



Workshop

**PRINCIPLES OF
LIGHT-INDUCED
CHARGE TRANSFER
FOR OPTOGENETICS**

July 3-5, 2023 | Modena (IT) | optogenetics.nano.cnr.it



DSFC
Dipartimento
di Scienze Fisiche
e Chimiche



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Centre Européen de Calcul Atomique et Moléculaire



REPORT

CT4OPTO 2023

Maria Bartolacelli, Susanna Cavicchioli, Anna Grazia Stefani,
and Laura Zanetti Polzi

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Introduction

The aim of the workshop was to gather leading experts in the experimental and theoretical investigation of photoactive proteins that find application in the field of optogenetics. After the successful virtual edition of the same workshop in 2021, we organized a new, fully in presence, edition of the “Principles of light-induced charge transfer for optogenetics” workshop to emphasize new results and point out new directions, challenges and opportunities in the following fields:

- Charge transfer processes in light-sensitive proteins,
- Excited state properties of biological matter,
- Photoreceptor thermodynamics and photocycle kinetics,
- Interplay between photoexcitation and protein conformations.

These and other issues were faced from a chemical physical perspective, highlighting the main recent achievements in this timely and stimulating research field.

Organization

The Workshop was held in Modena (Italy) from July 3 to July 5, 2023 at Complesso San Geminiano (via San Geminiano 3), in the historical city centre of Modena.

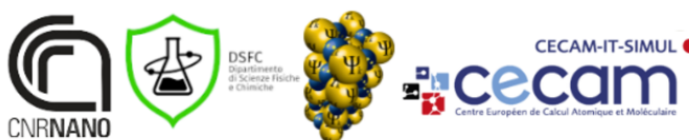
The event was organized by:

the Nanoscience Institute of the National Research Council of Italy - CNR Nano, the University of L'Aquila - Dipartimento di Scienze Fisiche e Chimiche (DSFC), the University of Southern California, and the Karlsruher Institut für Technologie.



The event was sponsored by:

the Nanoscience Institute of the National Research Council of Italy, the University of L'Aquila - Dipartimento di Scienze Fisiche e Chimiche (DSFC), Psi-k, Cecam-IT-Simul.



The event has been planned, defined, organized and realized by a team of people (researchers, technologists and collaborators) with different tasks and expertise.

The scientific program, the selection of the invited speakers, the selection of the contributed talks, the definition of the Book of Abstracts content, the assistance and relationship with the invited speakers, has been curated by a Scientific Committee.

Scientific Committee composition

Isabella Daidone | University of L'Aquila | isabella.daidone@univaq.it

Rosa Di Felice | USC and CNR Nano Modena | rosa.difelice@nano.cnr.it

Marcus Elstner | Karlsruhe Institute of Technology | marcus.elstner@kit.edu

Anna Krylov | University of Southern California | krylov@usc.edu

Laura Zanetti Polzi | CNR Nano Modena | laura.zanettipolzi@nano.cnr.it

The definition of the location, the agreement with the services suppliers (venue, catering, social dinner, hotels, etc), the overall monitoring of the registration process, the mailing activity, the web definition, implementation and updating, the communication process, the secretariat during the event has been realized by the Organizing Committee.

Organizing Committee composition

Maria Bartolacelli | CNR Nano Modena - coordinator

Susanna Cavicchioli | CNR Nano Modena

with the support of the CNR Nano colleagues: Anna Grazia Stefani (for the administrative aspects) and Maddalena Scandola (for the communication aspects).

The registration process, the fee collection and the definition of the single agreements with the different services suppliers chosen by the organizing committee has been realized through a framework agreement with [Planning Congressi srl](#), events organizer in Bologna. Roberta Suzzi, Simona Fontana, and Riccardo Corsolini flanked the organizing committee before, during and after the event.

A dedicated website <https://optogenetics.nano.cnr.it/> and an email address ct4opto@nano.cnr.it have been created for all information regarding the workshop.

CT4OPTO
Modena | July 3-5, 2023

Welcome Registration Program Accommodation Partnership Contacts

Workshop

PRINCIPLES OF LIGHT-INDUCED CHARGE TRANSFER FOR OPTOGENETICS

Welcome to the "Principles of light-induced charge transfer for optogenetics" workshop!

The Workshop will be held in **Modena** (Italy) from **July 3 to July 5, 2023**.
The program will bring together leading experts in the experimental and theoretical investigation of photoactive proteins that find application in the field of optogenetics.
The workshop will emphasize new results and point out new directions, challenges and opportunities in the following fields:

- Charge transfer processes in light-sensitive proteins,
- Excited state properties of biological matter,
- Photoreceptor thermodynamics and photocycle kinetics,
- Interplay between photoexcitation and protein conformations.

Deadlines

Abstract submission: expired.
Registration: is now closed. For info about the last available slots send an email to ct4opto@nano.cnr.it

About CT4OPTO

To learn more about the first edition of CT4OPTO visit the webpage: optogenetics2021.nano.cnr.it

Homepage of the <https://optogenetics.nano.cnr.it/> website

Participation

The Scientific Committee also defined the participation procedure and related costs.

A fee of € 150 has been requested to attend the workshop and cover part of the costs. Furthermore the Scientific Committee gave the possibility to 4 students/young researchers to attend the workshop for free and carefully selected the applications.

The workshop was attended by 39 participants (+ 5 organizers): 12 were invited speakers and 19 were contributing speakers.

The participants came from 8 different countries.

Participation fee: € 150

- The participation fee includes lunches, coffee breaks and the conference dinner.
- A separate online registration is required for each participant.

The participation fee will be waived to four PhD students/young researchers participating in the workshop with a contributed talk. More information on how to ask for the waiver of the registration fee can be found at the [Abstract Submission page](#).

Detailed Program

Monday, July 3	
Session 1	
14:30	15:00 Registration
15:00	15:15 Opening
15:15	16:00 Invited Massimo Olivucci University of Siena & Bowling Green State University <i>From Photon To Neuron: The Molecular Mechanism Of The Primary Event In Vision</i>
16:00	16:20 Katharina Spies Karlsruhe Institute of Technology <i>Active Site Structure And Absorption Spectrum Of The Channelrhodopsin Chrimson – Wild Type And Mutants</i>
16:20	16:45 Coffee break
16:45	17:30 Invited John Kennis Vrije Universiteit Amsterdam <i>Isomeric Switching Near The Conical Intersection In Bestrhodopsin, An Unusual Red-Absorbing Microbial Rhodopsin</i>
17:30	17:50 Raffaella Polito Sapienza University of Rome <i>Mid-IR Spectroscopy To Probe Conformational Changes Of Bacteriorhodopsin At The Nanoscale</i>
17:50	18:10 Maria Eleonora Temperini Sapienza University of Rome <i>A New IR Spectroscopy Platform To Study The Effect Of Static Electric Fields On Biomolecules</i>
18:10	18:30 Thanh Nhut Do Vrije Universiteit Amsterdam <i>Excitation-Fluence Dependent Two-Photon Induced Photoionization Of Bacterial Phytochrome</i>

Monday, July 3 - Session 1 - Chair: Rosa Di Felice

14:30-15:00 Registration

15:00-15:15 Opening

15:15-16:00 Invited | Massimo Olivucci | University of Siena & Bowling Green State University *“From Photon To Neuron: The Molecular Mechanism Of The Primary Event In Vision”*

16:00-16:20 Katharina Spies | Karlsruhe Institute of Technology *“Active Site Structure And Absorption Spectrum Of The Channelrhodopsin Chrimson – Wild Type And Mutants”*

16:20-16:45 Coffee break

16:45-17:30 Invited | John Kennis | Vrije Universiteit Amsterdam *“Isomeric Switching Near The Conical Intersection In Bestrhodopsin, An Unusual Red-Absorbing Microbial Rhodopsin”*

17:30-17:50 Raffaella Polito | Sapienza University of Rome *“Mid-IR Spectroscopy To Probe Conformational Changes Of Bacteriorhodopsin At The Nanoscale”*

17:50-18:10 Maria Eleonora Temperini | Sapienza University of Rome *“A New IR Spectroscopy Platform To Study The Effect Of Static Electric Fields On Biomolecules”*

18:10-18:30 Thanh Nhut Do | Vrije Universiteit Amsterdam *“Excitation-Fluence Dependent Two-Photon Induced Photoionization Of Bacterial Phytochrome”*

Tuesday, July 4	
Session 2	
09:00	09:45 Invited Nadia Rega University of Napoli Federico II & Scuola Superiore Meridionale <i>Photoinduced Charge Transfer Non-Equilibrium Processes: Theory And Modeling Strategies</i>
09:45	10:05 Daniele Narzi University of L'Aquila <i>Mechanism Of The Light-Induced Water Oxidation Reaction Occurring In The Natural Oxygenic Photosynthesis</i>
10:05	10:25 Abhishek Sirohiwal Stockholm University <i>Primary Events In Reaction Centre Of Photosystem II</i>
10:25	10:45 Coffee break
10:45	11:30 Invited Ciro A. Guido Università del Piemonte Orientale <i>Dispersion Interactions At The Excited State: Influence On Light-Responsive Properties Of Biosystems</i>
11:30	11:50 Sinjini Bhattacharjee Max-Planck-Institut <i>Multiscale Modeling Of Genetic Variants Of Photosystem II</i>
11:50	12:35 Invited Lyudmila Slipchenko Purdue University <i>Triplet Energy Transfer In The Fenna-Matthews-Olson (FMO) Pigment-Protein Complex</i>
12:35	12:55 Pavel Rukin CNR - Istituto Nanoscienze <i>Theoretical Study Of Vibrational-Mediated Interlayer Charge Transfer In A Cobalt Phthalocyanine-Graphene Heterojunction</i>
12:55	14:30 Lunch break

Tuesday, July 4 - Session 2 - Chair: Isabella Daidone

09:00-09:45 Invited | Nadia Rega | University of Napoli Federico II & Scuola Superiore Meridionale *"Photoinduced Charge Transfer Non-Equilibrium Processes: Theory And Modeling Strategies"*

09:45-10:05 Daniele Narzi | University of L'Aquila *"Mechanism Of The Light-Induced Water Oxidation Reaction Occurring In The Natural Oxygenic Photosynthesis"*

10:05-10:25 Abhishek Sirohiwal | Stockholm University *"Primary Events In Reaction Centre Of Photosystem II"*

10:25-10:45 Coffee break

10:45-11:30 Invited | Ciro A. Guido | Università del Piemonte Orientale *"Dispersion Interactions At The Excited State: Influence On Light-Responsive Properties Of Biosystems"*

11:30-11:50 Sinjini Bhattacharjee | Max-Planck-Institut *"Multiscale Modeling Of Genetic Variants Of Photosystem II"*

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12:55-14:30 Lunch break

Session 3	
14:30	15:15 Invited Jochen Blumberger University College London <i>Currents Of Bacterial Life Probed By Molecular Simulation And Pump-Probe Spectroscopy</i>
15:15	15:35 Matteo Capone University of L'Aquila <i>Multiscale Modeling Of Photo-Induced Stereoselective Radical Cyclization In A Flavoenzyme</i>
15:35	15:55 Lorenzo Cupellini University of Pisa <i>How Simulations Uncover The Photoactivation Mechanism Of Appa Bluf</i>
15:55	16:15 Coffee break
16:15	17:00 Invited Sharon Hammes-Schiffer Yale University <i>Nonequilibrium Excited State Dynamics Of Proton-Coupled Electron Transfer In Bluf Photoreceptor Proteins</i>
17:00	17:20 Laura Pedraza-Gonzales University of Pisa <i>How The pH Controls Photoprotection In The Light-Harvesting Complex Of Mosses</i>
17:20	18:05 Invited James Boedicker USC Dornsife <i>Optogenetic Tools To Control Charge Transfer Within Bacteria</i>
18:05	18:30 Discussion
19:30	Social Dinner

Tuesday, July 4 - Session 3 - Chair: Nadia Rega

14:30-15:15 Invited | Jochen Blumberger | University College London *“Currents Of Bacterial Life Probed By Molecular Simulation And Pump-Probe Spectroscopy”*

15:15-15:35 Matteo Capone | University of L'Aquila *“Multiscale Modeling Of Photo-Induced Stereoselective Radical Cyclization In A Flavoenzyme”*

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15:55-16:15 Coffee break

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17:20-18:05 Invited | James Boedicker | USC Dornsife *“Optogenetic Tools To Control Charge Transfer Within Bacteria”*

18:05-18:30 Discussion

19:30-Social Dinner

Wednesday, July 5		
Session 4		
09:00	09:45	Invited Gloria Mazzone Università della Calabria <i>Light Induced Charge Transfer For Enhanced Photodynamic Therapy Action</i>
09:45	10:05	Colin Coane University of Southern California <i>Unraveling The Mechanism Of Tip-Enhanced Molecular Energy Transfer</i>
10:05	10:25	Giovanni Parolin University of Padova <i>Modelling Plexcitonic States With Single-Molecule Resolution</i>
10:25	10:45	Coffee break
10:45	11:30	Invited Ksenia Bravaya Boston University <i>Predictive Methods For Simulating Charge Transfer And Redox Processes In Proteins</i>
11:30	11:50	Davide Accomasso University of Pisa <i>Uncovering A Carotenoid Quencher State In The CP29 Light-Harvesting Complex Of Plants</i>
11:50	12:10	Matteo Bruschi University of Padova <i>Simulating Action-2D Electronic Spectroscopy From Molecular Dimers To Photosynthetic Antennas</i>
12:10	12:30	Stefano Scoditti Università della Calabria <i>Unveiling The Photocatalytic Reduction Of Platinum(IV) Complexes By Riboflavin: Insights From Computational Analysis</i>
12:30	14:00	Lunch break

Wednesday, July 5 - Session 4 - Chair: John Kennis

- 09:00-09:45 Invited | Gloria Mazzone | Università della Calabria *"Light Induced Charge Transfer For Enhanced Photodynamic Therapy Action"*
- 09:45-10:05 Colin Coane | University of Southern California *"Unraveling The Mechanism Of Tip-Enhanced Molecular Energy Transfer"*
- 10:05-10:25 Giovanni Parolin | University of Padova *"Modelling Plexcitonic States With Single-Molecule Resolution"*
- 10:25-10:45 Coffee break
- 10:45-11:30 Invited | Ksenia Bravaya | Boston University *"Predictive Methods For Simulating Charge Transfer And Redox Processes In Proteins"*
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- 12:10-12:30 Stefano Scoditti | Università della Calabria *"Unveiling The Photocatalytic Reduction Of Platinum(IV) Complexes By Riboflavin: Insights From Computational Analysis"*
- 12:30-14:00 Lunch break

Session 5	
14:00	14:45 Invited Igor Schapiro The Hebrew University of Jerusalem <i>Insight Into The Photochemistry Of Cyanobacteriochromes By Qm/Mm Simulations</i>
14:45	15:05 Leonardo Barneschi University of Siena <i>Mechanism Of Fluorescence Enhancement In Rhodopsin Optogenetic Reporters</i>
15:05	15:25 Giacomo Salvadori University of Pisa <i>Transient Intermediates In A Bacteriophytochrome Photocycle Revealed By Multiscale Simulations</i>
15:25	15:45 Coffee break
15:45	16:05 Federico Gallina University of Padova <i>Simulating 2D Spectroscopic Responses Of Optical Systems With Digital Quantum Computers</i>
16:05	16:50 Invited Samer Gozem Georgia State University <i>Electrostatic Tuning Maps And Average Protein Configurations: Tools To Aid In Studying Flavoproteins</i>
16:50	17:00 Closing

Wednesday, July 5 - Session 5 - Chair: Massimo Olivucci

14:00-14:45 Invited | Igor Schapiro | The Hebrew University of Jerusalem *“Insight Into The Photochemistry Of Cyanobacteriochromes By Qm/Mm Simulations”*

14:45-15:05 Leonardo Barneschi | University of Siena *“Mechanism Of Fluorescence Enhancement In Rhodopsin Optogenetic Reporters”*

15:05-15:25 Giacomo Salvadori | University of Pisa *“Transient Intermediates In A Bacteriophytochrome Photocycle Revealed By Multiscale Simulations”*

15:25-15:45 Coffee break

15:45-16:05 Federico Gallina | University of Padova *“Simulating 2D Spectroscopic Responses Of Optical Systems With Digital Quantum Computers”*

16:05-16:50 Invited | Samer Gozem | Georgia State University *“Electrostatic Tuning Maps And Average Protein Configurations: Tools To Aid In Studying Flavoproteins”*

16:50-17:00 Closing

Best Oral Contribution Award

The Scientific Committee awarded the “Best Oral Contribution Award”.

The award recipient was selected under the following criteria: Excellence of the candidate and presentation; Relevance to the theme of the workshop; Juniority; Experimental/theoretical balance; Gender balance; Geographical balance.

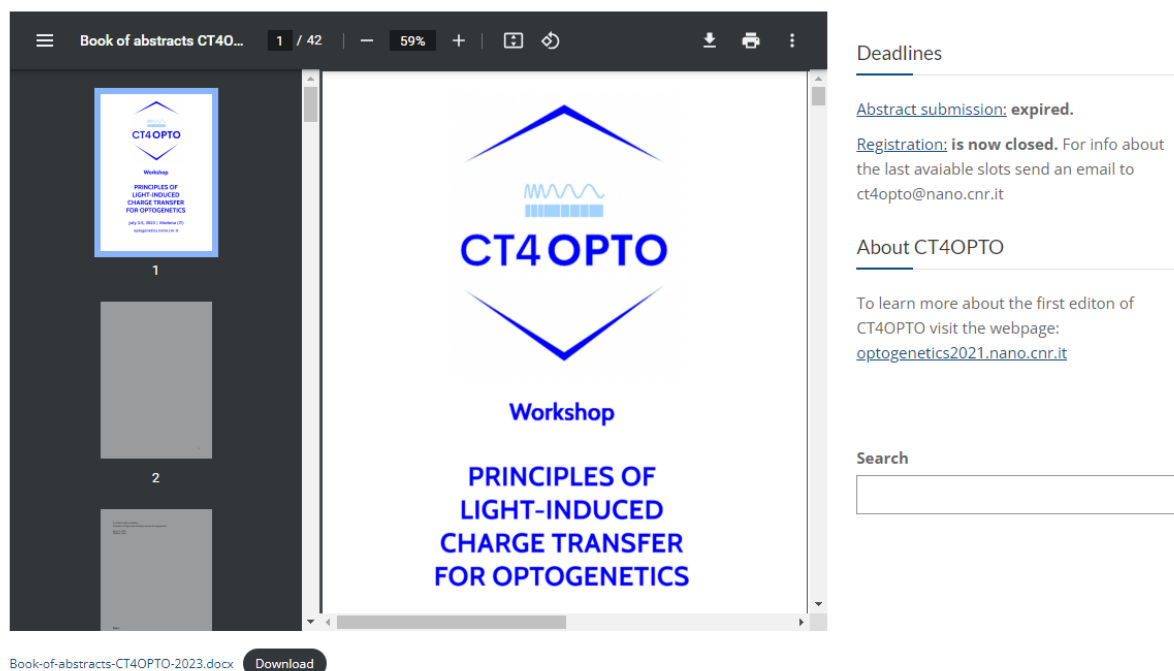
The award went to Giacomo Salvadori from University of Pisa.



Tweet about the Best Oral Contribution Award

Book of Abstracts

To keep records of the talks held during the workshop we realized a e-book of abstracts available on the workshop website and linked here [Book of abstracts](#)



Screenshot of the website, section Book of abstracts

General remarks

During the whole workshop all participants showed a very high level of interest and keen participation. The discussion was always fruitful and lively, showing the high competence of the participants in the workshop topics. The invited speakers delivered very interesting and inspiring talks, but we were also impressed by the high quality of the contributed talks. During Q&As and the discussion sessions, very interesting inputs came from the audience. Overall, the whole workshop was characterized by a fruitful exchange of ideas that will surely motivate new research on the topic.

Conclusions and prospects

We believe that the workshop was an exciting and fruitful scientific event: the invited speakers presented very well their excellent research work and the contributed speakers delivered well-prepared and interesting talks. All these excellent contributions stimulated very interesting discussions which we hope will also serve as inputs for further developments in the field. Research on the topic has reached impressive levels, both from an experimental

and from a theoretical point of view, and we also noticed that this is a very rapidly developing field. For this reason, we are already planning to organize the third edition of the workshop in two years.

Acknowledgements

We would like to thank Dr. Luisa Neri for the precious support and advice.



Group picture near Modena cathedral

Annex 1: participants list

1. Davide Accomasso | Università di Pisa (IT)
2. Andrea Amadei | Università degli Studi di Roma Tor Vergata (IT)
3. Leonardo Barneschi | Università di Siena - (IT)
4. Sinjini Bhattacharjee | Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr (DE)
5. Matteo Bruschi | Università degli Studi di Padova (IT)
6. Matteo Capone | University of L'Aquila (IT)
7. Colin Coane | University of Southern California, Dept. of Physics and Astronomy (US)
8. Lorenzo Cupellini | Università di Pisa (IT)
9. Isabella Daidone | University of L'Aquila (IT)
10. Thanh Nhut Do | Department of Physics and Astronomy, Vrije Universiteit Amsterdam (NL)
11. Gianluca Dell'Orletta | University of L'Aquila (IT)
12. Rosa Di Felice | USC and CNR Nano Modena (IT)
13. Federico Gallina | Università degli Studi di Padova (IT)
14. Daniele Narzi | University of L'Aquila (IT)
15. Bence Olsz | Jagiellonian University, Faculty of Biochemistry, Biophysics and Biotechnology (PL)
16. Gianluca Parisse | University of L'Aquila (IT)
17. Giovanni Parolin | Department of Chemical Sciences, University of Padova (IT)
18. Laura Milena Pedraza Gonzales | Università di Pisa (IT)
19. Alessio Petrone | Università degli Studi di Napoli "Federico II" (IT)
20. Raffaella Polito | University of Rome La Sapienza (IT)
21. Pavel Rukin | Cnr Nano (IT)
22. Giacomo Salvadori | Università di Pisa (IT)
23. Stefano Scoditti | University of Calabria (IT)
24. Abhishek Sirohiwal | Stockholm University, Stockholm (SE)
25. Katharina Spies | Karlsruhe Institute of Technology, Theoretical Chemical Biology (DE)
26. Maria Eleonora Temperini | Sapienza University of Rome (IT)
27. Laura Zanetti Polzi | Cnr Nano (IT)

Annex 2: invited speakers list

1. Jochen Blumberger | University College London
2. James Boedicker | USC Dornsife
3. Ksenia Bravaya | Boston University
4. Samer Gozem | Georgia State University
5. Ciro A. Guido | Università degli Studi del Piemonte Orientale
6. Sharon Hammes-Schiffer | Yale University (remote participation)
7. John Kennis | Vrije Universiteit Amsterdam
8. Gloria Mazzone | Università della Calabria
9. Massimo Olivucci | University of Siena & Bowling Green State University
10. Nadia Rega | Università degli Studi di Napoli “Federico II”
11. Igor Schapiro | The Hebrew University of Jerusalem
12. Lyudmila Slipchenko | Purdue University

Annex 3: [Flyer](#)

Annex 4: practical info for abstract submission

Abstract submission has expired on May 5, 2023.

Abstracts should be submitted by e-mail to ct4opto@nano.cnr.it following the template provided and the indications therein. [abstract template pdf](#) | [abstract template rtf](#).

The e-mail subject should contain “Abstract for opto2023”. Please specify in the e-mail body if you are applying for an oral presentation, a poster or both.

The participation fee will be waived to four PhD students/young researchers participating in the workshop with a contributed talk. If you want to apply for the waiver of the participation fee. Selection of the four contributors that will benefit from the waiver of the participation fee will be made on the basis of the applicant’s CV and abstract. Students or researchers affiliated to institutions of developing countries will be given priority.

Acceptance notifications (for both abstract and participation fee waiver) will be sent by May 15, 2023.

To support gender equality, abstract submission from women scientists are particularly welcome.

Abstracts will be collected in a Book of Abstracts available for download.

Annex 5: workshop materials

We realized a workshop bag with the logo of the event and the useful materials inside:

- pen
- notes
- printed program
- wifi credentials and access instructions
- [practical information about the workshop and Modena in general](#)
- map of the city centre of Modena



The workshop secretariat

Annex 6: collaterals and social aspects

During the workshop several coffee breaks and lunches were organized in the premises on Complesso San Geminiano. Furthermore a social dinner was organized on July 4, 2023 at Caffè Concerto, in the main square of Modena: piazza Grande.

