

**Event Title:** Photoinduced Processes in Embedded Systems (PPES)

**Organizers:** Claudia Filippi (University of Twente, The Netherlands)  
Filippo Lipparini (University of Pisa, Italy)  
Benedetta Mennucci (University of Pisa, Italy)

Location of meeting	Pisa, Italy
Dates of meeting	24-27 June 2018
Number of participants	114

## 1. Scientific summary

The scientific aim of the Psi-k workshop “Photoinduced Processes in Embedded Systems” was to bring together researchers from the physics, chemistry, and biophysics communities working on the computational study of photo-physical processes in complex systems. Modelling such phenomena is challenging since they involve very different space and time scales, from the extremely fast, localized absorption of light to the collective, slow motions of the environment.

The workshop has focused on some of the most recent theoretical and algorithmic developments in the field such as:

- DFT embedding for excited states
- Hybrid QM/Classical approaches
- Highly-correlated methods for excited-state dynamics
- TDDFT outside the Franck-Condon region
- Non-adiabatic dynamics

These methodological aspects have been framed in the context of realistic applications to materials and biosystems such as:

- Natural photosynthetic systems
- Photo-induced signal transduction in bio-systems
- Bio-mimetic light-driven molecular devices
- Photo-induced charge propagation in solar-energy devices

The workshop received funding from Psi-k, the MESA+ Institute for Nanotechnology at the University of Twente, and the University of Pisa. The workshop was open to both experts and newcomers and gathered a total of 114 participants.

## 2. Meeting Programme

The workshop began with two keynote lectures in the afternoon of Sunday, 24<sup>th</sup> June. A welcome reception for all participants was organized in the evening. Monday 25<sup>th</sup> and Tuesday 26<sup>th</sup> June were full conference days, with 8 invited lectures and 5 contributed lectures per day. There was a poster session at the end of each day. The workshop continued on Wednesday 27<sup>th</sup> with the last 6 invited lectures, which took place in the morning.

The abstracts are available on <https://www1.dcci.unipi.it/ppes/programme.html> and we report the program below with the invited speakers indicated in boldface.

Sunday 24 June	
15:00 16:30	Registration
16:30 16:40	Welcome

16:40	17:20	<b>M. Persico</b> Nonadiabatic excited state dynamics with semiclassical methods
17:20	18:00	<b>G. Scholes</b> Electronic Couplings and Energy Transfer in Photosynthesis
19:00	20:30	Welcome Cocktail

Monday 25 June		
9:00	9:30	<b>O. Prezhdo</b> Excited State Dynamics of Photoexcited Charge Carriers in Halide Perovskites: Time-Domain Ab Initio Studies
9:30	10:00	<b>I. Burghardt</b> Ultrafast Vibronic Dynamics of Functional Organic Polymer Materials: Coherence, Confinement, and Disorder
10:00	10:30	<b>A. Troisi</b> Making sense of charge and exciton dynamics in organic materials via model reduction
10:30	11:10	Coffee Break
11:10	11:40	<b>J. Gao</b> Toward a Method beyond Kohn-Sham Density Functional Theory
11:40	12:10	<b>M. Elstner</b> Multi-scale methods for electron and exciton transfer in biological and organic materials
12:10	14:10	LUNCH
14:10	14:40	<b>M. Garavelli</b> Towards an accurate computational photochemistry and photobiology: the paradigmatic case of vision
14:40	15:00	P. de Silva Static and Dynamic Energetic Disorder in the Emission Layer of an Organic Light-Emitting Diode
15:00	15:20	H. Ma Describing the Excited States in Organic Optoelectronics
15:20	15:40	E. Coccia Probing coherence in ultrafast photoinduced processes: a quantum chemistry perspective
15:40	16:20	Coffee Break
16:20	16:50	<b>V. Batista</b> Studies of PCET in Natural and Artificial Photosynthesis
16:50	17:20	<b>S. Hammes-Schiffer</b> Photoinduced Proton-Coupled Electron Transfer: Integrating Electronic and Nuclear Quantum Effects
17:20	17:40	C. Curutchet Assessing drug-binding through simulations of electronic energy transfer
17:40	18:00	M. Caricato Electronic Coupling for Donor-Bridge-Acceptor Systems with a Bridge-Overlap Approach
18:00	19:30	POSTER

Tuesday 26 June		
9:00	9:30	<b>L. González</b> Descriptors to characterize excited states and its time evolution in the presence of environment
9:30	10:00	<b>J. Blumberger</b> Charge transport in Organic Semiconductors From Fragment-orbital Non-adiabatic Molecular Dynamics Simulation
10:00	10:30	<b>I. Tavernelli</b> New strategies for non-adiabatic dynamics with trajectories
10:30	11:10	Coffee Break
11:10	11:40	<b>X. Li</b> Coupling Real-Time Time-Dependent Density Functional Theory with Polarizable Force Field
11:40	12:10	<b>N. Rega</b> Capturing nuclear photorelaxation in condensed phase through ab-initio molecular dynamics

12:10	14:10	LUNCH
14:10	14:40	<b>T. Martinez</b>
14:40	15:00	S. Ghosh Quantum Nuclear Effects in the Simulations of Non-adiabatic Dynamics of Ultrafast Charge Transfer Reactions
15:00	15:20	J. Cerezo The shape of electronic spectra of floppy molecules in solution: a hybrid quantum/classical description of the contribution of nuclear motion
15:20	15:40	M. Biczysko From 3-D structure to spectroscopic properties of complex molecular systems: the Q R route
15:40	16:20	Coffee Break
16:20	16:50	<b>F. Manby</b> Coupling electronic systems to harmonic environments
16:50	17:20	<b>J. Neugebauer</b> A Versatile Implementation of Frozen-Density Embedding TDDFT
17:20	17:40	L. Cupellini Exciton structure and optical spectra of multichromophoric biomatrices from ab initio multiscale methods
17:40	18:00	F. Di Maiolo Intermolecular energy transfer in real time
18:00	19:30	POSTER
20:30		Social Dinner

Wednesday 27 June		
9:00	9:30	<b>Y. M. Rhee</b> Characterizing energy fluctuations in the FMO Complex on a DFT level potential: covering timescales from femto to sub-microseconds
9:30	10:00	<b>F. Buda</b> Mechanism and Design Strategy in Photocatalytic Water Splitting
10:00	10:30	<b>R. Nifosi</b> Polarizable embedding effects in the spectral tuning of Fluorescent Proteins
10:30	11:10	Coffee Break
11:10	11:40	<b>J. Kongsted</b> Polarizable (Density) Embedding - from solvents to heterogeneous environments
11:40	12:00	A. Puglisi Fully Polarizable QM/MM Approach to the Study of Electronic Excitations of Flexible Solvated Dyes
12:00	12:20	I. Navizet Is the tautomerization of firefly oxyluciferin feasible at the excited state inside the protein?

### 3. List of participants

Davide	Accomasso	Università di Pisa	Italy
Alessandro	Agostini	Johannes Gutenberg-Universität Mainz	Germany
Neus	Aguilera-Porta	UAM-UNIFI-GSK	Italy
Prokopis C.	Andrikopoulos	Institute of Biotechnology CAS, v.v.i.	Czech Republic
Toshio	Asada	Osaka Prefecture University	Japan
Victor	Batista	Yale University	United States
Simon	Bennie	The University of Bristol	Great Britain
Fatma	Benyettou	Université d'Oran	Algeria
Malgorzata	Biczysko	Shanghai University	China
Jochen	Blumberger	University College London	Great Britain
Beatrix	Bold	Karlsruhe Institute of Technology	Germany
Mattia	Bondanza	Università di Pisa	Italy
Francesco	Bosia	ETH Zurich	Switzerland

Ksenia	Bravaya	Boston University	United States
Christoph	Brunken	ETH Zurich	Switzerland
Francesco	Buda	Leiden University	Netherlands
Timur	Burganov	FRC Kazan Scientific Center of RAS	Russian Federation
Irene	Burghardt	Goethe University Frankfurt	Germany
Dario	Calvani	Università di Pisa	Italy
Chiara	Cappelli	Scuola Normale Superiore	Italy
Felipe	Cardoso Ramos	Università di Pisa	Italy
Marco	Caricato	University of Kansas	United States
Javier	Cerezo	Universidad de Murcia	Spain
Jan	Chalabala	Univ. Chem. & Technology in Prague	Czech Republic
Robert	Charlton	Imperial College London	Great Britain
Kirsten	Claridge	University of Liverpool	Great Britain
Emanuele	Coccia	Università di Padova	Italy
Zeljko	Crljen	Rudjer Boskovic Institute	Croatia
Lorenzo	Cupellini	Università di Pisa	Italy
Carles	Curutchet	University of Barcelona	Spain
Alice	Cuzzocrea	University of Twente	Italy
Monika	Dash	University of Twente	Netherlands
Piotr	de Silva	Technical University of Denmark	Denmark
Francesco	Di Maiolo	University of Parma	Italy
Marcus	Elstner	Karlsruhe Institute of Technology	Germany
Milica	Feldt	KU Leuven	Belgium
Jonas	Feldt	University of Gottingen	Germany
Xibo	Feng	Dalhousie University	Canada
Claudia	Filippi	University of Twente	Netherlands
Maria	Fumanal	Université de Strasbourg	France
Jiali	Gao	University of Minnesota	USA
Marco	Garavelli	Università di Bologna	Italy
Cristina	Garcia Iriepa	Université Paris-Est Marne-la-Vallée	France
Soumya	Ghosh	University College London	Great Britain
Samuele	Giannini	University College London	Great Britain
Gabriel José	Gil Pérez	Università di Padova	Italy
Leticia	González	Universität Wien	Austria
Robert	Góra	Wroclaw Univ. Science & Technology	Poland
Giovanni	Granucci	Università di Pisa	Italy
Luca	Grisanti	SISSA, Trieste	Italy
Sharon	Hammes-Schiffer	Yale University	United States
Nicole	Holzmann	Science & Technology Facilities Council	Great Britain
Michael	Horbury	University of Warwick	Great Britain
Zhongming	Jiang	Shanghai University	China
Xiuyun	Jiang	University College London	Great Britain
Jacob	Kongsted	University of Southern Denmark	Denmark
Laura	Le Bras	Chimie ParisTech, IRCP, PSL Univ	France
Guohui	Li	Chinese Academy of Science	China
Xiaosong	Li	University of Washington	United States
Filippo	Lipparini	Università di Pisa	Italy
Daniele	Loco	Sorbonne Universités	France
Haibo	Ma	Nanjing University	China

Tristan	Mackenzie	Imperial College London	Great Britain
Sebastian	Mai	University of Vienna	Austria
Fred	Manby	University of Bristol	Great Britain
Marco	Marazzi	Univeridad de La Rioja	Spain
María del Carmen	Marín Pérez	University of Siena	Italy
María Elena	Martín Navarro	Universidad de Extremadura	Spain
Todd	Martínez	Stanford University	United States
Toshiaki	Matsubara	Kanagawa University	Japan
Jakub	Med	Univ. Chem. & Technology, Prague	Czech Republic
Elena	Meneghin	University of Padova	Italy
Maximilian	Menger	Universität Wien	Austria
Benedetta	Mennucci	Università di Pisa	Italy
Jan Paul	Menzel	Leiden University	Netherlands
Isabelle	Navizet	labo MSME, UPEM	France
Artur	Nenov	Università di Bologna	Italy
Johannes	Neugebauer	University of Münster	Germany
Riccardo	Nifosi	CNR-NANO NEST	Italy
Michele	Nottoli	Università di Pisa	Italy
Daniele	Padula	University of Liverpool	Great Britain
Elisa	Palacino González	Technische Universität München	Germany
Xiaojuan	Pang	Technische Universität München	Germany
Laura Milena	Pedraza-González	University of Siena	Italy
Maurizio	Persico	Università di Pisa	Italy
Gennaro	Pescitelli	Università di Pisa	Italy
Alessio	Petrone	University of Washington	United States
David	Picconi	Goethe-Universität Frankfurt am Main	Germany
Elisa	Pieri	Aix Marseille Université	France
Martin	Pizl	Acad. Sciences of the Czech Republic	Czech Republic
Thomas	Plehn	Humboldt-University Berlin	Germany
Ingrid	Prandi	Universidade Federal de Lavras	Brazil
Oleg	Prezhdo	University of Southern California	United States
Alessandra	Puglisi	Scuola Normale Superiore	Italy
Umberto	Raucci	Università di Napoli	Italy
Nadia	Rega	Università di Napoli	Italy
Young Min	Rhee	Korea Adv. Inst. Science & Technology	South Korea
Niccolo	Ricardi	University of Geneva	Switzerland
Antonio	Rizzo	CNR IPCF	Italy
Silvia	Santoni	Università di Pisa	Italy
Fabrizio	Santoro	ICCOM CNR	Italy
Gregory	Scholes	Princeton University	United States
Karno	Schwinn	Aix-Marseille University	France
Souloke	Sen	Vrije Universiteit Amsterdam	Netherlands
André	Pereira Gomes	CNRS / Université de Lille	France
Vladislav	Slama	Charles University	Czech Republic
Attila	Takti	ELTE Eötvös Loránd University	Hungary
Ivano	Tavernelli	IBM	Switzerland
Alessandro	Troisi	University of Liverpool	Great Britain
Matt	Turner	University of Warwick	Great Britain
Omar	Valsson	Max Planck Institute	Germany

Meilani	Wibowo	University of Pisa	Italy
Andrew	Wildman	University of Washington	United States
Weiwei	Xie	Technische Universität München	Germany

#### **4. Geographical and Gender distribution**

The 114 participants were coming from 22 different countries with the following distribution:

Algeria 1  
Austria 3 (of which 1 was an invited speaker)  
Belgium 1  
Brazil 1  
Canada 1  
China 5  
Croatia 1  
Czech Republic 5  
Denmark 2 (of which 1 was an invited speaker)  
France 8  
Germany 12 (of which 3 were invited speakers)  
Hungary 1  
Italy 31 (of which 3 were invited speakers)  
Japan 2  
Netherlands 5 (of which 1 was an invited speaker)  
Poland 1  
Russia 1  
South Korea 1 (invited speaker)  
Spain 4  
Switzerland 4 (of which 1 was an invited speaker)  
UK 14 (of which 3 were invited speakers)  
USA 10 (of which 5 were invited speakers)

The gender distribution was of 83 male and 31 female participants.