

# Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems

3-7 May 2021 – Online Les Houches Workshop

## Monday 3 May 2021

- 09:45-10:00 Welcome & introduction  
*Chair: J. Léonard*
- 10:00-10:40 **M. Chergui**  
Spin cross-over dynamics in photoexcited haem proteins
- 10:40-11:20 **O. Johansson**  
Observation of coherent wavepacket along the Jahn-Teller axis in a Mn-based single molecule magnet
- 11:20-12:00 **S. K. Min**  
Development of theoretical/computational tools for excited state molecular dynamics
- 12:00-14:00 Break  
*Chair: I. Burghardt*
- 14:00-14:25 **O. Kornilov**  
Electronic relaxation of aqueous aminoazobenzenes studied by time-resolved photoelectron spectroscopy and surface hopping TDDFT dynamics calculations
- 14:25-14:50 **F. Remacle**  
Quantum parallelism by coherent excitonic dynamics of an ensemble of CdSe quantum dots with size dispersion
- 14:50-15:15 **S. Haacke**  
Femtosecond vibrational coherence spectroscopy reveals excited branching in Fe(II)-NHC complexes for photo-sensitizing applications
- 15:15-15:45 **SSP 1: G. Karras, V. Brenner, O. Kefer**
- 15:45-16:00 **Discussion**
- 16:00-17:00 Break  
*Chair: J. Anna*
- 17:00-17:40 **B. Curchod**  
In silico photochemical experiments with Non-Born-Oppenheimer Molecular Dynamics
- 17:40-18:20 **D. McCamant**  
Femtosecond Stimulated Raman Spectroscopy as a Test of Theoretical Predictions of Excited-State Structural Changes
- 18:20-19:00 **A. De Sio**  
Light-induced ultrafast coherent exciton-phonon dynamics in functional materials

## Tuesday 4 May 2021

- Chair: Y. M. Rhee*
- 10:00-10:40 **T. Joo**  
Role of coherent nuclear motions in ultrafast processes in liquid by time-resolved spectroscopies and molecular dynamics simulation
- 10:40-11:20 **Y. Zhao**  
The Hierarchical Stochastic Schrödinger Equations: Theory and Application
- 11:20-12:00 **J. C. Tremblay**  
Light-driven electron dynamics in molecules and nanostructures

- 12:00-17:00 Break  
*Chair: D. Picconi*
- 17:00-17:40 **J. Asbury**  
Separation and Trapping of Triplet Pair Intermediates in Amorphous Singlet Fission Materials Measured with Ultrafast Infrared Spectroscopy
- 17:40-18:20 **R. Frontiera**  
Probing singlet fission and exciton transport with femtosecond stimulated Raman spectro-microscopy
- 18:20-19:00 **J. Krich**  
Efficient and fast prediction of ultrafast spectroscopies
- 19:00-20:00 Break  
*Chair: J. Cina*
- 20:00-21:10 **SSP 2: A. Dunnett, J. Runeson, M. Erakovic, D. Romanin, A. Klinger, J. Green, F. Di Maiolo**
- 21:10-22:00 **Discussion**

## Wednesday 5 May 2021

- Chair: B. Blasiak*
- 10:00-10:25 **X. Sun**  
Photoinduced Charge Transfer Dynamics via Semiclassical Methods
- 10:25-10:50 **D. Gorelova**  
Imaging electron currents in molecules and clusters with ultrafast resonant x-ray scattering
- 10:50-11:15 **J. Fregoni**  
Controlling photochemical reactions through strong light-molecule coupling
- 11:15-11:45 **SSP 3: K. H. Cho, H. W. Kim, A. Paz**
- 11:45-12:00 **Discussion**
- 12:00-14:00 Break  
*Chair: T. Renger*
- 14:00-15:10 **SSP 4: H. Masood, M. Horz, J. Mannouch, M. Papai, M. Reuner, J. Léonard, I. Burghardt**
- 15:10-16:00 **Discussion**
- 16:00-17:00 Break  
*Chair: A. De Sio*
- 17:00-17:40 **A. Olaya-Castro**  
Vibronic quantum dynamics and coherence in light-harvesting systems
- 17:40-18:20 **J. Ogilvie**  
Multispectral multidimensional spectroscopy studies of excitonic structure and charge separation in the Heliobacterial Reaction Center
- 18:20-19:00 **I. Rivalta**  
Hunting Electronic States in Two-Dimensional Electronic Spectra
- 19:00-20:00 Break  
*Chair: J. Anna, T. Renger*
- 20:00-22:00 **Discussion**

## Thursday 6 May 2021

- Chair: J. C. Tremblay*
- 10:00-10:40 **F. Lépine**  
UV induced femtosecond and attosecond dynamics in 2D and 3D carbon-based molecular structures
- 10:40-11:20 **D. Picconi**  
Molecular photodynamics and its manifestation in UV-Vis and X-ray time-resolved spectra: Insights from quantum chemistry and quantum dynamics
- 11:20-12:00 **M. Vacher**  
Light-matter interactions: from ab initio molecular dynamics and machine learning to x-ray spectroscopy
- 12:00-17:00 Break
- Chair: E. Thyryhaug*
- 17:00-17:40 **L. Huang**  
Exciton transport in molecular aggregates imaged by ultrafast microscopy
- 17:40-18:20 **I. Schapiro**  
Insight into the Spectral Tuning and Photoisomerization of Proteorhodopsin
- 18:20-19:00 **J. Yuen-Zhou**  
Optical spectroscopy of molecular polaritons
- 19:00-20:00 Break
- Chair: B. Curchod*
- 20:00-20:25 **G. Levi**  
Exploring excited-state and solvation dynamics through multi-scale atomistic simulations
- 20:25-20:50 **D. Lindorfer**  
Non-conservative circular dichroism of photosystem II reaction centers: Is there an enhancement by a coupling with charge transfer states?
- 20:50-21:15 **S. Cavaletto**  
Monitoring molecular coherences by time-resolved x-ray Raman spectroscopy and diffraction with stochastic free-electron-laser pulses
- 21:15-21:45 **SSP 5: V. Freixas, A. Hanes, O. Carrillo-Bohórquez**
- 21:45-22:00 **Discussion**

## Friday 7 May 2021

- Chair: Y. M. Rhee*
- 10:00-10:25 **W. Glover**  
UV Photoresponse of the Green Fluorescent Protein Chromophore
- 10:25-10:50 **M. Hervé**  
Controlled Ultrafast Charge Transfer Dynamics in Peptides with Tailored Micro-environment
- 10:50-11:15 **I. Navizet**  
Modelling absorption and emission spectra taking into account the dynamic environment: example of firefly bioluminescent systems
- 11:15-11:45 **SSP 6: X. Li, D. Brey, Z. Shen**
- 11:45-12:00 **Discussion**
- 12:00-14:00 Break

*Chair: J. Léonard*

- 14:00-14:40 **E. Collini**  
How the environment can tune the energy, the coupling, and the ultrafast dynamics of interacting chromophores: the effect of hydrogen-bonds
- 14:40-15:20 **T. Kramer**  
Finding good polarization sequences for tracking dynamics in 2DES with HEOM and machine learning
- 15:20-16:00 **E. Thyryhaug**  
Exciton Dynamics in Biological Rings
- 16:00-17:00 **Discussion**



**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)