

Quantum Dynamics and Spectroscopy of Functional Molecular Materials and Biological Photosystems

21-26 May 2017

École de Physique des Houches

Monday

- 07:45-08:45 Breakfast
Chair: J. Anna
- 09:00-09:40 Welcome & introduction
Chair: J. Anna
- 09:40-10:20 **S. Haacke**
Ultrafast Spectroscopy of Functional Molecular Materials and Biological Photosystems: Some Case Studies
- 10:20-10:50 Coffee break
- 10:50-11:30 **M. Cho**
Two-dimensional Electronic Spectroscopy of Surface Plasmonic Resonance Modes of Gold Nanorods and Intraband Transitions of Colloidal Quantum Dots
- 11:30-12:10 **T. Pullerits**
Coherent Multidimensional Action Spectroscopy
- 12:30 Lunch
- 13:30-17:00 Free time
Chair: J. Bredenbeck
- 17:00-17:40 **E. J. Heller**
Checks and Balances: The Chemical Physics Mindset in Condensed Matter Spectroscopy
- 17:40-18:20 **A. B. McCoy**
Using Diffusion Monte Carlo to Decode Signatures of Large Amplitude Motion in Molecules and Ions
- 18:20-19:00 **Y. Tanimura**
Multi-state Quantum Hierarchical Fokker-Planck Equation Approach to Photoisomerization Processes
- 19:00 Reception
- 19:30 Dinner
Chair: J. Wachtveitl
- 20:50-21:10 **J. Hummert**
Isomerization of Azo Dyes Investigated by Time-Resolved Photoelectron Spectroscopy in Solution
- 21:10-21:30 **M. Mayes**
Towards Understanding the Molecular Structures and Interactions of Aromatic Dipeptide Nanotubes
- 21:30-21:10 **O. Johansson**
Directly Probing Femtosecond Spin Dynamics in a Molecular Magnet

Tuesday

- 07:45-08:45 Breakfast
Chair: J. Cina
- 09:00-09:40 **C. Fang**
Tuning Ultrafast Raman to Watch Chemical Reactions in Solution: New Insights for Biological and Materials Sciences

- 09:40-10:20 **A. Bragg**
Structural (Dis)Order and Charge Separation in Conjugated Molecular Materials
- 10:20-10:50 Coffee break
- 10:50-11:30 **M. Elstner**
QM/MM Simulations of Electron/Exciton Transfer Reactions
- 11:30-12:10 **H. Tamura**
Charge and Exciton Dynamics in Organic Photovoltaics and Singlet Fission
- 12:30 Lunch
- 13:30-16:00 Free time
- 16:00-17:00 Poster session I
Chair: J. Hauer
- 17:00-17:40 **J. Anna**
Two-Dimensional Electronic Spectroscopy of Photosystem I and Light-Harvesting Chromophores
- 17:40-18:20 **T. Renger**
Structure-Based Theory of Light-Harvesting in Photosystem II
- 18:20-19:00 **D. Zigmantas**
Coherence Shift Mechanism for Long-Lived Coherences
- 19:30 Dinner
Chair: O. Johansson
- 20:50-21:10 **L. Wang**
Imaging Ultrafast Carrier Dynamics of Two-Dimensional Materials by Femtosecond Time-Resolved Photoemission Electron Microscopy
- 21:10-21:30 **A. Sevink**
Molecular Dynamics Simulations Reveal Intrinsic Curvature Formation in Chlorosomes
- 21:30-21:50 **J. Cerezo**
Developing Accurate Molecular Mechanics Force Fields for Photosystems: A First Step Towards Reliable Hybrid QM/MM Simulations

Wednesday

- 07:45-08:45 Breakfast
Chair: M. Mayes
- 09:00-09:40 **M. Chergui**
Ultrafast Charge Carrier Dynamics in Solar Materials: Multidimensional Deep-UV Spectroscopies and Core-Level Spectroscopies
- 09:40-10:20 **K. Ohmori**
Ultrafast Many-Body Electron Dynamics in a Strongly Correlated Ultracold Rydberg Gas
- 10:20-10:50 Coffee break
- 10:50-11:30 **B. Mennucci**
Modeling Linear and Nonlinear Optical Spectra of Multichromophoric Biosystems: A Multiscale Strategy
- 11:30-12:10 **J. Cao**
Quantum Coherence in Light-Harvesting Systems and Organic Semiconductors
- 12:30 Lunch
- 13:30-17:00 Free afternoon & excursion
- 19:30 Dinner

- Chair: Y. M. Rhee*
- 20:50-21:10 **L. Bolzonello**
Novel Analysis of 2DES Data: The Example of TPPS J-Aggregates
- 21:10-21:30 **J. Cina**
Mixed Quantum/Semiclassical Simulations of Ultrafast Spectroscopy Signals
- 21:30-21:50 **I. Burghardt**
High-Dimensional Quantum Dynamics of Exciton Migration and Dissociation in Polymeric J- and H-Aggregates

Thursday

- 07:45-08:45 Breakfast
- Chair: A. Bragg*
- 09:00-09:40 **S. Mukamel**
Probing Electronic Coherence in Conical Intersections by Stimulated X-Ray Raman Spectroscopy
- 09:40-10:20 **D. Egorova**
Detection of Conical Intersections via Coherence in Time-Resolved Signals
- 10:20-10:50 Coffee break
- 10:50-11:30 **P. Foster**
Nonadiabatic Eigenfunctions Can Have Conical Nodes
- 11:30-12:10 **J. Hauer**
The Functional Roles of Vibronic Coupling in Carotenoids
- 12:30 Lunch
- 13:30-16:00 Free time
- 16:00-17:00 Poster session II
- Chair: T. Renger*
- 17:00-17:40 **D. Coker**
First Principles Models for Biological Light-harvesting: Phycobiliprotein Complexes from Cryptophyte Algae
- 17:40-18:20 **U. Kleinekathöfer**
Mixed Quantum-Classical Simulations to Study Exciton and Charge Transfer: Applications to Light Harvesting and Molecular Wires
- 18:20-19:00 **S. Jang**
Optimality of Light Harvesting 2 (LH2) Complex and its Mutants as Exciton Carriers and Hidden Effects of Hydrogen Bonding
- 19:30 Workshop Dinner

Friday

- 07:45-08:45 Breakfast
- Chair: P. Foster*
- 09:00-09:40 **J. Bredenbeck**
Subensemble-Selective Photochemistry by Mixed IR/VIS Two-Dimensional Spectroscopy
- 09:40-10:20 **W. J. Buma**
High-Resolution Laser Spectroscopy of Photoactive Materials: Light on the Dark Side of the Force

10:20-10:50 Coffee break
11:30-12:10 **J. Wachtveitl**
Photomodulation of Electronic and Vibrational Communication in Molecular Dyads
10:50-11:30 **Y. M. Rhee**
Realizing "Ab Initio" Spectroscopy: Dreaming a Realistic Dream
12:10-12:30 Concluding Remarks
12:30 Lunch
Departure



Organizers: Irene Burghardt (Goethe University Frankfurt), Jeff Cina (University of Oregon)