

Conference on the Complex Interactions of Light and Biological Matter: Experiments meet Theory | (smr 3120)

Monday, 21 May 2018

08:30 - 09:00 REGISTRATION & ADMINISTRATIVE FORMALITIES

ATTENTION:

All Participants paid by the ICTP and staying in the ICTP Guesthouses are automatically registered at the time of check-in at the reception desk. Therefore, on Monday morning, please go directly to the Finance Office at the Enrico Fermi Building from 8.30 to 9.00 am, ground floor to collect your expenses. Badges, Passports and Travel Receipts are needed.

Additional Shuttle Bus service will be provided and pick-up available from carpark area at the main entrance of the Adriatico Guest House

Finance office opening times are:

Monday, Tuesday and Friday from 8.30 – 12.00 and 13.30 to 14.30

PLEASE NOTE:

To all Directors/Conference Speakers and to all Participants NOT staying in the ICTP Guesthouses Please register with the Conference Secretary in office no. 1 Adriatico Guest House, lower level 1

Location: As specified above

09:00 - 09:25 Welcome Address & Opening

A. HASSANALI and L. GRISANTI

Time for each talk:

Conference Speakers: 40 mins + 10 mins discussion time

Contributed talks by Participants: 20 mins + 5 mins discussion time

Location: Adriatico Guest House (Kastler Lecture Hall)

09:25 - 14:00 Session 1 - Excited state, photophysics and dynamics of small biological molecules - I

09:25 **New strategies for non-adiabatic dynamics with trajectories 50'**

Speaker: Ivano TAVERNELLI (Zurich Research Laboratory, Switzerland)

Material:  **Abstract - Tavernelli**

10:15 **Coffee break 25'** (AGH Terrace)

10:40 **Nonadiabatic decay of photoexcited nucleobases in water studied by mixed quantum/classical dynamical approaches 50'**

Speaker: Fabrizio SANTORO (ICCOM-CNR, Pisa, Italy)

Material:  **Abstract - Santoro**

11:30 **Study of dynamical observables involved in photoionization process 25'**

Speaker: Aurora PONZI (Ruder Boskovic Institute, Zagreb, Croatia)

Material:  **Abstract - Ponzi**

11:55 **Nuclear quantum effects in an HIV/cancer inhibitor: The case of ellipticine 25'**

Speaker: Subrahmanyam SAPPATI (IISER, Pune, India)

Material:  **Abstract - Sappati**

12:20 **Lunch break 1h40'** (AGH Cafeteria)

14:00 - 16:05 Session 2 - Bio-functional materials, complex living systems and interaction with light - I

- 14:00 **Molecular-self-assembly of peptides, peptide nucleic acids and metabolites into optically active assemblies 50'**
Speaker: Ehud GAZIT (Tel Aviv University, Israel)
Material: [Abstract - Gazit](#)
- 14:50 **Live-cell super-resolution microscopy reveals a primary role for diffusion in polyglutamine aggresome assembly 25'**
Speaker: Meng LU (University of Cambridge, U.K.)
Material: [Abstract - LU](#)
- 15:15 **Assembly of a tripeptide an anti-inflammatory drugs into supramolecular hydrogels for sustained release 25'**
Speaker: Marina KURBASIC (University of Trieste, Italy)
Material: [Abstract - Kurbasic](#)
- 15:40 **Coffee break 25'**
- 16:05 - 17:45 Session 3 - Excitonic behaviours, charge and energy transfer in biological systems - I
- 16:05 **Photoinduced charge transfer processes in oligonucleotides: from base pairs up to DNA duplexes 50'**
Speaker: Roberto IMPROTA (IBB-CNR, Napoli, Italy & Universite' Paris-Saclay, France)
Material: [Abstract - Improta](#)
- 16:55 **Modulating the charge recombination to DNA 50'**
Speaker: Mahesh HARIHARAN (IISER, Kerala, India)
Material: [Abstract - Hariharan](#)
- 18:00 - 19:30 Session 4
- Welcome Drink – outside on Terrace (weather permitting)*

Tuesday, 22 May 2018

- 09:00 - 10:40 Session 5 - Excitonic behaviours, charge and energy transfer in biological systems - II
- 09:00 **Photoinduced symmetry-breaking charge transfer 50'**
Speaker: Eric VAUTHEY (University of Geneva, Switzerland)
Material: [Abstract - Vauthey](#)
- 09:50 **Using fluorescence as a tool for studying biomolecular dynamics 25'**
Speaker: Debjani BAGCHI (University of Baroda, Vadodara, India)
Material: [Abstract - Bagchi](#)
- 10:15 **Coffee break 25'** (AGH Terrace)
- 10:40 - 14:30 Session 6 - Fluorescence and emerging phenomena of biological matter - I
- 10:40 **GFP: a model system for understanding proton transfer, photoisomerization and optogenetics 50'**
Speaker: Steven G. BOXER (Stanford University, U.S.A.)
Material: [Abstract - Boxer](#)
- 11:30 **Ultrafast nonlinear dynamics of the structure-specific fluorescence in protein structures 25'**
Speaker: Giancarlo SOAVI (University of Cambridge, U.K.)
Material: [Abstract - Soavi](#)
- 11:55 **On the optical properties of L-glutamine and pyroglutamic acid 25'**
Speaker: Nawaz QAISRANI MUHAMMAD (ICTP, Trieste, Italy)
Material: [Abstract - Qaisrani Muhammad](#)

12:20 **Lunch break 1h40'**

Free afternoon – Excursion activity

Wednesday, 23 May 2018

- 09:00 - 10:40 Session 7 - Imaging of biological matter, cell, tissues - I
- 09:00 **Organic and hybrid photosensitizers for photodynamic therapy and imaging 50'**
Speaker: Nadia BARBERO (University of Torino, Italy)
Material: [Abstract - Barbero](#)
- 09:50 **Cerium oxide (CeO₂-x) nanoparticles for visualization of redox processes in biological systems 25'**
Speaker: Vladyslav V. SEMINKO (Institute of Scintillation Materials, Kharkiv, Ukraine)
Material: [Abstract - Seminko](#)
- 10:15 **Coffee break 25'** (AGH Terrace)
- 10:40 - 14:00 Session 8 - Photochemistry in biological matter and its building blocks - I
- 10:40 **Mechanistic aspects of solar energy harvesting with organic heterocycles 50'**
Speaker: Wolfgang DOMCKE (Technical University of Munich, Germany)
Material: [Abstract - Domcke](#)
- 11:30 **Photoactivating C-H bonds inside artificial photoenzymes 50'**
Speaker: Jyotishman DASGUPTA (TIFR, Mumbai, India)
Material: [Abstract - Dasgupta](#)
- 12:20 **Lunch break 1h40'** (AGH Cafeteria)
- 14:00 - 16:05 Session 9 - Excited state, photophysics and dynamics of small biological molecules - II
- 14:00 **Exploring nuclear photorelaxation through an integrated ab-initio molecular dynamics and time resolved vibrational analysis approach 50'**
Speaker: Nadia REGA (Universita' degli Studi di Napoli, Italy)
Material: [Abstract - Rega](#)
- 14:50 **Time-dependent DFT investigation of the optical response in biological materials 50'**
Speaker: Yavar TAGHIPOUR AZAR (NSTRI, AEOI, Tehran, Iran)
Material: [Abstract - Taghipour Azar](#)
- 15:40 **GROUP PHOTO - Coffee break 25'** (AGH Terrace)
- 16:05 - 17:45 Session 10 - Advanced linear and non-linear spectroscopies for biological systems - I
- 16:05 **Tunable UV resonant raman spectroscopy at Elettra: a tool for exploring the structural dynamics in biological matter 50'**
Speaker: Barbara ROSSI (Elettra-Sincrotrone, Basovizza, Trieste, Italy)
Material: [Abstract - Rossi](#)
- 16:55 **Raman spectroscopy for the characterization of antimicrobial photodynamic therapy against staphylococcus epidermidis 25'**
Speaker: Taha FATHIAWAD (Red Sea University, Sudan)
Material: [Abstract - Fathi Awad](#)
- 17:20 **Vibrational study of a self-assembling globular protein 25'**
Speaker: Sara CATALINI (LENS, Sesto Fiorentino, Italy)
Material: [Abstract - Catalini](#)
- 18:00 - 19:30 Session 11

Poster Session

Location: outside the Kastler Lecture Hall

Thursday, 24 May 2018

09:00 - 14:00

Session 12 - Excitonic behaviours, charge and energy transfer in biological systems - III

09:00 **Excitonic interactions in biological systems: from the understanding to manipulation** 50'

Speaker: Benedetta MENNUCCI (University of Pisa, Italy)

Material: [Abstract - Mennucci](#)

09:50 **Probing coherence in ultrafast molecular processes: a theoretical perspective** 25'

Speaker: Emanuele COCCIA (Universita' di Padova, Italy)

Material: [Abstract - Coccia](#)

10:15 **Coffee break** 25' (AGH Terrace)

10:40 **Energy transfer and charge separation in a hybrid bio-conjugate bacterial reaction center** 50'

Speaker: Mariangela DI DONATO (LENS, Sesto Fiorentino & INO-CNR, Firenze, Italy)

Material: [Abstract - Di Donato](#)

11:30 **Photoinduced charge transfer transitions in charged amino acids: New label free spectroscopic markers to probe protein structure and dynamics** 50'

Speaker: Ravindra VENKATRAMANI (TIFR, Mumbai, India)

Material: [Abstract - Venkatramani](#)

12:20 **Lunch break** 1h40' (AGH Cafeteria)

14:00 - 16:05

Session 13 - Advanced linear and non-linear spectroscopies for biological systems - II

14:00 **In silico time-resolved infrared spectroscopy of biomolecules in solution** 50'

(presentation given on behalf of Massimiliano ASCHI)

Speaker: Isabella DAIDONE (University of Aquila, Italy)

Material: [Abstract - Daidone](#)

14:50 **Probing low-barrier hydrogen bonds in biologically-relevant systems with low-frequency vibrational spectroscopy and quantum mechanical simulations** 25'

Speaker: Michael T. RUGGIERO (University of Cambridge, U.K. & University of Vermont, U.S.A.)

Material: [Abstract - Ruggiero](#)

15:15 **Chiroptical properties of supramolecular assemblies: a combined experimental and theoretical study** 25'

Speaker: Cristina SISSA (University of Parma, Italy)

Material: [Abstract - Sissa](#)

15:40 **Coffee break** 25' (AGH Terrace)

16:05 - 17:45

Session 14 - Bio-functional materials, complex living systems and interaction with light - II

16:05 **Interfacial structure and hydration of model membranes elucidated with non-linear scattering techniques** 50'

Speaker: Halil I. OKUR (LBP, IMX, STI, LACUS, EPFL, Laussane, Switzerland)

Material: [Abstract - Okur](#)

16:55 **Spectroscopic investigation and theoretical modelling of benzothiadiazole-based charge-transfer chromophores: from solution to nanoaggregates** 25'

Speaker: Brunella BARDI (Universita' degli Studi di Parma, Italy)

Material: [Abstract - Bardi](#)

17:20 **The divergent path of homochiral and heterochiral tripeptides for self-assembly into hydrogels** 25'

Speaker: Ana Maria GARCIA FERNANDEZ (University of Trieste, Italy)

Material: [Abstract - Garcia Fernandez](#)

Friday, 25 May 2018

09:00 - 10:40 Session 15 - Bio-functional materials, complex living systems and interaction with light - III

09:00 **Design of tailored fluorescent colloidal probes using thermodynamically stable nanovesicles as scaffolds 50'**

Speaker: Nora VENTOSA (ICMAB-CSIC, Barcelona, Spain)

Material: [Abstract - Ventosa](#)

09:50 **Luminescent hydrogels: self-assembly of a tripeptide and carbon nanodots 25'**

Speaker: Maria Cristina CRINGOLI (University of Trieste, Italy)

Material: [Abstract - Cringoli](#)

10:15 **Coffee break 25'** (AGH Terrace)

10:40 - 12:30 Session 16 - Excited state, photophysics and dynamics of small biological molecules - III

10:40 **Excited state proton transfer in systems of chemical and biological interest 50'**

Speaker: Nadja DOSLIC (Ruder Boskovic Institute, Zagreb, Croatia)

Material: [Abstract - Doslic](#)

11:30 **Nonadiabatic dynamics simulations of organic materials with optical activity 50'**

Speaker: Mario BARBATTI (CNRS-ICR, Marseille, France)

Material: [Abstract - Barbatti](#)

12:20 **Closing Session 10'**