Les Houches Workshop:

Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems

3 - 8 September 2023

Monday 4 September 2023

07:45-08:45	Breakfast
09:00-09:20	Welcome & introduction
	Chair: J. Léonard
09:20-10:00	**T. Brixner**
	Electrochemical, chirality-sensitive, single-molecule, and higher-order ultrafast spectroscopies
10:00-10:20	**T. Renger**
	Quantification of short-range effects in the special pair of photosystem II reaction centers:
	The non-conservative nature of the circular dichroism spectrum
10:20-10:50	Coffee break
10:50-11:30	**T. Kramer**
	Tracking electronic coherence with time- and frequency resolved spectroscopy:
	The HEOM approach
11:30-12:10	**J. Hauer**
	Isolating pure donor and acceptor signals by polarization-controlled transient
	absorption spectroscopy
12:30	Lunch
13:30-17:00	Free time
	Chair: T. Renger
17:00-17:40	**S. Mukamel**
	Novel ultrafast probes of elementary molecular events using X-ray pulses, quantum light,
	and optical cavities
17:40-18:20	**Y. Tanimura**
	Numerically “exact” simulations of a quantum Carnot cycle:
	Analysis using thermodynamic work diagrams
18:20-19:00	**P. Malý**
	Multi-excitonic probes of coherent to diffusive dynamics
19:00	Reception
19:30	Dinner
	Chair: D. Picconi
20:50-21:10	**J. Seibt**
	Theoretical investigations on 2D electronic spectroscopy of ”Water Soluble
	Chlorophyll-Binding Protein” (WSCP)
21:10-21:30	**R. Rouxel**
	Light-harvesting processes in green sulfur bacteria in vivo
21:30-21:50	**F. Sanda**
	2D line-shape analysis of fifth order signals
21:50-22:10	**L. Bolzonello**
	Photoelectrochemical detection in 2D electronic spectroscopy of Photosystem I:
	What do we really gain? What can we optimize?

Tuesday 5 September 2023

07:45-08:45	Breakfast
	Chair: J. Hauer
09:00-09:40	**E. Bittner**
	Looking under the hood and unraveling dark processes in excitonic systems
09:40-10:20	**A. De Sio**
	Field-driven exciton Rabi oscillations in functional materials
10:20-10:50	Coffee break
10:50-11:30	**O. Johansson**
	Towards optical control of the magnetic anisotropy in single-molecule magnets
11:30-12:10	**Y. Kurashige**
	Molecular mechanism of SCO in Fe complexes and methods in non-adiabatic molecular dynamics
12:30	Lunch
13:30-16:00	Free time
16:00-17:00	Poster session I
	Chair: I. Burghardt
17:00-17:40	**J. Cao**
	Quantum diffusion in organic materials: Disorder, phonons, and photons
17:40-18:20	**R. Hildner**
	Energy Transport in Supramolecular (Super-)Structures with Tailored Excited-State Energy Landscapes
18:20-19:00	**C. Silva**
	Many-body exciton-polariton quantum dynamics in Ruddlesden-Popper metal halide optical microcavities
19:30	Dinner
	Chair: T. Kramer
20:50-21:10	**L. Joubert-Doriol**
	Light-matter interaction in natural conditions: Estimating timescales in the nonequilibrium steady state
21:10-21:30	**A. Sarmah**
	Rational design of photo-active optical switches and molecular motors for the quantum energy devices
21:30-21:50	**F. Di Maiolo**
	Inverted singlet-triplet emitters: The path towards highly efficient OLEDs
21:50-22:10	**J. Green**
	Charge transfer symmetry breaking and singlet fission: Solvent and vibrational effects

Wednesday 6 September 2023

07:45-08:45	Breakfast
	Chair: P. Malý
09:00-09:40	**M. Delor**
	Imaging and controlling ballistic polarons and polaritons
09:40-10:20	**G. Groenhof**
	Photochemistry in the collective strong coupling regime: Insights from multi-scale molecular dynamics simulations
10:20-10:50	Coffee break

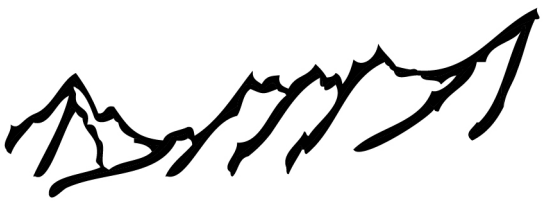
10:50-11:30	**L. van Wilderen** Vibrational pre-excitation enables new applications in photochemistry
11:30-12:10	**M. Joffre** Multiscale vibrational spectroscopy in Fatty Acid Photodecarboxylase from picoseconds to microseconds
12:30	Lunch
13:30-19:30	Free afternoon
19:30	Dinner
	Chair: J. Krich
20:50-21:10	**J. van Thor** Coherence structure from non-linear optical crystallography and coherent control of ultrafast structural dynamics with femtosecond X-ray crystallography
21:10-21:30	**O. Kornilov** Electronic structure and excited state reactions of aqueous aminoazobenzenes studied by time-resolved XUV photoelectron spectroscopy
21:30-21:50	**J. Léonard** Revealing the exciton diffusion coefficient from exciton-exciton annihilation kinetics in efficient light-harvesting nanoparticles
21:50-22:10	**I. Burghardt** Quantum dynamical simulations of coherent diffusive exciton transport in organic polymer materials

Thursday 7 September 2023

07:45-08:45	Breakfast
	Chair: O. Kornilov
09:00-09:40	**E. Collini** Coherent dynamics in solutions of colloidal plexcitonic nanohybrids at room temperature
09:40-10:20	**A. Ishizaki** Probing exciton dynamics with spectral selectivity through the use of quantum entangled photons
10:20-10:50	Coffee break
10:50-11:30	**M. Chergui** Non-linear Extreme Ultraviolet to hard X-ray spectroscopy
11:30-12:10	**J. Krich** New spectroscopic pathways: Information content and interpretation of high order transient absorption spectroscopy
12:30	Lunch
13:30-16:00	Free time
16:00-17:00	Poster session II
	Chair: D. Coker
17:00-17:40	**R. Borrelli** Hierarchical equation of motions in tensor train format and their application to complex vibronic systems
17:40-18:20	**S. Jang** Theories of exciton and charge transfer based on Fermi's golden rule and beyond
18:20-19:00	**D. Picconi** Photophysics, photochemistry and spectroscopy using high-dimensional quantum wave packets
19:30	Workshop dinner

Friday 8 September 2023

07:45-08:45	Breakfast
	Chair: T. Renger
09:00-09:40	**D. Coker**
	Vibronic dynamics in light harvesting
09:40-10:20	**D. Zigmantas**
	Exposing vibronic mixing in chlorophylls
10:20-10:50	Coffee break
10:50-11:10	**D. Brey**
	Intra-chain exciton dynamics in conjugated polymers: Reduced-dimensional quantum dynamics and computation of 2DES signals
11:10-11:30	**E. Carnio**
	Quantized fields for optimal control in the strong coupling regime
11:30-11:50	**F. Camargo**
	Ultrafast transient holography: pump-probe microscopy goes widefield
11:50-12:10	**Y. M. Rhee**
	Early stage photodynamics of photoactive yellow protein simulated: The role of hydrogen bonding environment
12:10	Closing remarks
12:30	Lunch
	Departure



Organizers: **Jessica Anna** (University of Pennsylvania, USA)
Irene Burghardt (Goethe University Frankfurt, Germany)
Jeff Cina (University of Oregon, USA)
Jérémie Léonard (University of Strasbourg, France)
Thomas Renger (University of Linz, Austria)
Young Min Rhee (KAIST, South Korea)