Topical school
"MOLECULAR PHOTOCHEMISTRY"

Auditorium IPCMS, May 23rd-25th 2022

Program *at-a-glance*

Topical School on Molecular Photochemistry					
May 23rd	**Basic concepts in photochemistry**	***May 24th***	**Techniques**	***May 25th***	**Advanced topics and applications**
8h35-10h05	Electronic structure of molecules (V. Robert)	*8h30-9h15*	Fluorimetry (M. Mauro)	*8h30-9h15*	Ultrafast photophysics involved in natural photosynthesis (J. Leonard)
10h05 - 10h30	*coffee break*				
10h30-11h30	Introduction to molecular photochemistry (M. Mauro)	*9h15-10h00*	Time-resolved techniques (M. Mauro)	*9h15-10h45*	Artificial photosynthesis and photocatalysis (A. Aukauloo)
		10h-10h30	*coffee break*	*10h45-11h15*	*coffee break*
11h30-12h15	Elements of photophysics: absorption and emission spectra (S. Haacke)	*10h30-11h15*	Polarisation effects (A. Barsella)	*11h15-12h15*	Light-emitting materials and devices (M. Mauro)
12h15-13h30	*lunch break (not included)*			*12h15-13h45*	*lunch break (not included)*
13h30-14h30	Elements of photophysics: energy and electron transfer (S. Haacke)	*11h15-12h45*	Chiroptical techniques (L. Di Bari)	*13h45-15h15*	Electrochemiluminescence (F. Polo)
		12h45-14h	*lunch break (not included)*		
14h30-15h15	Photochromic compounds (G. Ragazzon)	*14h-15h15*	Transient and ultrafast techniques: experimental femtochemistry (J. Leonard)	*15h15-16h*	Light-driven molecular machines (G. Ragazzon)
15h15-15h45	*coffee break*	*15h15-15h45*	*coffee break*	*16h-16h30*	*coffee break*
15h45-16h45	Non-linear optical phenomena (A. Barsella)	*15h45-16h45*	Computational Photochemistry part II (C. Daniel)	*16h30-17h30*	Questions&Answers session
16h45-17h45	Computational Photochemistry part I (C. Daniel)	*16h45-17h45*	Single molecule fluorescence microscopy (P. Didier)		

Syllabus

Monday May 23th Basic concepts in photochemistry

8:30 – 8:35 Welcome address and general information

Dr. Matteo Mauro (ICPMS-DMO, Université de Strasbourg & CNRS)

8:35 – 10:05 Electronic structure of molecules

Pr. Vincent Robert (LCQ, Institut de Chimie, Université de Strasbourg & CNRS)

Hamiltonian model: Huckel; from Atomic Orbitals to Molecular Obitals; exact Hamiltonian: wavefunction structure; electron-electron correlation; Hartree Fock and beyond HF; ground state, excited states.

10:05– 10:30 coffee break

10:30 – 11:30 **Introduction to molecular photochemistry**

Dr. Matteo Mauro (ICPMS-DMO, Université de Strasbourg & CNRS)

Photochemical and photophysical processes; intramolecular vs. intermolecular processes; spin states; Born-Oppenheimer approximation; Fermi Golden rule; Frank-Condon factor; Jablonski diagram; radiative and non-radiative processes; Kasha-Vavilov rule; Stokes shift; relationship between oscillator strength and epsilon; fluorescence vs. phosphorescence; Lambert-Beer law and its deviations; photoluminescence quantum yield.

11:30 – 12:15 **Elements of photophysics: absorption and emission spectra**

Pr. Stefan Haacke (ICPMS-DON, Université de Strasbourg & CNRS)

"Quantum size effect" (coherence length & lambda_max); spectral line shapes of absorption /emission spectra as a result of vibronic eigenstates, (Franck-Condon factors). Selection rules; breaking the selection rules (vibronic coupling, spin-orbit coupling, El-Sayed rule); mirror image symmetry; effects of environment (polarity, H-bonding) on absorption and emission spectra. Strickler-Berg relationship, radiative rate, fluorescence quantum yield.

12:15 – 13:30 **lunch break** (not included)

13:30 – 14:30 **Elements of photophysics: energy and electron transfer**

Pr. Stefan Haacke (ICPMS-DON, Université de Strasbourg & CNRS)

Introduction to bimolecular quenching processes: static vs dynamic quenching, Stern-Volmer equation; Fermi's Golden Rule & FRET, transition dipole moment coupling, resonance effect through spectral overlap. Förster radius. Dexter energy transfer. Electron transfer as described by Marcus theory, driving force and re-organization energy, regular and inverted regimes, experimental demos.

14:30 – 15:15 **Photochromic compounds**

Dr. Giulio Ragazzon (ISIS, Université de Strasbourg & CNRS)

Excited state processes leading to isomerization; P-type photochromes (e.g. Diarylethene); T-type photochromes (e.g. azobenzene); photoacids; isomerization quantum yield; photostationary states; chemical actinometry; industrial applications of photochromes

15:15 – 15:45 **coffee break**

15:45 – 16:45 **Non-linear optical phenomena**

Dr. Alberto Barsella (IPCMS-DON, Université de Strasbourg & CNRS)

Introduction to the nonlinear optics considering the non linear polarization from the molecule to the materials; various examples will be treated in order to give a very first approach of different nonlinear

optical phenomena and the conditions required for their observation; harmonics generation; soliton; two photon absorption.

16:45 – 17:45 **Computational photochemistry (part I)**

Dr. Chantal Daniel (LCQ, Institut de Chimie, Université de Strasbourg & CNRS)

This course is an introduction to the computation of molecular electronic excited state properties and to the simulation of their reactivity and ultrafast decay. The first session will be dedicated to a static view: i) the quantum chemical methods, more specifically adapted to the calculation of electronic excited state properties, namely their transition energies, oscillator strengths and characters; ii) the concept of multi-dimensional potential energy surfaces associated to electronic excited states; iii) the photoreactivity and concurrent deactivation pathways.

Tuesday May 24th Spectroscopy and microscopy techniques

8:30 – 9:15 **Fluorimetry**

Dr. Matteo Mauro (ICPMS-DMO, Université de Strasbourg & CNRS)

Spectrophotometry; fluorimetry: steady state vs. time-resolved techniques. Instrumental aspects such as detectors sensitivity, spectral corrections, monochromators and second-order transmission; filter effects, deviations from linearity; Photoluminescence quantum yield and its determination methods;

9:15 – 10:00 **Time-resolved techniques**

Dr. Matteo Mauro (ICPMS-DMO, Université de Strasbourg & CNRS)

Time vs. phase domain, principles of Time-Correlated Single Photon Counting (TCSPC) method; Multi-Channel Scaling (MCS); detectors (single-photon PMT, SPAD, streak camera); instrumental response function; fitting methods (mono vs. multi-exponential decays).

10:00 – 10:30 **coffee break**

10:30 – 11:15 **Polarization effects**

Dr. Alberto Barsella (IPCMS-DON, Université de Strasbourg & CNRS)

The polarization of light will considered from a phenomenological point of view. Different polarization-related phenomena will be described and examples of applications will be given. Polarization of light; linear polarization; circular polarization; linear dichroism; circular dichroism; birefringence; control of light polarization; electrooptic effect; Faraday effect.

11:15 – 12:45 **Chiroptical techniques**

Pr. Lorenzo di Bari (Department of Chemistry, Università di Pisa, Italy)

Electronic Circular Dichroism (ECD) and Circularly Polarized Luminescence (CPL); ECD: local chirality and exciton coupling; how to "read" an ECD spectrum; molecular and supramolecular ECD; very brief overview on approaches to absolute configurations with chiroptical methods; ECD of solid-state samples: crystals and films; ECD imaging; anisotropy of ECD and joint effect of linear birefringence and linear dichroism; the LDLB effect and apparent non reciprocity; CPL of organic molecules: isolated chromophores, interacting chromophores and excimers; CPL of lanthanide compounds and brief overview of d-metal systems; applications in polarization-sensitive optoelectronic devices.

12:45 – 14:00 **lunch break** (not included)

14:00 – 15:15 **Transient and ultrafast techniques: experimental femtochemistry**

Dr. Jérémie Léonard (IPCMS-DON, Université de Strasbourg & CNRS)

Ultrafast fluorescence and absorption spectroscopies; introduction to femtochemistry: vibrational dynamics and photochemistry beyond the Born-Oppenheimer approximation.

15:15 – 15:45 **coffee break**

15:45 – 16:45 **Computational photochemistry (part II)**

Dr. Chantal Daniel (LCQ, Institut de Chimie, Université de Strasbourg & CNRS)

The second session will address a dynamical view: i) wavepacket propagation on potential energy surfaces; ii) coupling between electronic and nuclear vibrational motion beyond the Born-Oppenheimer approximation; iii) ultrafast decay (ps-fs time scale).

16:45 – 17:45 **Single molecule fluorescence microscopy**

Pr. Pascal Didier (Faculté de Pharmacie, Université de Strasbourg & CNRS)

Optical microscopy (contrast, resolution); fluorescence microscopy, labeling strategies, confocal and widefield geometries; characterizing bio-molecular interactions at the single molecule level (fluorescence correlation spectroscopy, Förster energy transfer); overcoming the diffraction limit.

Wednesday May 25th Accounts on advanced topics and applications

8:30 – 9:15 **Ultrafast photophysics involved in natural photosynthesis**

Dr. Jérémie Léonard (IPCMS-DON, Université de Strasbourg & CNRS)

Ultrafast energy and electron transfers as observed in natural light-harvesting complexes and in the reaction center: photophysical concepts and experimental evidence.

9:15 – 10:45 **Artificial photosynthesis and photocatalysis**

Pr. Ally Aukauloo (ICMMO, Université Paris-Saclay)

*Photosynthesis is the process that uses sunlight as sole energy input to flush carbon dioxide (CO_2) from our atmosphere and convert it into a chemical energy vector. Chemists worldwide are devoting much effort to develop advanced materials that can capture light to activate and transform very stable molecules i.e., water and carbon dioxide, the key ingredients, into energy rich molecules. I will discuss on the three aspects of **C**apturing photons, **C**onverting them into a chemical potential and performing multi-electron **C**atalysis, the three **C**s of Artificial Photosynthesis research.*

10:45 – 11:15 **coffee break**

11:15 – 12:15 **Light-emitting materials and devices**

Dr. Matteo Mauro (ICPMS-DMO, Université de Strasbourg & CNRS)

Exciton types and their generation; Organic Light-Emitting Diodes: working principles and materials requirements; fluorescent vs. phosphorescent vs. TADF vs. hyperfluorecence; Light-emitting Electrochemical Cell: working principle and materials requirements; selected literature examples (Alq_3, metal complexes and SOC management), TADF.

12:15 – 13:45 **lunch break** (not included)

13:45 – 15:15 **Electrochemiluminescence**

Pr. Federico Polo (DMSN, Università di Venezia Ca' Foscari, Italy)

The electrochemical activation of suitable molecules or ions can generate species that undergo sufficiently exergonic electron-transfer reactions to form excited state species (emitters) capable of causing luminescence. This fascinating phenomenon is known as electrogenerated chemiluminescence or electrochemiluminescence (ECL). The aim of the seminar is to provide students the basic knowledge of the main electrochemical techniques employed to trigger and investigating ECL: cyclic voltammetry, chronoamperometry. Radical ion formation at the electrodes and the luminescence produced by annihilation reactions between radical cations and anions will be investigated to understand how ECL is triggered. Singlet and triplet state formation will be briefly discussed with some examples (e.g. metal complexes, organic molecules).

15:15 – 16:00 **Light-driven molecular machines**

Dr. Giulio Ragazzon (ISIS, Université de Strasbourg & CNRS)

Light-controlled natural molecular machines; concept of directed motion; stepwise actuation; autonomous motors; nano and macro-scale light-driven tasks

16:00 – 16:30 **coffee break**

16:30 – 17:30 **Q&A session and Closing remarks**

General information

The courses will take place in the Auditorium of the *Institut de Physique et Chimie des Matériaux de Strasbourg* (IPCMS), Campus Cronenbourg, following the program displayed above. The campus can be easily reached by public transport, bus line G, stop "Arago".

External participants are required to register at the CNRS reception by going through the main gate entrance, located at the 23 rue du Loess.

Coffee breaks are included during the whole duration of the school. **Lunch breaks are not included**.

PhD students that are enrolled to either the Ecole Doctorale 182 "Physics and Physical Chemistry" or the Ecole Doctorale 222 "Sciences Chimiques" may validate their participation to the Topical School on "Molecular photochemistry" as part of their scientific formations.

For the ED182: if the PhD student has followed the whole duration of the delivered courses, it will be counted as **one scientific formation**. Otherwise, only the exact hours of participation will be counted.

For the ED222: for the validation of the hours, please refer to the following table: *http://ed.chimie.unistra.fr/doctorat/formations-durant-la-these/*

Their participation needs to be signed in the AMETHIS platform. For more information, please contact the secretary of the corresponding Ecole Doctorale.

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