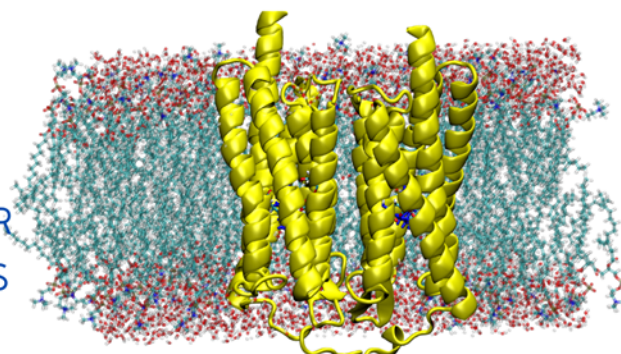


Workshop
 PRINCIPLES OF
 LIGHT-INDUCED
 CHARGE TRANSFER
 for OPTOGENETICS
 - Virtual Edition -



CT4OPTO WORKSHOP PROGRAMME

CEST	Monday, June 14
2:45 PM	Main zoom room opens
Session 1/1	Investigating optical properties (1)
3:00 – 3:10 PM	Opening remarks
3:10 – 3:50 PM	Massimo Olivucci <i>University of Siena & Bowling Green State University</i> “On the fluorescence enhancement of arch neuronal optogenetic reporters”
3:50 - 4:30 PM	Dongping Zhong <i>The Ohio State University</i> “Light-induced charge transfer triggers dimer dissociation of UVR8 photoreceptor for possible optogenetics”
4:30 – 4:55 PM	Contributed talks: Nadja K. Singer <i>University of Vienna</i> “From taco to banana: turn-on mechanism of a fluorescent probe for imaging GABA _A receptors” Laura Pedraza-González <i>University of Siena</i> “Automated QM/MM model screening of rhodopsin variants displaying enhanced fluorescence” Volha Chukhutsina <i>Imperial College London</i> “The keto group in β2 of the carotenoid tunes the orange carotenoid protein photocycle kinetics” Ciro A. Guido <i>University of Padova</i> “Exploring the spatial features of electronic transitions in biomolecular systems by swift electrons”

4:55 – 5:25 PM	Coffee break & breakout rooms
Session 1/2	Investigating optical properties (2)

5:25 – 6:05 PM **Igor Schapiro** *The Hebrew University of Jerusalem*
 “Insight into the spectral tuning mechanism of retinal proteins”

6:05 – 6:45 PM **Roberta Croce** *Vrije Universiteit Amsterdam*
 “Breaking the red-limit: driving oxygenic photosynthesis with far-red light”

	Tuesday, June 15
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2:45 PM	Main zoom room opens
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Session 2/1	Interplay between CT events and environmental factors
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3:00 – 3:40 PM **Petra Imhof** *Freie Universität Berlin*
 “Interplay of hydration, water mobility, and proton transfer in cytochrome c oxidase”

3:40 – 4:20 PM **Andrea Amadei** *University of Rome “Tor Vergata”*
 “On the modeling of charge transfer processes in complex chemical systems”

4:20 – 4:50 PM **Contributed talks**

Puja Goyal *State University of New York*
 “Modulation of adenosylcobalamin photochemistry by the CarH photoreceptor protein”

Bryan Kudisch *Princeton University*
 “Active-site environmental factors customize the photophysics of photoenzymatic old yellow enzymes”

Matteo Capone *University of L’Aquila*
 “Multiscale modelling of the photoactivation of electron donor acceptor complexes in ene reductases”

Ruibin Liang *Texas Tech University*
 “Light-activation mechanism of Channelrhodopsin 2”

Fulvio Perrella *University of Naples Federico II*
 “Proton transfer in fluorescent proteins: a dynamical viewpoint on hydrogen bonds networks”

4:50 – 5:25 PM	Coffee break & breakout rooms
Session 2/2	Excited states dynamics (1)

5:25 – 6:05 PM **Gregory Scholes** *Princeton University*
 “Electron transfer reactions: vibration and dielectric tuning”

6:05 – 6:45 PM **Benedetta Mennucci** *University of Pisa*
 “From the light absorption by the embedded chromophore to the conformational change of the protein: can we simulate such a long travel in space and time?”

Wednesday, June 16	
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10:45 AM	Main zoom room opens
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Session 3/1	Excited states dynamics (2)
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11:00 – 11:40 AM **Nadia Rega** *University Federico II of Napoli & Center for Advanced Biomaterials for Healthcare*
 “Probing relaxation mechanisms of photoinduced charge transfer phenomena: combining time-resolved vibrational analysis and ab-initio molecular dynamics”

11:40 – 12:20 AM **Basile Curchod** *Durham University*
 “In silico photochemical experiments with non-Born-Oppenheimer molecular dynamics”

12:20 – 12:45 AM **Contributed talks**

Uriel N. Morzan *International Centre for Theoretical Physics*
 “Optical signature of strong hydrogen bonds”

James Green *CNR-IBB*
 “A fragment based approach to the quantum dynamics of multichromophoric systems: application to the GC DNA base pair”

F. Di Maiolo *Goethe Universität*
 “Quantum molecular dynamics in out of equilibrium environments: redfield-smoluchowski and hydrodynamic approaches”

Pavel S. Rukin *CNR-S3 Institute of Nanoscience*
 “Theoretical study of internal conversion between B and Q bands in a functionalized porphyrin”

12:45 AM – 2:30 PM	Lunch break (breakout rooms 12:45 AM - 1:15 PM)
Session 3/2	Retinal and flavin based systems (1)
2:30 – 3:10 PM	Marco Garavelli <i>University of Bologna</i> “Modelling accurate photoinduced events and transient spectroscopies in biomolecules: the paradigmatic case of retinal systems”
3:10 - 3:50 PM	Sharon Hammes-Schiffer <i>Yale University</i> “Nonequilibrium excited state dynamics of proton-coupled electron transfer in BLUF photoreceptor proteins”
3:50 – 4:15 PM	Contributed talks Valeria Giliberti <i>Istituto Italiano di Tecnologia</i> “Conformational changes of light-sensitive membrane proteins determined by infrared difference nanospectroscopy” Luca Bellucci <i>CNR-NEST Institute of Nanoscience</i> “Relating retinal isomerization and deprotonation mechanism in Channelrhodopsin-2” Himanshu Bansal <i>Dayalbagh Educational Institute</i> “Improved optogenetic retinal prostheses with Chrmine” Xiankun Li <i>Princeton University</i> “Ultrafast dynamics of light-induced charge transfer in Lactate Monooxygenase”
4:15 – 4:45 PM	Coffee break & breakout rooms
Session 3/3	Retinal and flavin based systems (2)
4:45 – 5:25 PM	Ana-Nicoleta Bondar <i>Freie Universität Berlin</i> “Proton transfers with dynamic hydrogen-bond networks”
5:25 – 6:05 PM	Andreas Möglich <i>University of Bayreuth</i> “Interplay of signals in Light-Oxygen-Voltage receptors”
18:05 – 18:30 PM	Prizes and closing remarks

CONTACTS:

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