

# TIMETABLE

(invited talks: 40 min, contributed talks: 20 min)

	<b>Sunday</b> <i>August 25</i>	<b>Monday</b> <i>August 26</i>	<b>Tuesday</b> <i>August 27</i>	<b>Wednesday</b> <i>August 28</i>	<b>Thursday</b> <i>August 29</i>
<b>Morning Session</b> <i>9:00 – 12:05</i>		<i>I1: Clark</i> <i>C2: Di Donato</i> <i>C3: Furché</i> <i>Coffee</i> <i>I2: Scuseria</i> <i>C4: Lüchow</i>	<i>I6: Hellmann</i> <i>Lecture</i> <i>I7: Mukamel</i> <i>Coffee</i> <i>I8: Saalfrank</i> <i>C8: Paulus</i>	<i>I9: Nitzan</i> <i>C9: Koch</i> <i>C10: Kaupp</i> <i>Coffee</i> <i>I10: de Vivie-Riedle</i> <i>C11: Kühn</i>	<i>I13: Drummond</i> <i>I14: Großmann</i>  <i>Coffee</i> <i>I15: Pollak</i> <i>C15: Käb</i>
<i>12:10 – 14:00</i>			<i>Lunch</i>		
<b>Afternoon Session</b> <i>14:00 – 18:00</i>	Registration starting 15:00	<i>I3: Rösch</i> <i>I4: Koslowski</i> <i>Coffee</i> <i>I5: May</i> <i>C5: Elstner</i> <i>C6: Frank</i> <i>C7: Mladenović</i>	Excursion Free afternoon	<i>I11: Ernsting</i> <i>C12: Dreuw</i> <i>C13: Sommerfeld</i> <i>Coffee</i> <i>I12: Rötthlisberger</i> <i>C14: Seifert</i> Meeting AGTC	End of conference Departure
<i>18:00 – 20:00</i>		<i>Dinner</i>			
<b>Evening Session</b> <i>20:00 – 22:00</i>	<i>C0: Schreiber</i> <i>C1: Helfrich</i>	<b>Poster session I</b> (even numbers)	BBQ Dinner starting 19:00	<b>Poster session II</b> (odd numbers)	

# SYMPOSIUM PROGRAMME

## Sunday, 25 August

- 15:00      *Start of registration*
- 18:00      *Dinner*
- 20:00      *C0*: Michael Schreiber (International University Bremen):  
– 20:30 IUB – A challenging alternative to public universities
- 20:30      *C1*: Klaus Helfrich (Technische Universität Berlin):  
– 21:00 Wigner and the Technical University of Berlin -  
Wigner and Theoretical Chemistry
- 21:00      *Get Together*

## Monday, 26 August

### Morning session

- Chair: Werner Jakubetz**
- 8:50      Gerhard Haerendel (Dean, School of Engineering and Science IUB):  
– 9:00      Opening
- 9:00      *I1*: Thomas Herz, Daniel Barthel, Timothy Clark  
(Universität Erlangen-Nürnberg):  
– 9:40      Semiempirical CI calculations on electron-transfer in proteins
- 9:45      *C2*: Mariangela Di Donato and Andrea Peluso  
(Università di Salerno, Baronissi):  
– 10:05      Electron transfer between quinones in photosynthetic reaction centers
- 10:10      *C3*: Philipp Furche (Universität Karlsruhe):  
– 10:30      Photoinduced charge transfer in DMABN: exploring excited  
potential energy surfaces by TDDFT
- 10:35      *Coffee break*
- Chair: Christoph van Wüllen**
- 11:00      *I2*: Gustavo E. Scuseria (Rice University, Houston):  
– 11:40      Linear scaling quantum chemistry methods for periodic systems:  
Applications to polymers, surfaces, and solids
- 11:45      *C4*: Sebastian Manten and Arne Lüchow (Universität Düsseldorf):  
– 12:05      Linear scaling with quantum Monte Carlo
- 12:10      *Lunch break*

## Monday, 26 August

### Afternoon session

Chair: Franz Mark

14:00 *I3*: Notker Rösch (TU München): Quantum chemical  
– 14:40 and molecular dynamics modeling of charge transfer in DNA

14:45 *I4*: Thorsten Koslowski (Universität Freiburg):  
– 15:25 Variational approach to the energetics of electron transfer  
reactions: molecules, condensed matter and biopolymers

15:30 *Coffee break*

Chair: Bernd Hess

16:00 *I5*: Volkhard May (HU Berlin):  
– 16:40 External field control of electron transfer processes

16:45 *C5*: Markus Elstner (Universität Paderborn):  
– 17:05 An approximate DFT Method for QM/MM  
simulations of biomolecular structures and processes

17:10 *C6*: Christel Nonnenberg and Irmgard Frank (LMU München):  
– 17:30 Reactions in the rocket propellant MMH + NTO  
on a picosecond time scale: CPMD simulation

17:35 *C7*: Mirjana Mladenović (Universität Göttingen):  
– 17:55 Tetratomic molecules: From theory to algorithms  
and their application

18:00 *Dinner*

### Evening session

20:00  
– 22:00 Poster session I (even numbers)

## Tuesday, 27 August

### Morning session

Chair: Gernot Frenking

- 9:00 *Award ceremony:* Fritz Schaumann (President of IUB),  
– 9:05 Walter Thiel (AGTC): Hellmann award
- 9:05 *I6* N.N. (Recipient of the Hellmann award 2002):  
– 9:45 Hellmann lecture
- 9:45 *I7* Shaul Mukamel (University of Rochester):  
– 10:25 Multidimensional infrared coherent spectroscopies of peptides
- 10:30 *Conference photo and coffee break*
- Chair: Gerhard Stock
- 11:00 *I8* Peter Saalfrank (Universität Regensburg):  
– 11:40 Theory of (field-driven electron) dynamics at interfaces
- 11:45 *C8* Beate Paulus (MPI-PKS Dresden):  
– 12:05 Ab-initio electron correlation calculation for metals
- 12:10 *Lunch break*

14:00 Free afternoon

Possible excursions:

- train ride to the city center of Bremen (starting at 14:10 from the front gate of IUB or 14:26 from Schönebeck station) or 15:00 in front of the main station: three different guided tours (up to 30 people each, one in English), tickets sold at the conference office until Monday evening
- trip to the artists village Worpswede (private cars, self-organized)
- bike tour (there is the possibility to rent some bikes on campus), tickets sold at the conference office until Monday evening
- walk to Bremen-Vegesack and the sailing ship Deutschland

19:00 *Barbeque dinner*

## Wednesday, 28 August

### Morning session

Chair: Jörn Manz

9:00 *I9* Michael Galperin, Abraham Nitzan, Uri Peskin (Tel Aviv Uni.):  
– 9:40 Inelastic effects in electron transmission through water

9:45 *C9* Christiane P. Koch, Thorsten Klüner, Hans-Joachim Freund  
– 10:05 and Ronnie Kosloff (Fritz-Haber-Institut, Berlin)  
Charge transfer in condensed phase with a Surrogate Hamiltonian

10:10 *C10* Martin Kaupp (Universität Würzburg):  
– 10:30 Quantum chemical insight into the function of photosystem I

10:35 *Coffee break*

Chair: Stefan Grimme

11:00 *I10* Regina de Vivie-Riedle (MPI für Quantenoptik, Garching):  
– 11:40 Coherent control of molecular systems: Reaction dynamics,  
quantum computer, molecular BEC

11:45 *C11* Oliver Kühn (FU Berlin):  
– 12:05 Dynamics and spectroscopy of intramolecular hydrogen bonds  
in the condensed phase

12:10 *Lunch break*

### Afternoon session

Chair: Christel Marian

14:00 *I11* S.A. Kovalenko, J.L. Peres-Lustres, N.P. Ernsting (HU Berlin):  
– 14:40 Symmetry breakage upon photoinduced electron transfer in  
bianthryl in solution: new experimental results and interpretation

14:45 *C12* Andreas Dreuw, Barry D. Dunietz  
– 15:05 and Martin Head-Gordon (Lawrence Berkeley National Lab.):  
Characterization of the relevant excited states  
in the photodissociation process of CO ligated Myoglobin

15:10 *C13* Thomas Sommerfeld (Universität Heidelberg):  
– 15:30 Coupling between dipole-bound and valence states:  
Nitromethane as a prototype

15:35 *Coffee break*

Chair: Peter Botschwina

16:00 *I12* Ursula Röthlisberger (EPFL Lausanne):  
– 16:40 QM/MM Car-Parrinello simulations of photoreactions in proteins

16:45 *C14* Gotthard Seifert and Gerd Fischer (TU Dresden):  
– 17:05 Molecular dynamics simulation of formation of  
hydrocarbon molecules in interstellar space

17:15 Meeting: Mitgliederversammlung der AG Theoretische Chemie

18:00 *Dinner*

## Wednesday, 28 August

### Evening session

20:00  
– 22:00 Poster session II (odd numbers)

## Thursday, 29 August

### Morning session

Chair: Joachim Reinhold

9:00 *I13* Peter D. Drummond (University of Queensland, Brisbane):  
– 9:40 Superchemistry

9:45 *I14* Frank Grossmann, Rafael Gutierrez,  
– 10:25 and Rüdiger Schmidt (TU Dresden):  
Electronic transport calculations for real systems on the nanoscale

10:30 *Coffee break*

Chair: Bernd Hartke

11:00 *I15* Eli Pollak (Weizmann Institute, Rehovot):  
– 11:40 Theory of photoinduced polyatomic reactions

11:45 *C15* Günter Käß, Oliver Henrich and Gert D. Billing  
– 12:05 (MPI für Biophysikalische Chemie) :  
Semiclassical dynamics of large molecular systems

12:10 Concluding remarks

12:15 *Lunch*

14:00 End of conference; Departure

In case of several authors, the presenting author is underlined.  
The affiliation included in parentheses refers to this author.