

Timetable

AW: Award, CT: Contributed Talk, IS: Invited Speaker, IT: Invited Talk.

last updated: 02/09/2022

Sunday, 18th of September

15:00–18:00	Registration	
18:00–19:00	IT	Lorenz Cederbaum Heidelberg University Evening Lecture
from 19:00	Welcoming Reception	

Monday, 19th of September

	Chair: Vera Krewald		
9:00–9:40	IS	Patrick Norman KTH Royal Institute of Technology	Liouville-space response theory in the self-consistent field approximation
09:40–10:00	CT	Tim Neudecker University of Bremen	Simulating Molecules Under Hydrostatic Pressure
10:00–10:20	CT	Greta Heydenrych Wiley	Chemistry Europe: Open Access and DORA
10:30–11:00	Coffee Break		
	Chair: Christoph van Wüllen		
11:00–11:40	IS	Shirin Faraji ¹ University of Groningen	On-the-fly hybrid quantum/classical dynamics simulations of excited-state processes in complex environments
11:40–12:00	CT	Lena Bäuml Ludwig-Maximilians-University Munich	Observing the nuclear and electronic wavepacket dynamics in uracil via simulated X-ray absorption spectra
12:00–12:20	CT	Patrick Zobel University of Vienna	Simulating and Screening Photophysics of Transition-Metal Complexes
12:30–14:00	Lunch Break		

The program continues on the next page.

¹Chemistry Europe Lecturer

Monday, 19th of September

	Chair: Bernd Engels		
14:00–14:40	IS	Benjamin Helmich-Paris Max-Planck-Institute for Coal Research	CASSCF Methods for Ground- and Excited States: How the Hessian May Help You
14:40–15:30	AW	Hückel Award	
15:30–16:00	Coffee Break		
	Chair: Carolin König		
16:00–16:40	IS	Alicia Palacios Universidad Autónoma de Madrid	XUV and X-Ray induced ultrafast electron dynamics in atoms and molecules
16:40–17:00	CT	Richard Beckmann Ruhr University Bochum	The Effect of Helium Microsolvation on Structure and Structural Correlation of Protonated Acetylene
17:00–17:20	CT	Arne Lüchow RWTH Aachen University	Many-Electron Probability Density Analysis as Tool for Analysis of Chemical Bonding
from 18:00	Poster Session		

Tuesday, 20th of September

		Chair: Peter Saalfrank	
9:00–9:40	AW	Hellmann Award	
9:40–10:30	AW	Peyerimhoff Award	
10:30–11:00		Coffee Break	
		Chair: Axel Groß	
11:00–11:40	IS	Martin Head-Gordon University of Berkeley	
11:40–12:00	CT	Maren Podewitz TU Vienna	Building Better Models to Uncover The Reaction Dynamics of A Supramolecular Cu-calix[8]arene Catalyst with QM/MM MD
12:00–12:20	CT	James Green Goethe-University Frankfurt	Solvent Effects on Ultrafast Charge Transfer Population: Insights from the Quantum Dynamics of Guanine-Cytosine in Chloroform
12:30–14:00		Lunch Break	
14:00–18:00		Social Activities	
from 18:00		Conference Dinner Party	

Wednesday, 21st of September

	Chair: Wim Klopper		
9:00–9:40	IS	Irene Burghardt Goethe University Frankfurt	Quantum Dynamical Simulations of Coherent Excitonic Processes and 2D Electronic Spectroscopy of Functional Organic Polymer Materials
9:40–10:00	CT	Thomas Schnappinger Albanova University Centre, Stockholm University	A non-adiabatic dynamics perspective on strongly coupled molecule-cavity systems
10:00–10:20	CT	Johann Mattiat University of Zurich	Spectroscopic simulations with real-time TDDFT – linear response and gauge dependence
10:30–11:00	Coffee Break		
	Chair: Oliver Kühn		
11:00–11:40	IS	Spiridoula Matsika Temple University	Theoretical description of nonadiabatic events in photon and electron driven processes
11:40–11:00	CT	Christoph Bannwarth RWTH Aachen	Approaching Photochemistry with Low-Cost Electronic Structure Theory
11:00–11:20	CT	Joern Manz Freie Universität Berlin	Effects of Nuclear Spins on Quantum Dynamics and Symmetry: A Case Study for Molecular Boron Rotors
12:30–14:00	Lunch Break		

The program continues on the next page.

Wednesday, 21st of September

		Chair: Leticia Gonzalez	
14:00–14:40	IS	Todd Martinez Stanford University	Reaction Discovery for Ground and Excited States
14:40–15:00	CT	Denis Artiukhin Freie Universität Berlin	The Frozen-Density Embedding Diabatization Scheme: Recent Progress and New Directions
15:00–15:20	CT	Mickael Delcey KTH Royal Institute of Technology	Multiconfigurational simulations of X-ray spectra of transition metals
15:30–16:00	Coffee Break		
		Chair: Tonner-Zech	
16:00–16:40	IS	Fabien Gatti University of Paris-Saclay	Quantum Dynamics with motions of large amplitude
16:40–17:00	CT	Anna Skitnevskaya Heidelberg University	Nonlocal electronic decay processes: the role of donor-acceptor interactions
17:00–17:20	AGTC Meeting		
from 18:00	Poster Session		

Thursday, 22nd of September

	Chair: Doreen Mollenhauer		
9:00–9:40	IS	Philipp Marquetand University of Vienna	Machine learning and beyond – from ground-state wave functions to excited-state dynamics
9:40–10:00	CT	Jan-Michael Mewes University of Bonn	ROKS/PCM for the description of charge-transfer states in solution: Faster, more accurate, and more robust than TD-DFT
10:00–10:20	CT	Rhiannon Zarotiadis ETH Zurich	A nonadiabatic generalised-dividing-surface (NGD) instanton rate theory
10:30–11:00	Coffee Break		
	Chair: Beate Paulus		
11:00–11:40	IS	Henrik Larsson University of California	Tensor network states for computing vibrational and electronic states
11:40–12:00	CT	Christoph Schran University of Cambridge	Understanding complex aqueous systems with machine learning
12:00–12:20	CT	Caio O. da Silva Federal University of ABC (UFABC)	Newton's Method for Hartree–Fock: Lagrange and Riemann
from 12:30	Departure		