Transfer Mechanisms in Basic Solutions and at the Oxide/Water Interface Revealed by Neural Networks
<b>16:30 – 16:50</b>	<b>C8</b>	Janine George	Ab Initio Anisotropic Displacement Parameters of Molecular Crystals
<b>16:50 – 17:10</b>	<b>C9</b>	Ralf Tonner	Strain and Non-covalent Interactions as Driving Forces for Surface Reactivity

**17:10 – 17:40 Coffee Break**

<b>17:40 – 18:10</b>	<b>Poster Slam A</b>
<b>18:10 – 18:50</b>	<b>AGTC Meeting</b>

**19:00 – 22:00 Poster Session A (odd numbers)**

## 2. Program

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### Tuesday, 18. September 2018

Session Chairs: Leticia González & Christian Ochsenfeld		
9:00 – 9:40	Hellmann Award	
9:40 – 10:20	Hückel Award	

10:20 – 10:50 Coffee Break & “Sekt-Empfang”

Session Chair: Ricardo Mata		
10:50 – 11:10	C10	Thomas Jagau
		Coupled-Cluster Treatment of Molecular Strong-Field Ionization
11:10 – 11:30	C11	Peter Pinski
		Analytical Gradient for a Pair Natural Orbital-based Local MP2 Method, and for Faster Double-hybrid Density Functional Geometry Optimizations
11:30 – 11:50	C12	Michael Roemelt
		On the Importance of Choosing an Adequate Active Space for Large-Scale Multireference Calculations
11:50 – 12:10	C13	Stella Stopkowicz
		Closed-shell Paramagnetism Revisited: A Low-field Effect Due to a Strong-field Three-state Avoided Crossing

12:10 – 13:40 Lunch Break

Session Chair: Ralf Ludwig		
13:40 – 14:20	I5	Marialore Sulpizi
		Water at Interfaces: Structure and Vibrational Spectroscopy from ab initio Simulations
14:20 – 14:40	C14	Ganna Gryn'ova
		Conceptual Framework of Molecular Electronics
14:40 – 15:00	C15	Richard Henchman
		Hierarchical Method to Determine the Entropy of Molecular Systems

15:00 – 15:30 Coffee Break

<b>Session Chair:</b> Ralf Ludwig			
<b>15:30 – 16:10</b>	I6	<b>Michael Thoss</b>	Electron Transport in Molecular Junctions
<b>16:10 – 16:30</b>	C16	Jan-Michael Mewes	Twist and Shine: Organic TADF Emerges from the Interplay of Non-covalent Interactions, Triplet-exciton Delocalization, and Post Franck-Condon Effects
<b>16:30 – 16:50</b>	C17	Wolfgang Quapp	Simple Models for Mechanochemistry

**16:50 – 17:20 Coffee Break**

<b>Session Chair:</b> Daniel Sebastiani			
<b>17:20 – 17:40</b>	C18	Jan Wilhelm	Applying Quantum Chemistry to Reactivity in the Condensed Phase
<b>17:40 – 18:00</b>	C19	Gerd Berghold	Digital Finance at Deutsche Bahn AG
<b>18:00 – 18:20</b>	C20	Alfred Blume	History of Chemistry in Halle
<b>18:20 – 18:50</b>	<b>Poster Slam B</b>		

**19:00 – 22:00 Poster Session B (even numbers)**

## Wednesday, 19. September 2018

<b>Session Chair:</b> Michael Thoss			
<b>9:00 – 9:40</b>	I7	<b>Ricardo Mata</b>	Non-covalent Interactions: from Gas Phase Benchmarks to Communication in Enzymes
<b>9:40 – 10:00</b>	C21	Julia Maria Westermayr	Neural Networks Trained on Ab-initio Data for Executing Surface Hopping Molecular Dynamics
<b>10:00 – 10:20</b>	C22	Christian Wiebeler	Structural Basis of the Red/Green Spectral Tuning in the Cyanobacteriochrome Slr1393

**10:20 – 10:50 Coffee Break**

## 2. Program

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Session Chair: Michael Thoss			
10:50 – 11:30	I8	Rodolphe Vuilleumier	Vibrational Circular Dichroism Spectra From First-Principle Molecular Dynamics Simulations
11:30 – 11:50	C23	Ingo Barth	Non-zero Electron Current Densities for the Vibrating Hydrogen Molecular Ion in a Single Electronic Born-Oppenheimer Ground State
11:50 – 12:10	C24	Hossam Elgabarty	The Mechanism of Overhauser Dynamical Nuclear Polarization in Insulating Solids

**12:10 – 13:40** Lunch Break

Session Chair: Anna Krylov			
13:40 – 14:20	I9	Thomas Kühne	Teaching New Tricks to an Old Dog to Quantify the Degree of Covalency of Hydrogen Bonding
14:20 – 14:40	C25	Eike Caldeweyher	DFT-D4: An Accurate and Generally Applicable Tight-binding Based Dispersion Correction for Density Functional Theory
14:40 – 15:00	C26	Thomas Weymuth	Statistical Analysis of Semiclassical Dispersion Corrections

**15:00 – 19:00** Excursions

**19:00 – 23:00** Conference Dinner (*Dormero Hotel “Rotes Ross”, Leipziger Straße 76*)

Please note:

- You will need your name badge to enter.
- The food is for free.
- Standard drinks (beer, wine, softdrinks) are free from 19:00 to 22:00. Starting from 22:00, all drinks have to be paid.

## Thursday, 20. September 2018

<b>Session Chair:</b> Thomas Kühne			
<b>9:00 – 9:40</b>	<b>I10</b>	<b>Gerhard Hummer</b>	Molecular simulations of lipid membrane sensing
<b>9:40 – 10:00</b>	<b>C27</b>	<b>Annika Bande</b>	Can You Do More? – Yes! Quantum Dot Inter-Coulombic Decay with Three Electrons
<b>10:00 – 10:20</b>	<b>C28</b>	<b>David Picconi</b>	Photodynamics and Spectroscopy of Halogens Embedded in Rare Gas Solids. Quantum Dynamical Description of the I <sub>2</sub> :Kr system

**10:20 – 10:50 Coffee Break**

<b>Session Chair:</b> Thomas Kühne			
<b>10:50 – 11:10</b>	<b>C29</b>	<b>Fabian Pauly</b>	Robust Periodic Fock Exchange with Atom-centered Gaussian Basis Sets
<b>11:10 – 11:30</b>	<b>C30</b>	<b>Florian Bischoff</b>	The Accurate Computation of Molecular Properties Using Multiresolution Analysis
<b>11:30 – 11:50</b>	<b>C31</b>	<b>Dorothea Golze</b>	Accurate Core-level Spectra from GW: An Efficient Approach within a Localized Basis
<b>11:50 – 12:10</b>	<b>C32</b>	<b>Dirk Rehn</b>	Inelastic X-ray scattering amplitudes in the ADC/ISR framework
<b>12:10 – 12:50</b>	<b>I11</b>	<b>Anna Krylov</b>	Solvent Effects in Core- and Valence-level Photoionization Spectroscopy

**12:50 – 13:10 Closing & Poster Prize**

## 2.3. Excursions

On Wednesday afternoon, we offer the following excursions to participants of our conference. All of these excursions are fully covered by the conference fee (*no additional cost*). The sign-in to the excursions will be managed at the conference desk. Please pick one single “excursion ticket” at registration time.

- **Visit to “Leopoldina”**

Founded in 1652, the Leopoldina is the oldest scientific learned society in Germany, and even the oldest continuously existing national science academy of the world. We offer a guided tour through the building.

- **Visit to “Landesmuseum für Vorgeschichte”**

The State Museum of Prehistory in Halle (Saale) is the archaeological museum of the German state of Saxony-Anhalt. Its collection, comprising more than 15 million items, is among the most extensive and important in Germany. We offer a guided tour through the museum.

- **Visit to “Franckesche Stiftungen”**

The Francke Foundations (Franckesche Stiftungen) were founded in 1695 as a Christian, social and educational work by August Hermann Francke. Francke Foundations are today a modern educational cosmos closely connected with their history. The Francke Foundations are on the German proposal list as a UNESCO World Heritage Site since 1999. We offer a guided tour through the foundations.

- **Guided city tour**

Within 2 hours, a good survey of the historical city and the related facts is given.

- **Hike along the Saale river with a view over Halle**

The hike will have a length of around 5 km, and will lead over a hill directly at the Saale river, from where you will have a view over Halle. The Hike ends at the “Peißenitzhaus” (*Peißenitzinsel 4*), where a picnic at the Saale shore is anticipated (depending on the weather). Probably you can buy some food and drinks at the Peißenitzhaus, but it is better to bring your own stuff. It is another 2 km walk from Peißenitzhaus back to the conference venue.

On our conference homepage, you will find internet links with additional information to some of these locations (see section “Program” and scroll down to “Excursions”):

<https://stc2018.de/>

### **3. List of Talks / Posters**

#### **3.1. List of Invited Talks**

The author names are links to the list of participants. The contribution numbers and titles are links to the book of abstracts. Click to jump to the corresponding sections.

I1	Jungwirth, P.	Exploring Solvated Electrons by Explosive as well as Non-Explosive Experiments and Simulations
I2	Nafie, L.	Chirality and Electron Transition Current Density in Molecular Vibrations: VCD and ROA
I3	Ludwig, R.; Knorr, A.; Niemann, T.; Neumann, J.; Paschek, D.	Competing Interactions in Ionic Liquids: When Cooperative Hydrogen Bonding Overcomes Coulomb Repulsion Between Ions of Like Charge
I4	Andrienko, D.	Molecular Understanding of Organic-organic Interfaces and Mixtures
I5	Sulpizi, M.	Water at Interfaces: Structure and Vibrational Spectroscopy from ab initio Simulations
I6	Thoss, M.	Electron Transport in Molecular Junctions
I7	Mata, R.	Non-covalent Interactions: from Gas Phase Benchmarks to Communication in Enzymes
I8	Vuilleumier, R.; Scherrer, A.; Jähnigen, S.; Sebastiani, D.	Vibrational Circular Dichroism Spectra From First-Principle Molecular Dynamics Simulations
I9	Kühne, T.	Teaching New Tricks to an Old Dog to Quantify the Degree of Covalency of Hydrogen Bonding
I10	Hummer, G.	Molecular simulations of lipid membrane sensing
I11	Krylov, A.	Solvent Effects in Core- and Valence-level Photoionization Spectroscopy

## 3.2. List of Contributed Talks

The author names are links to the list of participants. The contribution numbers and titles are links to the book of abstracts. Click to jump to the corresponding sections.

C1	Götze, J. P.; Ostroumov, E. E.; Reus, M.; Holzwarth, A. R.	QM/QM Models of a Molecular Mechanism Controlling Photoprotective Quenching in Higher Plants
C2	Wolter, M.; Looz, M. V.; Meyerhenke, H.; Jacob, C. R.	Improved Partitioning of Biomolecules for Quantum-Chemical Embedding Calculations Based on Graph Theory
C3	Sidler, D.; Bleiziffer, P.; Riniker, S.	Beyond Rosenfeld Equation: Computation of Vibrational Circular Dichroism Spectra for Anisotropic Solutions
C4	Springborg, M.	On the Theoretical Optimization of Properties
C5	Bahmann, H.; Klawohn, S.	Hybrid Exchange Density Functionals within the Local Range Separation Scheme
C6	Hartke, B.; Freibert, A.; Dieterich, J. M.	Global Geometry Optimization of Molecular Assemblies on Surfaces
C7	Hellström, M.; Quaranta, V.; Behler, J.	Proton Transfer Mechanisms in Basic Solutions and at the Oxide/Water Interface Revealed by Neural Networks
C8	George, J.; Englert, U.; Dronskowski, R.	Ab Initio Anisotropic Displacement Parameters of Molecular Crystals
C9	Tonner, R.; Pecher, L.	Strain and Non-covalent Interactions as Driving Forces for Surface Reactivity
C10	Jagau, T.	Coupled-Cluster Treatment of Molecular Strong-Field Ionization
C11	Pinski, P.; Neese, F.	Analytical Gradient for a Pair Natural Orbital-based Local MP2 Method, and for Faster Double-hybrid Density Functional Geometry Optimizations

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C12	Roemelt, M.; Khedkar, A.; Krewald, V.; Pantazis, D.	On the Importance of Choosing an Adequate Active Space for Large-Scale Multireference Calculations
C13	Stopkowicz, S.; Borgoo, A. B.; Hampe, F. H.; Tellgren, E. I. T.; Klopper, W. K.; Gauss, J. G.; Teale, A. M. T.; Helgaker, T. H.	Closed-shell Paramagnetism Revisited: A Low-field Effect Due to a Strong-field Three-state Avoided Crossing
C14	Gryn'ova, G.; Corminboeuf, C.	Conceptual Framework of Molecular Electronics
C15	Henchman, R.; Higham, J.; Chakravorty, A.; Gräter, F.	Hierarchical Method to Determine the Entropy of Molecular Systems
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C23	Barth, I.; Renziehausen, K.; AlBaraghtheh, T.	Non-zero Electron Current Densities for the Vibrating Hydrogen Molecular Ion in a Single Electronic Born-Oppenheimer Ground State

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