

Time	Monday, March 31	Time	Tuesday, April 1	Time	Wednesday, April 2	Time	Thursday, April 3
	Boat departing at 9:00		Boat departing at 9:00		Boat departing at 9:00		
9:20	Welcome						
9:30	Ivo Leito, University of Tartu Acidic and superacidic molecules: design and acidity measurements	9:30	Herbert Mayr, LMU München Nucleophilicity versus Lewis Basicity: The Role of Intrinsic Barriers	9:30	Michael Groll, TUM München Protein Crystallography at the Intersection of Chemistry and Biology	9:30	Bern Kohler, Montana State University On the Road to Nowhere: The Ultrafast Events that Inhibit DNA Photodamage
10:20	Amir Hoveyda, Boston College Design of Selective Catalytic Cycles that are Fuelled by a Proton	10:20	Jeremy Harvey, University of Bristol Structure and Reactivity in Organic Chemistry: Insights from Electronic Structure Theory	10:20	Marc Fontecave, Collège de France, Paris tRNA modification: new enzyme mechanisms	10:20	AK Zacharias DNA damage recognition studied by Molecular Dynamics Simulations
11:10	coffee break	11:10	coffee break	11:10	coffee break	10:40	AK Herres-Pawlis Hiking on the potential energy surface of a functional tyrosinase model
11:40	AK Knochel Key dynamic features for organometallic synthesis	11:40	short presentation of posters II	11:40	AK Carell Mechanisms of DNA and RNA base modifications	11:00	AK Bein Dynamics and Inclusion Chemistry in Mesoporous Channel Systems
12:00	AK Ochsenfeld Quantum-chemical insights into the repair process of oxidative DNA damages			12:00	AK Zinth DNA - from Photophysics to Photochemistry	11:20	closing remarks
	Lunch 12:20-14:20		Lunch 12:20-14:20		Lunch 12:20-14:20		
14:20	Walter Thiel, MPI für Kohlenforschung Surface-hopping excited-state dynamics	14:20	Josef Wachtveitl, Universität Frankfurt Triggering molecular processes with light	14:30	Mitgliederversammlung		
15:10	AK Trauner Photochemical Formation of Intricarene: Experiment	15:10	AK Riedle Increasing the benzhydryl cation yield by a delayed second light pulse	15:30	AK Zipse Radicals in Enzymatic Catalysis		
15:30	AK de Vivie-Riedle Photochemical Formation of Intricarene: Theory	15:30	AK Kiefhaber Dynamic heterogeneity in native proteins as a mechanism to control	15:50	AK Schneider Targeting structured RNA- elements: expressed cyclic		

			protein function		peptides as selective inhibitors for Protein-RNA interactions		
15:50	coffee break	15:50	coffee break	16:10	coffee break		
16:20	AK Sieber Small molecules as tools to determine enzyme active site dynamics	16:30	AK Dube Hemithioindigo - a toolbox for photoswitches	16:40	AK Mathias Simulation of proteins in dielectric solvent continua by a Hamiltonian reaction field dynamics		
16:40	AK Tavan The Microscopic Physical Cause for the Density Maximum of Liquid Water	16:50 - 18:50	Poster Session	17:00	AK Antes Computational investigation of the energetics of protein-ligand binding		
17:00	short presentation of posters I						