Massimo Olivucci

E-mail: molivuc@bgsu.edu or olivucci@unisi.it **Web:** https://www2.bgsu.edu/departments/chem/faculty/massimo/

September 2020

PROFILE

FULL NAME: Massimo Olivucci

DATE OF BIRTH: February 28, 1958

NATIONALITY: Italian

MARITAL STATUS: Married with MATILDE

FAMILY: 2 SONS (Paolo and Enrico) and 1 DAUGHTER (Lidia)

I. Appointments

Position	**Date**	**Place**
Research Professor and Director of the Laboratory of Computational Photochemistry and Photobiology.	**2006-**	**Bowling Green State University (BGSU)**
Full Professor of Organic Chemistry	**2001-**	**Università di Siena (UNISI)**
Associate Professor of Organic Chemistry	1998-2001	Università di Siena
Ricercatore (Lecturer)	1992-1998	Università di Bologna
Post Doc (with Prof. Michael A. Robb)	1989-1992	King's College London (UK)

Visiting Professorships	**Date**	**Place**
Invited Professorship	March **2017**	**Nagoya Institute of Technology**
USIAS Fellow	July **2015**-June **2018**	**Université Luis Pasteur Strasbourg**
Professeur Invité	February **2012**	**Université Luis Pasteur Strasbourg**

II. Education

Qualification	**Date**	**Institution**
Ph.D. in Chemistry[b] (with Prof. Fernando Bernardi)	October 1989	Università di Bologna
Laurea in Chimica[a] (equivalent to UK-USA MSc)	March 1984	Università di Bologna

a Project title: "Diabatic Decomposition of Adiabatic Surfaces at the Theoretical Level."
b Thesis title: "Adiabatic and Diabatic Surfaces in Chemical Reactivity".

III. Academic Duties

Position	Date	Institution
Member of the Committee for the Bachelor and Master Degree in Chemistry	October 2004-	Università di Siena
Faculty Board for the Graduate Program in Chemical and Pharmaceutical Sciences	October 2011-	Università di Siena
Member of the ERASMUS Program Committee (Chemistry, Pharmacy)	October 2005-	Università di Siena
Research Delegate for the Department of Excellence	October 2018-	Università di Siena

TEACHING

I Courses

King's College London (UK): 1989-90/1990-91 Theoretical Chemistry.
Università di Bologna (IT): 1996-97 Organic Reaction Mechanisms - 1997-98 Organic Chemistry.
Università di Siena (IT): 1998-2000 Organic Chemistry Lab.; 2000- Advanced Organic Chemistry (BSc-level); 1999- Organic Chemistry 3rd Course (Mechanistic and Physical Organic Chemistry); 1999- Advanced and Computational Organic Chemistry (MSc-level). 2020- Quantum Chemistry with Application to Thermal and Photochemical Organic Reactions.

Bowling Green State University (USA): 2007-2016 PCS-704 Introduction to Computational Chemistry and Photochemistry (Graduate Course).

II Advisees (Graduate Students and PostDoc)

Current MSc students:
Germana Calce (UNISI) and Tayler Douglas (BGSU), Laleh Allahkaram (UNISI), Quinn Eberhard (BGSU). Riccardo Palombo (UNISI), Simone Bonfrate (UNISI), Mikhal Marszałek (ERASMUS, UNISI), Razan Daud (UNISI).

Current Graduate Students:
Laura Milena Pedraza Gonzales (UNISI), Dmitrii Nikolaev (UNISI, visiting from St. Petersburg State University, Russia), Aljandro Blanco Gonzalez (BGSU), Leonardo Barneschi (UNISI), Martina Nucci (UNISI, visiting from the University of Alcalà, Spain), Riccardo Palombo (UNISI).

Current Postdocs/Assistant Professors/Associate Professor:
Samira Gholami (BGSU), Luca De Vico (Associate Professor, UNISI), Daniele Padula (Tenure-Track Associate Professor, UNISI), Xuchun Yang (BGSU), Marco Paolino (Tenure-Track Associate Professor, UNISI)

Former Graduate Students (current position in brackets):
L. De Vico (Ph.D. 2004, presently Assistant Professor, U. Siena, Italy), A. Sinicropi (Ph.D. 2002, presently Lecturer, U. of Siena, Italy), Angela Strambi (Ph.D. 2007, presently working at Pfitzer & U. of Stocholm, Sweden), Laura Parisi (Ph.D. 2008, presently PostDoc U. Siena, Italy), Mikhail Ryazantsev (Ph.D. 2010, presently Assistant Professor, St Petersburg

Academic U. and St. Petersburg State U., Russia), P. El-Khuory (Co-Adv., Ph.D. 2010, presently Researcher at PNNL, USA), L. A. Estrada (Co-Adv., Ph.D. 2010, presently PostDoc U. of Florida, Gainesville), Federico Melaccio (Ph.D. 2012, Presently Programmer & System Manager, EPSRC, UK), Mark Huntress (Ph.D. 2012, presently Instructor at Patrick Henry Community College, USA), Elena Laricheva (Ph.D. 2012, presently Instructor at the Utah Valley U., USA), Samer Gozem (Ph.D. 2013, presently Assistant Professor at the Georgia State U., USA), Silvia Rinaldi (Ph.D. 2014, PostDoc at CNR-Milan, Italy), Venjamin Borin (Co-Adv Ph.D. 2016, Presently PostDoc Hbrew U. of Jerusalem, Israel), Daryna Smirnova (Siena-Leuven), Alessio Valentini (PhD 2016, Presently PostDoc at Universitè de Liegè, Belgium), Madushanka Sugath (PostDoc at Michigan State University), Maria del Carmen Marin (Siena), Maria del Carmen Marin (Siena).

Former Postdocs/Assistant Professors (present position in brackets):
A. Sinicropi (Assistant Professor, U. Siena, Italy), C. Page (Researcher at the Imperial Cancer Research, London, UK), N. Ferré (Professor at the U. de Provence, France), T. Andruniów (Professor at the U. of Wroclaw, Poland), Luis Manuel Frutos (Professor at the U. of Alcalà, Spain), E. Martin-Navarro (Professor at the U. Extremadura, Spain), D. Sampedro (Professor at the U. Rioja, Spain), P. Braña Coto (Faculty at CFM-CSIC, San Sebastián, Basque Country, Spain), A. Migani (Researcher at the U. of Barcelona, Spain), C. Reynaud (Researcher at U. Montpellier, France), A. Melloni, (working at Zambon, Vicenza, Italy), A. Perrier, (Assistant Professor at U. Paris, France), B. Durbeej (Assitant Professor at U. Upsala, Sweden), Xuebo Chen (Professor at the Bejing Normal U., China), Wan Jian Ding (Professor at the Bejing Normal U., China), Laura Parisi (PostDoc at the U. of Siena), Uksha Saini (PostDoc Univ. of Pittsburgh Medical Center), Igor Schapiro (Assistant Professor at the Hebrew U. of Jerusalem), Riccardo Rossi-Paccani (working at NOVARTIS, Siena, Italy), Joseph Saju (PostDoc at KAUST, Saudi Arabia), Samer Gozem (Assistant Professor at Georgia State U., USA), Federico Melaccio (Programmer & System Manager, EPSRC, UK), Calvin Luk (PostDoc at the U. of Jyväskylä, Finland), Alessio Valentini (PostDoc at Universitè de Liegè, Belgium), Yoelvis Orozco (PostDoc, U. Strasbourg, France, PostDoc at Georgia State University), Maria del Carmen Marin (PostDoc, Tokyo), Marco Paolino (Associate Professor, University of Siena).

III PhD Dissertation committee chair (research advisor) 2018-2019, 2019-2020:

Xuchun Yang (BGSU, graduated in the a.a. 2018-2019), Alejandro Blanco Gonzalez (BGSU, current), Yorrick Boeije (University of Amsterdam, Netherland, a.a. 2019-2020)

RESEARCH

Over 240 research papers published in international journals. These include 70 papers in the Journal of the American chemical society, 9 papers in Angewandte Chemie International Edition, 15 papers in multidisciplinary science journals such as the Proceedings of the National Academy of Science USA (10 papers) and the Science Magazine (1 paper) and Nature's Scientific Reports (1 paper), Nature Communications (2 papers) and Nature Chemistry (1 paper). Our work focuses on the investigation of organic and bio-organic reactivity using theoretical and computational tools. The current work is focuses on two research lines: The investigation of the light energy conversion processes in biological photoreceptors and the design of biomimetic photo-driven molecular switches/rotary motors. The development of novel (or more effective) computational methodologies and strategies is also part of our research activity. Further information on the research group (The Laboratory for Photochemistry and Photobiology) and activities can be found in the group homepage: http://www2.bgsu.edu/departments/chem/faculty/massimo/LCPP.html).

I. Research Achievements

Three different objectives have been achieved over the years. The first objective aimed to a deeper understanding of the Woodward-Hoffmann selection rules for pericyclic reactions to

the development of new computational tools capable of treating reactivity problems in small to medium size (few tens of atoms) organic molecules.
The second objective involved the development of protocols for mapping excited state energy surfaces and a systematic characterization of the photochemical reactivity of different classes of organic and biological chromophores. The corresponding results provided the first "statistical" demonstration of the ubiquity of *conical intersections* and *singlet/triplet crossings* in organic chromophores and of their role, equivalent to that of transition states in thermal chemistry, as basic mechanistic elements in photochemistry.
The third and present objective includes the development and application of excited state reaction path and semi-classical trajectory computations using a quantum mechanics/molecular-mechanics protocol. In this context, Olivucci's group is one of the first and few with expertise in the development and application of quantum mechanics/molecular mechanics methods for excited states and in particular for photochemical reactions occurring in complex molecular environment such as in a protein cavity. Notice that the quantum mechanical part is usually treated at the *ab initio* multiconfigurational level (mainly employing the CASPT2//CASSCF level of theory). This methodology is being intensively exploited for the investigation of photoisomerization reactions in biological photoreceptors and for the design of novel photoresponsive biomimetic molecular switches and motors. Recently, the group has reported on these achievements in the Science Magazine, Nature Chemistry and Nature Communications.[1,2,3] For recent (last 10 years) work in these areas see:

1) Sinicropi A. et al. (2008) An Artificial Molecular Switch that Mimics the Visual Pigment and Completes its Photocycle in Picoseconds. **Proc. Nat. Acad. Sci. USA** 105:17642-17647.
2) Melloni, A. et al. (2010) Modeling, Preparation and Characterization of a Dipole Moment Switch Driven by Z/E Photoisomerization **J. Am. Chem. Soc.** 132:9310-9319.
3) Altoè, P. et al. (2010) An aborted double bicycle-pedal isomerization with hydrogen bond-breaking is the primary event in the Bacteriorhodopsin proton-pumping **Proc. Natl. Acad. Sci. USA** 107:20172-20177.
4) Strambi, A. et al. (2010) Anabaena sensory rhodopsin is a light-driven unidirectional rotor **Proc. Natl. Acad. Sci. USA** 107:21322-21326.
5) Schapiro, I. et al. (2011) The Ultrafast Photoisomerizations of Rhodopsin and Bathorhodopsin are Modulated by Bond Alternation and HOOP driven Electronic Effects **J. Am. Chem. Soc.** 133:3354–3364.
6) Grilj, J. et al. (2011) Fluorescence of Radical Ions in Liquid Solution: Wurster's Blue as a Case Study **Angew. Chem. Int. Ed.** 50:4496-4498.
7) Gozem S., Schapiro, I., Ferré, N. & Olivucci, M. (2012) The Molecular Mechanism of Dark Noise in Rod Photoreceptors. **Science** 337:1225-1228.
8) Rinaldi S., Melaccio, F., Gozem, S., Fanelli, F. & Olivucci, M. (2014) Comparison of the isomerization mechanisms of human melanopsin and invertebrate and vertebrate rhodopsins **Proc. Natl. Acad. Sci. USA** 111:1714-1719.
9) Luk H. L., Melaccio, F., Rinaldi, S., Gozem, S. & Olivucci, M. (2015) Molecular bases for the selection of the chromophore of animal rhodopsins. **Proc. Natl. Acad. Sci. USA** 112:15297-15302.
10) Schnedermann, C.; Yang, X.; Liebel, M.; Spillane, K. M.; Lungtenburg, J.; Fernandez, I.; Valentini, A.; Schapiro, I.; Olivucci, M.; Kukura, P.; Mathies, R. A. Evidence for a Vibrational Phase-Dependent Isotope Effect on the Photochemistry of Vision. **Nature Chemistry** 2018, 10.1038/s41557-018-0014-y.
11) Gueye, M.; Manathunga, M.; Agathangelou, D.; Orozco, Y.; Paolino, M.; Fusi, S.; Haacke, S.; Olivucci, M.; Léonard, J. Engineering the vibrational coherence of vision into a synthetic molecular device. **Nat. Commun**. 2018, 9, 313.
12) Marín, M.; Carmen, D.; Agathangelou, D.; Orozco-Gonzalez, Y.; Valentini, A.; Kato, Y.; Abe-Yoshizumi, R.; Kandori, H.; Choi, A.; Jung, K.-H.; Haacke, S.; Olivucci, M. Fluorescence Enhancement of a Microbial Rhodopsin via Electronic Reprogramming. **J. Am. Chem. Soc.** 2019, 141, 262-271.

II International Collaborations

We had a long standing collaboration with Prof. M. A. Robb at the Imperial College London (UK). Over the years this collaboration has yielded outstanding applicative and methodological developments. **Past** fruitful collaborations also involving joined experimental and theoretical work involved the groups of Prof. W. Nau (University of Bremen, Germany), Prof. M. Merchàn (University of Valéncia, Spain), Dr. W. Fuss (Max-Planck-Institüt für Quantenoptik, Garching, Germany), Waldemar Adam (University of Wurzburg, Germany), Peter Hamm (University of Zurich, Switzerland), Bernd Giese (University of Basel, Switzerland) and Alesandro Lami & Fabrizio Santoro (CNR-Pisa, Italy), Dr. F. De Angelis & Dr. Simona Fantacci (CNR-Perugia, Italy). **Recent and Current Collaborations** involve Nicolas Ferré (Université de Provence, France), Tadeusz Andruniów (University of Wrolcaw, Poland), Luis Manuel Frutos (Univerity of Alcalà, Spain), Jan Helbing (University of Zurich, Switzerland), Loredana Latterini & Fausto Elisei (University of Perugia, Italy), Vinicio Zanirato (University of Ferrara, Italy), Stefan Haacke (University of Strasbourg, France), Alexander Tarnovsky (Bowling Green State University), Roland Lindh (Department of Theoretical Chemistry, University of Uppsala, Sweden), Alex Granovsky (the Firefly Project, Moscow), Celestino Angeli (University of Ferrara, Italy), Francesca Fanelli (Department of Biology, University of Modena and Reggio Emilia, Italy), Fleming Crim (University of Wisconsin, Madison), Tatjana Domratcheva (Max-Planck Institute for Medical Research - Heidelberg, Germany), Eric Vauthey (University of Geneva, Switzerland), Ksenija Glusac (Bowling Green State University), Belinda Chang (Department of Evolutionary Biology, University of Toronto), Anna Krylov (USC), Krzysztof Palczewski (Case Western University), Jeanne Serb (Iowa State), Hideki Kandori (Nagoya Institute of Technology, Japan), Kwang-Hwan Jung (Sogang University, South Korea), Richard Mathies (University of California at Berkeley), Philipp Kukura (University of Oxford), Laura Gagliardi (University of Minnesota), Donald Truhlar (University of Minnesota), Laura Ragona (CNR, Milano), ANdrea Cappelli (Università di Siena), Ilya Ioffe (Moscow State University), Micahel Filatov (Kyungpook National University, South Korea).

III Current Research Activity

(1) Computational investigation of the "primary event" in biological photoreceptors.
(2) Structure of potential energy surfaces near conical intersections.
(3) Development and application of accurate QM/MM methods for investigating excited states and photochemical reactivity.
(4) Computer Design and Synthesis of Biomimetic Molecular Motors and Switches.
(5) Methods for the Design of Photoreceptors Mutants with Programmed Optical and Photochemical Properties
(6) Automated and interfaced methods for the construction of QM/MM models of proteins.

IV Research Funding

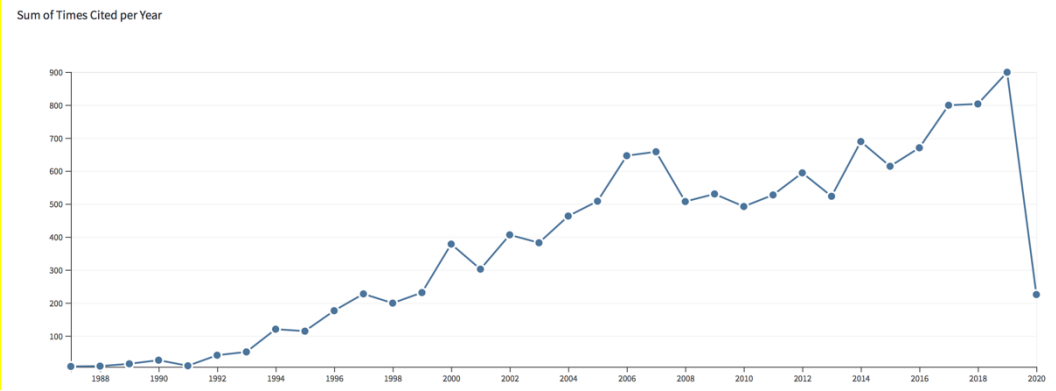
1. EU TMR Network Grant (ERB 4061 PL95 1290, Quantum Chemistry for the Excited State).
2. NATO Collaborative Research Grant (CRG 950748, Theoretical Study of the Excited State Relaxation and Phototransformations of Polyenes).
3. Marie Curie Fellowship HPMF-CT-1999-00384
4. Human Frontier Science Program- RG 0229/2000-M
5. Marie Curie Fellowship HPMF-CT-2001-00089
6. Marie Curie Fellowship HPMF-CT-2002-01769
7. FIRB Italian Ministry of Education, 2002-2005
8. MIUR Italian Ministry of Education, 2004-2006 (U. Siena PI, €60000)
9. Marie Curie Fellowship HPMF-CT-2005-(Proposal N° 023430 - EXCPROT - PI, €227000)
10. Bowling Green State University Startup Funds, 2006 (PI, $200000)
11. MIUR Italian Ministry of Education, 2007-2009 (U. Siena PI, €60000)
12. RCGE, Bowling Green State University, 2008 (BGSU, PI $50000)
13. RIG Bowling Green State University, 2010 (BGSU, PI $50000)
15. Ohio Supercomputer Center, 2010 - Computer time.
16. Yearly funded by MITSUBISHI CHEMICAL since 2002-2011
17. NSF Grant 2012-2015 CHE-CLP 1152070 (PI, $223245)

18. HFSP Research Grant No. RGP0049/2012 (PI, $750000)
19. NSF-XSEDE Grant, 2012 - Computer time
20. NSF-XSEDE Grant 2013 - Computer time
21. MIUR Grant 2012-2014 (U. Siena PI, €53000)
22. Ohio Supercomputer Center, 2012.
23. FP7 People Marie-Curie (International Outgoing) PIOF-GA-2012-332233 (PI, €227000)
24. NSF-XSEDE Grant 2015. - Computer time.
25. USIAS Fellowship 2015-2017 (PI, €105000)
26. Ohio Supercomputer Center, 2015 - Computer time.
27. NSF Grant 2015 CHE-CLP-1551416 (PI, $38236).
28. MIUR-PRIN Grant 2015-2018. (U. of Siena PI, €66000)
29. CINECA - Grant 2017 Computer time.
30. Support as a Host for a PRACE Visiting scientist (Nicolaev) from the University of St. Petersburg 2017.
31. NSF Grant 2017-2020 CHE-CLP-1551416 (PI, $350120).
32. NIH, 2018-2021R15 GM126627 01 (PI, $336540)
33. Support as a Host for a PRACE Visiting scientist (Ryazantsev) from the University of St. Petersburg 2019.
34. Fondazione Banca D'Italia. Grant 2019-2020 to U. Siena (PI, €65368)
35. Support as a Host for a PRACE Visiting scientist (Martina Nucci) from the University of Alcalà (Madrid) 2020.
36. ERASMUS+ Internship 2019-2020 (Michał Marszałek) Wrocław University of Science and Technology, Poland.

V. Laboratory of Computational Photochemistry and Photobiology

The Laboratory for Computational Photochemistry and Photobiology (LCPP) is a bi-national lab (BGSU-University of Siena) devoted to the development of tools for mapping excited state potential energy surfaces and for the systematic characterization of the photochemical reactivity of different classes of organic and biological chromophores. The main target of LCPP is to help to establish and consolidate a branch of computational chemistry entirely devoted to the investigation of light-induced phenomena in molecular and bio-molecular materials. This also includes the introduction of new generations of MSc and Graduate students to the methods of theoretical and computational photochemistry. The research activity focuses on the development and application of state-of-the-art computational protocols for the simulation of photophysical and photochemical processes in both isolated chromophores and in the condensed phase. Ultimately, these methodologies will be used to provide an atomic-level description of the mechanism of light energy transduction from the single-molecule level to complex systems and includes the design of molecular devices or biological molecules (i.e. peptides or proteins) with certain desired optical or photochemical properties.

HONOURS



I HIRSH (H) FACTOR

64 (based on **ISI-Web of Science. Average citation 47.38, Total Citation per Year, see picture**)

Invited Visiting Professor at the University of Strasbourg, Strasbourg, France, October **2012**.

USIAS Fellow at the University of Strasbourg, Strasbourg, France, July **2015**-June 2018.

Visiting Professor at the Nagoya Institute of Technology, **March 2017**.

Doctoris Honoris Causa at the Aix-Marseille Université, **2019-2020**.

Seven among the most cited papers:

1. Bernardi, F., Olivucci, M. & Robb, M. A. Potential energy surface crossings in organic photochemistry. Chemical Society Reviews **25,** 321 (1996).
2. Garavelli, M., Celani, P., Bernardi, F., Robb, M. A. & Olivucci, M. The C5H6NH2+ Protonated Shiff Base: An ab Initio Minimal Model for Retinal Photoisomerization. Journal of the American Chemical Society **119,** 6891-6901 (1997).
3. González-Luque, R., Garavelli, M., Bernardi, F., Merchán, M., et al. Computational evidence in favor of a two-state, two-mode model of the retinal chromophore photoisomerization. Proceedings of the National Academy of Sciences of the United States of America **97,** 9379-9384 (2000).
4. Andruniów T, Ferré N, Olivucci M Structure, initial excited-state relaxation, and energy storage of rhodopsin resolved at the multiconfigurational perturbation theory level. Proceedings of the National Academy of Sciences of the United States of America **101,**17908-17913 (2004).
5. Sinicropi A, Andruniow T, Ferré N, Basosi R, Olivucci M Properties of the Emitting State of the Green Fluorescent Protein Resolved at the CASPT2//CASSCF/CHARMM Level. Journal of the American Chemical Society **127**, 11534-11535 (2005).
6. Frutos L. M., Andruniów, T., Santoro, F., Ferré, N. & Olivucci, M. (2007) Tracking the excited-state time evolution of the visual pigment with multiconfigurational quantum chemistry. Proc Natl Acad Sci U S A 104:7764-7769.
7. Sinicropi A., Martin, E., Ryasantsev, M., Helbing, J., Briand, J., Sharma, D., Léonard, J., Haacke, S., Cannizzo, A., Chergui, M., Zanirato, V., Fusi, S., Santoro, F., Basosi, R., Ferré, N. & Olivucci, M. (2008) An Artificial Molecular Switch that Mimics the Visual Pigment and Completes its Photocycle in Picoseconds. Proceedings of the National Academy of Sciences of the United States of America 105:17642-17647.

One of the 4 Invited Speakers at the **Optochemical and Optogenetic Session** of the International Symposium on New Horizon in Membrane Transport and Communication 2017, Oct 4th - Oct 7th, 2017 in Frankfurt, Germany.

Invited to Nominate candidates for the Nobel Prize for Chemistry several years since year 2000

II RECENT INVITED AND PLENARY LECTURES (2007-2018)

Invited Lecture Retinal Proteins: Experiments and Theory, September 23-26 2007, Bremen, Germany (declined).
Invited Lecture Progress in ab initio modelling of biomolecules: towards computational spectroscopy, April 2-4 2007, Rome, Italy.
Invited Lecture TheoBio07, June 16-20, Cetraro, Italy.
Invited Lecture 393 WE-Heraeus-Seminar, Trends in Molecular Biophysical Spectroscopy, April 27-28 2007, Bonn, Germany.

Invited Lecture ICP2007 July 29 – August 3 2007, Cologne, Germany.
Invited Lecture SFB533 Light-induced Dynamics of Proteins Freising, September 9 – October 5 2007, Germany.
Invited Lecture COMET XX, June 3-7 2007, Arcachon, France (decline).
Invited Lecture ACS symposium "Excited Electronic States in Chemistry and Biology: Theory and Experiment", August19-23 2007, Boston USA.
Invited Lecture Frontiers in Photochemistry, September 9-13 2007, Villars-sur-Ollon, Switzerland.
Invited Lecture Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy July 24-27 2007, Telluride, USA (declined).
Invited Lecture WATOC 2008, September 14-18 2008, Sidney, Australia (declined).
Invited Lecture ICRP 2008, June 15-19 2008, Barcelona, Spain.
Invited Lecture CSC 2008, May 24-28 2008, Edmonton, Canada**.**
Invited Lecture Theoretical Biochemistry - Methods and Applications, 14-17 May 2008, Stockholm, Sweden.
Invited Lecture TACC 2008, September 23-27, 2008, Shanghai, China (declined).
Invited Lecture Laboratoire Chimie Provence Universite' de Provence – March, 5 - March 7 2009, Marseille, France.
Invited Lecture International Conference in Photochemistry 2009, July, 19 - July 21 2009, Toledo, Spain.
Invited Lecture ICQC Satellite Symposium entitled "Molecular Properties - Bridging the Gap between Theory and Experiment" 2009, June, 18 - June 2121 2009, Oslo, Norway.
Plenary Lecture CREST International Symposium on Theory and Simulations of Complex Molecular Systems, July, 19 - July 2121 2009, Kyoto, Japan. (declined)
Plenary Lecture CERMM Centre for Research in Molecular Modeling Montreal, Canada, May 1-3 21 2009.
Invited Lecture MIB 09 "Modeling Interaction in Biomolecules IV", September 14-19 2009 at Hrubá Skála
Plenary Lecture XXIII IUPAC Symposium on Photochemistry 2010, July, 11 - July 16, Ferrara, Italy.
Invited Lecture 6th International Symposium on Organic Photochromism 2010, October, 17 – October 21, Yokohama, Japan.
Plenary Lecture XX IUPAC Symposium on Physical Organic Chemistry 22-28, August 2010, Busan, South Korea.
Plenary Lecture 8th European Conference on Computational Chemistry 25-28, August 2010, Lund, Sweden.
Invited Lecture IX Congress of the World Association of Theoretical and Computational 17-22 Spain, Chemists 2011, Santiago de Compostela, Spain.
Plenary Lecture Workshop on Modeling of biologically-inspired photoactive systems 8th European Conference on Computational Chemistry, March 30-April 1, 2011 Marseille, France.
Invited Lecture at the 242nd ACS National Meeting, August, 28 - 2011 September 1, Denver, CO, USA.
Invited Lecture at the 8th Seminars of Advanced Studies on Molecular Modeling and Bioinformatics, Havana and Varadero, Cuba, July 10 to 15, 2011.
Invited Lecture "Dynamics of molecular mechanisms of biological photoreceptors: interplay between experiments and theory" DFG, Ringberg Castle in Bavaria, Germany October 9th-12th, 2011.
Invited Lecture at the CECAM Workshop "In Silico Spectroscopy", March 2012, Ecole Normal Superior, Lyon, France.
Invited Lecture, PA60 Conference on Electronic Structure Theory for Strongly Correlated Systems", Palermo Italy, May 30-June 1, 2012.
Invited Lecture at the 34th Reaction Mechanisms Conference, University of Missouri, Columbia, Missouri June 19-22, 2012.
Invited Lecture at the 244th ACS National Meeting, August, 19 - August, 23, 2012, Philadelphia, PA, USA.
Plenary Lecture at the 7th International Meeting on Photodynamics October, 14 - 20, Maresias, 2012, Brazil.

Invited Lecture Quantum Effects in Biological Systems Workshop, June 29th – July 3rd 2013 in Vienna, Austria.
Invited Lecture Radicals in the Rockies. Workshop, July 21-25, 2013, Telluride, USA.
Invited Lecture International Conference on Theoretical and High Performance Computational Chemistry (ICT-HPCC13), July 21-25, 2013, Dalian, China. (Declined)
Invited Lecture Modeling Interaction In Biomolecules (MIB) September, 16-19, 2013, Marianske lazne, Czech Republic. (Declined)
Invited Lecture 7th International Symposium on Photochromism (ISOP 2013), September 23-25, 2013, Berlin, Germany.
Invited Lecture Theory Fest LMU-Muenchen November 5, 2013, Munich, Germany.
Invited Series of Lecture Invited Lecture Winter School on Modeling Chemical and Biological (Re)activity. 2-22 Jan 2014, CCNSB, IIIT-H, Hyderabad, India.
Invited Lecture Light in Chemistry, Materials and Biology"(LCMB – 2014), February 24-25, 2014, Indian Institute of Techonology Kharagpur, India (Declined).
Invited Lecture 8th International Meeting on Photodynamics and Related Aspects (Oaxaca, Mexico, October 2014).
Invited Lecture American Physical Society meeting, Quantum Mechanics Applied to Biological Problems (Denver, Colorado, March 2014).
Invited Lecture 16th International Conference on Retinal Proteins 2014 (Nagahama, Japan, October 2014).
Invited Theoretical Session Presentation 16th International Conference on Retinal Proteins 2014 (Nagahama, Japan, October 2014).
Invited Lecture Löwdin Minisymposium 20-21 November 2014 (Uppsala, Sweden, November 2014).
Keynote Lecture at the International Conference on Physical Organic Chemistry 22 August 10-15, 2014, Ottawa, Canada.
Invited Lecture at the 249th ACS National Meeting, March, 22 - March, 26, 2015, Denver, CO, USA.
Invited Lecture at the Modeling Photoactive Molecules, April, 21 - April, 24, 2015, Nantes, France.
Invited BFG Colloquium at the Physics Department - Freie Universität Berlin July, 6, 2015, Berlin, Germany.
Invited Lecture, at the Symposium "Molecular Theory for Excited-state Electronic Structure and Dynamics", Pacifichem 2015 Honolulu. Hawaii, USA.
Invited Lecture at the 8th IUPAC Symposium on Photochemistry, March, 3 - 8, 2016, Osaka, Japan.
Invited Lecture at the 8th Molecular Quantum Mechanics conference, June, 26 - July, 1st, 2016, Uppsala, Sweden.
Invited Lecture at the HRSMC Photochemistry School 2016, August 27-31, 2016 Castle Vaeshartelt. The Netherlands.
Invited Lecture at the 17th International Conference on Retinal Proteins 2016, October 2nd - 7th, 2016 in Potsdam, Germany.
Invited Lecture at IGER International Symposium on Physics of Life, March 29-30 2017 in Nagoya, Japan.
Invited Lecture at the at the 249th ACS National Meeting, April, 2 - 6, 2017, San Francisco, CA, USA.
Invited Lecture at the 17th WATOC 2017, August 27th - September 1st, 2017 in Munich, Germany. (Declined)
Invited Lecture at the 17th CSC 2017, May 28th - June 1st, 2017 in Toronto, Canada.
Invited Lecture at the International Symposium on New Horizon in Membrane Transport and Communication 2017, Oct 4th - Oct 7th, 2017 in Frankfurt, Germany.
Invited Lecture at the Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy workshop, July 17-21, 2017, Telluride, Colorado (declined).
Invited Lecture at International Workshop on Conical intersections and Nonadiabatic Couplings, November 10, 2017 NYU, New York City, USA.
Invited Lecture, at the QSCP-XXII, October 16-24, 2017, Hunan, China.
Invited Lecture, Symposium Excited States and Non-adiabatic Dynamics, American Pysical Society March Meeting (March 5-9, 2018 Los Angeles).

Invited Lecture, Gordon Research Conference on Photosensory Receptors and Signal Transduction, Il Ciocco, Lucca, March 4 - 9, 2018.
Invited Lecture, Nonadiabatica 2018: Theory of Nonadiabatic Processes, Hebrew University of Jerusalem, 12-15 March 2018.
Plenary Lecture, Photoinduced Processes in Embedded Systems, Pisa, 24-27 June 2018.
Invited Lecture, International Conference on Retinal Proteins, Toronto, Canada, 24-29 September 2018.
Invited Lecture, VIth Jornadas Ibéricas de Fotoquimica, Aveiro, Portugal, 12-14 September 2018.
Invited Lecture, "Computational Spectroscopy In Natural sciences and Engineering" (COSINE),MACS2018, Scuola Normale Superiore, November 22-23, 2018 Pisa, Italy.
Invited Lecture, Collaborative Research Center 749 (SFB749) "Dynamics and Intermediates of Molecular Transformations", Venice International University (VIU) San Servolo, Italy, 10-15 March 2019.
Invited Lecture, Gordon Research Conference on Artificial Molecular Switches and Motors, Holderness School in Holderness NH United States, June 9 - 14, 2019.
Invited Lecture, European School of Medicinal Chemistry - ESMEC 2019, June 30-July 4 2019, Urbino, Italy.
Invited Lecture, CECAM Tel Aviv, Israel, September 3 - 5, 2019.
Invited Lecture, International Conference on Retinal Proteins, ISE-SHIMA, Shima, Japan, Japan, 1-6 June 2020.
Invited Lecture, Workshop Psi-K: light-induced charge transfer for optogenetics, Modena, Italy, 15-17 June 2020.
Invited Class*,* Photochemistry Course, University of Amsterdam, May 7, Lecture on Conical Intersection.
Invited Communication*,* WATOC 2020, Vancouver, Canada.
Invited Lecture*,* New Horizons in Scientific Software: from Legacy Codes to Modular Environments, South Korea, Nov. 23-26 2020.

III PRIZES, MEDIA & OUTREACH

1. National Prize "FEDERCHIMICA", 11th edition, 1999.
2. Finalist of the European Community 2001 Descartes Prize for scientific excellence.
3. Documentary on the Chemistry of Conical Intersection: "Paysage" by Vincent Gaullier & Angelo Caperna, broadcasted in France/Europe for the TV-Program "ARCHIMEDES".
4. Movie of the Lecture "Computational Photobiology". Available and broadcasted on-line from the Universite de Marseille, France.
5. Research Prize 2004 of the Organic Chemistry Division of the Italian Chemical Society.
6. "Angelo Mangini" (Gold) Medal for Research 2010 of the Organic Chemistry Division of the Italian Chemical Society.
7. Doctor Honoris Causa, Aix-Marseille Université - Academic Year 2019-2020.

MEMBERSHIP, EDITOR and OTHER SYNERGISTIC ACTIVITIES

Member of the Italian Chemical Society
Member of the American Chemical Society
Member of the Driving Committee of the Italian Computational Chemistry Group (GICC) 2000-2006.
IUPAC member of the sub-commission in photochemistry 2001-
Member of the Theoretical Chemistry Accounts Editorial Board 2001-2008
Member of the Driving Committee of the Italian Photochemistry Group (GIF) 2003-2006.
Member of the European Photochemical Society.
One of the Five Members of the MIUR Committee for the National Qualification to the Roles of Associate and Full Professor of Organic Chemistry. 2012-2014.
Member of the European COST ACTION "CODECS" for "Computational Spectroscopy" 2011-2014.
Italian Delegate for CNR/IUPAC committee 2013-.

Editor of the Computational Photochemistry, Theoretical and Computational Chemistry Vol.

16, Elsevier, Amsterdam, 2005.
Editor of the Special Issue of Molecular Physics dedicated to Prof. M. A. Robb, 2006, Vol. 104.
Member of the Editorial Board of Topics in Current Chemistry 2009-
Editor-in-Chief, Topics in Current Chemistry 2015-

Member of the Organizing Committee of the E-WISPOC (European Winter School of Physical Organic Chemistry) 1-6 February, 2008-2010.
Member of the Organizing Committee of the Symposium "Ultrafast Processes in Proteins: Theory and Experiment", 247th ACS National American Chemical Society Meeting, Dallas, 16-20 March, 2014.
Member of the Scientific Advisory Board of the International Conference of Retinal Proteins. 2014-.
Organizer of the Symposium "Chemistry and Applications of Retinal Proteins: From Microbes to Humans", Pacifichem 2015.
Organizer of the MOLCAS Developer Workshop, Siena, 12-14 April, Italy 2015.
Member of the Organizing Committee of the Symposium "Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photo-activities", 253rd ACS National American Chemical Society Meeting, San Francisco, 2-6 April, 2017.
International Scientific Advisory Board of IUPAC Conference in Photochemistry, Amsterdam, 2020.
Organizer of the Symposium "Chemistry of Retinal Proteins", Pacifichem 2020.

Member of the European Research Council, 2020 panel PE4 "*Physical and Analytical Chemical Sciences*".

REFEREE DUTIES

Funding Agencies: Scuola Normale Superiore (Italy), DFG (Germany), NSF (US), HFSP (international), RSC (UK), MIUR (Italy), ANR (France), FWF (Austria), SRC (Sweden), Israel Science Foundation (Israel), National Science Center, Poland, EU-PRACE (Europe), ERC ADVANCED (Europe), NWO (The Netherlands), ERC-ADG, ERC-SYR.
Peer-reviewed Journals: Nature, Nature Comm, Science, PNAS, ACR, JACS, JCTC, JPC A, JPC B, JOC, PCCP, PPS, Proteins, JCC, TCA, THEOCHEM, IJQC, Biophysical J., ChemPhotoChem, Progress in Retinal and Eye Research.
PhD Thesis: ETH-Lausanne (Switzerland), University of Fribourg (Switzerland), Universidad de Alcalá (Spain), University of Gröningen (The Netherlands)
International Recruiting: University of Hidelberg (Germany), Michigan State University (US), The Hebrew University of Jerusalem (Israel), Ariel University (Israel), MacArthur Fellows Program (US).

PUBLICATIONS (Total: 257)

SELECTED RECENT PUBLICATIONS (Last 12 Years - Since 2007)

1. Santoro F, Lami A, Olivucci M (2007) Complex excited dynamics around a plateau on a retinal-like potential surface: chaos, multi-exponential decays and quantum/classical differences. Theo Chem Acc 117:1061–1072.

2. Strambi A, Coto PB, Ferré N, Olivucci M (2007) Effects of water re-location and cavity trimming on the CASPT2//CASSCF/AMBER excitation energy of Rhodopsin. Theo Chem Acc 118:185–191.

3. Bravslasky S et al. (2007) Glossary of terms used in photochemistry 3rd edition:(IUPAC Recommendations 2006). Pure Appl Chem 79:293–465.

4. Migani A, Bearpark MJ, Olivucci M, Robb MA (2007) Photostability versus Photodegradation in the Excited-State Intramolecular Proton Transfer of Nitro Enamines: Competing Reaction Paths and Conical Intersections. J Am Chem Soc 129:3703–3713.

5. Lumento F et al. (2007) Quantum chemical modeling and preparation of a biomimetic photochemical switch. Angewandte Chemie, International Edition 46:414–420.

6. Santoro F, Barone V, Improta R, Lami A, Olivucci M (2007) Quantum Dynamics of Ultrafast Photoinduced Processes in Biological Molecules. AIP Conf Proc 963:667.

7. Zanirato V et al. (2007) Synthesis of biomimetic light-driven molecular switches via a cyclopropyl ring-opening/nitrilium ion ring-closing tandem reaction. Tetrahedron 63:4975–4982.

8. Castaño O, Sancho U, Garavelli M, Olivucci M, Frutos LM (2007) The Role of Intersection Space Segments in Photochemical Reactions. AIP Conf Proc 963:594.

9. Frutos LM, Sancho U, Garavelli M, Olivucci M, Castano O (2007) The Role of the Intersection Space in the Photochemistry of Tricyclo[3.3.0.02,6]octa-3,7-diene. J Phys Chem A 111:2830–2838.

10. Frutos LM, Andruniów T, Santoro F, Ferré N, Olivucci M (2007) Tracking the Excited-state Time Evolution of the Visual Pigment with Multiconfigurational Quantum Chemistry. Proc Natl Acad Sci U S A 104:7764–7769.

11. Sinicropi A et al. (2008) An Artificial Molecular Switch that Mimics the Visual Pigment and Completes its Photocycle in Picoseconds. Proc Natl Acad Sci U S A 105:17642–17647.

12. Olivucci M, Santoro F (2008) Chemical Selectivity Through Control of Excited-state Dynamics. Angewandte Chemie, International Edition 47:6322–6325.

13. Coto PB, Strambi A, Olivucci M (2008) Effect of Opsin on the Shape of the Potential Energy Surfaces at the Conical Intersection of the Rhodopsin Chromophore. Chem Phys 347:483–491.

14. Sinicropi A, Olivucci M (2008) Molecole e Luce al Calcolatore. Sapere 5:10–21.

15. Coto PB et al. (2008) Origin of the Absorption Maxima of the Photoactive Yellow Protein Resolved via Ab Initio Multiconfigurational Methods. J Phys Chem B 112:7153–7156.

16. Sinicropi A, Basosi R, Olivucci M (2008) Recent applications of a QM/MM scheme at the CASPT2//CASSCF/AMBER (or CHARMM) level of theory in photochemistry and photobiology. Journal of Physics: Conference Series 101:012001.

17. Strambi A, Coto PB, Frutos LM, Ferré N, Olivucci M (2008) Relationship between the Excited State Relaxation Paths of Rhodopsin and Isorhodopsin. J Am Chem Soc 130:3382–3388.

18. El-Khoury PZ, Olivucci M, Tarnovsky AN (2008) Switching on molecular iodine elimination through isomerization: The F2C-I-I isomer of difluorodiiodomethane. Chem Phys Lett 462:192–195.

19. Sinicropi A, Bernini C, Basosi R, Olivucci M (2009) A novel biomimetic photochemical switch at work: design of a photomodulable peptide. Theo Chem Acc 8:1639–1649.

20. Rivado-Casas L et al. (2009) Fluorenylidene-Pyrroline Biomimetic Light-Driven Molecular Switches. J Org Chem 74:4666–4674.

21. Andruniów T, Olivucci M (2009) How Does the Relocation of Internal Water Affect Resonance Raman Spectra of Rhodopsin? An Insight from CASSCF/Amber Calculations. J Chem Theory Comput 5:3096–3104.

22. Pistolesi S et al. (2009) Modeling the Fluorescence of Protein-Embedded Tryptophans with ab Initio Multiconfigurational Quantum Chemistry: The Limiting Cases of Parvalbumin and Monellin. J Phys Chem B 113:16082–16090.

23. Soİderhjelm P, Husberg C, Strambi A, Olivucci M, Ryde U (2009) Protein Influence on Electronic Spectra Modeled by Multipoles and Polarizabilities. J Chem Theory Comput 5:649–658.

24. El-Khoury PZ, Tarnovsky AN, Schapiro I, Ryazantsev MN, Olivucci M (2009) Structure of the Photochemical Reaction Path Populated via Promotion of CF(2)I(2) into Its First Excited State. J Phys Chem A 113:10767–10771.

25. Briand J et al. (2009) Ultrafast Isomerization Dynamics of Biomimetic Photoswitches. Spinger Series Chemical Physics 92:343–345.

26. Altoè P, Cembran A, Olivucci M, Garavelli M (2010) An aborted double bicycle-pedal isomerization with hydrogen bond-breaking is the primary event in the Bacteriorhodopsin proton-pumping. Proc Natl Acad Sci U S A 107:20172–20177.

27. Strambi A, Durbeij B, Ferré N, Olivucci M (2010) Anabaena sensory rhodopsin is a light-driven unidirectional rotor. Proc Natl Acad Sci U S A 107:21322–21326.

28. Briand J et al. (2010) Coherent Ultrafast Torsional Motion and Isomerisation of a Biomimetic Dipolar Photoswitch. Phys Chem Chem Phys 12:3178 – 3187.

29. Schapiro I et al. (2010) Computational Photochemistry and Beyond. Aust J Chem 63:413–429.

30. El-Khuory P et al. (2010) Matrix isolation and computational studies of the CF2I radical. Chem Phys Lett 496:68–73.

31. Melloni A et al. (2010) Modeling, Preparation and Characterization of a Dipole Moment Switch Driven by Z/E Photoisomerization. J Am Chem Soc 132:9310–9319.

32. Zhou D et al. (2011) Fast Excited-State Deactivation in N(5)-Ethyl-4a-hydroxyflavin Pseudobase. J Phys Chem B 115:7136–7143.

33. Grilj J, Laricheva EN, Olivucci M, Vauthey E (2011) Fluorescence of Radical Ions in Liquid Solution: Wurster's Blue as a Case Study. Angewandte Chemie, International Edition 50:4496–4498.

34. Réhault J, Zanirato V, Olivucci M, Helbing J (2011) Linear Dichroism Amplification - Adapting a Long-Known Technique for Ultrasensitive Femtosecond IR spectroscopy. J Chem Phys 134:124516 –1124525.

35. Schapiro I et al. (2011) The Ultrafast Photoisomerizations of Rhodopsin and Bathorhodopsin are Modulated by Bond Alternation and HOOP driven Electronic Effects. J Am Chem Soc 133:3354–3364.

36. Melaccio F, Olivucci M, Lindh R, Ferré N (2011) Unique QM/MM potential energy surface exploration using microiterations. Int J Quantum Chem 111:3339–3346.

37. Schapiro I, Melaccio F, Laricheva EN, Olivucci M (2011) Using the computer to understand the chemistry of conical intersections. Photochem Photobiol Sci 10:867–886.

38. El-Khoury P et al. (2012) in CRC Handbook of Organic Photochemistry and Photobiology. Third Edition, eds Griesbeck A, Ghetti F (CRC Press, Boca Raton, FL), pp 1029–1056.

39. Gozem S, Krylov A, Olivucci M (2012) Conical Intersections and Potential Energy Surface Features of a Model Retinal Chromophore: Comparison of EOM-CC and Multireference Methods. J Chem Theory Comput 9:284–292.

40. Gozem S et al. (2012) Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model. J Chem Theory Comput 8:4069–4080.

41. Léonard J et al. (2012) Mechanistic Origin of the Vibrational Coherence Accompanying the Photoreaction of Biomimetic Molecular Switches. Chem Eur J 18:15296–15304.

42. Laricheva E et al. (2012) Origin of fluorescence in 11-cis locked bovine rhodopsin. J Chem Theory Comput 8:2559–2563.

43. Dunkelberger AD et al. (2012) Photoisomerization and relaxation Dynamics of a Structurally Modified Biomimetic Photoswitch. J Phys Chem A 116:3527–3533.

44. Melaccio F, Ferré N, Olivucci M (2012) Quantum Chemical Modeling of Rhodopsin Mutants Displaying Switchable Colors. Phys Chem Chem Phys 14:12485–12495.

45. Gozem S, Schapiro I, Ferré N, Olivucci M (2012) The Molecular Mechanism of Dark Noise in Rod Photoreceptors. Science 337:1225–1228.

46. Rossi Paccani R et al. (2012) Towards a Stable α-cycloalkyl Amino Acid with a Photoswitchable Cationic Side-chain. J Org Chem 77:1738–1748.

47. Huix-Rotllant M et al. (2013) Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. J Chem Theory Comput 9:3917–3932.

48. Xu X, Gozem S, Olivucci M, Truhlar DG (2013) Combined Self-Consistent-Field and Spin-Flip Tamm–Dancoff Density Functional Approach to Potential Energy Surfaces for Photochemistry. J Phys Chem Lett 4:253–258.

49. Bernini C et al. (2013) Effects of the Protein Environment on the Spectral Properties of Tryptophan Radicals in Pseudomonas aeruginosa Azurin. J Am Chem Soc 135:4822–4833.

50. Perrier A, Aloise S, Olivucci M, Jacquemin D (2013) Inverse versus Normal Dithienylethenes: Computational Investigation of the Photocyclization Reaction. J Phys Chem Lett 4:2190–2196.

51. Léonard J et al. (2013) Isomer-dependent Vibrational Coherence in Ultrafast Photoisomerization. New J Phys 15:105022.

52. Gozem S et al. (2013) Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and EOM-CC Methods. J Chem Theory Comput 9:4495–4506.

53. El-Khoury P et al. (2013) Probing Vibrationally Mediated Ultrafast Excited State Reaction Dynamics with Multireference (CASPT2) Trajectories. J Phys Chem A 117:11271–11275.

54. Huntress M et al. (2013) Towards an Understanding of the Retinal Chromophore in Rhodopsin Mimics. J Phys Chem B 117:10053–10070.

55. Gozem S et al. (2014) A Conical Intersection Controls the Deactivation of the Bacterial Luciferase Fluorophore. Angewandte Chemie, International Edition 53:9870–9875.

56. Rinaldi S, Melaccio F, Gozem S, Fanelli F, Olivucci M (2014) Comparison of the Isomerization Mechanisms of Human Melanopsin and Invertebrate and Vertebrate Rhodopsins. Proc Natl Acad Sci U S A 111:1714–1719.

57. Filatov M, Olivucci M (2014) Designing conical intersections for light-driven single molecule rotary motors: From precessional to axial motion. J Org Chem 79:3587–3600.

58. Schapiro I et al. (2014) Initial Excited-State Dynamics of an N-Alkylated Indanylidene-Pyrroline (NAIP) Rhodopsin Analog. J Phys Chem B 118:12243–12250.

59. Gozem S, Melaccio F, Luk HL, Rinaldi S, Olivucci M (2014) Learning from photobiology how to design molecular devices using a computer. Chem Soc Rev 43:4019–4036.

60. Gozem S et al. (2014) Shape of Multireference, EOM-CC, and DFT Potential Energy Surfaces at a Conical Intersection. J Chem Theory Comput 10:3074–3084.

61. Schapiro I, Roca-Sanjuán D, Lindh R, Olivucci M (2015) A surface hopping algorithm for nonadiabatic minimum energy path calculations. J Comput Chem 36:312–320.

62. Tuna D et al. (2015) Assessment of approximate coupled-cluster and algebraic-diagrammatic-construction methods for ground-and excited-state reaction paths and the conical-intersection seam of a retinal-chromophore model. J Chem Theory Comput 11:5758–5781.

63. Luk HL, Melaccio F, Rinaldi S, Gozem S, Olivucci M (2015) Molecular bases for the selection of the chromophore of animal rhodopsins. Proc Natl Acad Sci U S A 112:15297–15302.

64. Marchand G et al. (2015) On the Directionality of Double Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center. J Phys Chem Lett 6:599–604.

65. Zen A, Coccia E, Gozem S, Olivucci M, Guidoni L (2015) Quantum Monte Carlo Treatment of the Charge Transfer and Diradical Electronic Character in a Retinal Chromophore Minimal Model. J Chem Theory Comput 11:992–1005.

66. Udvarhelyi A, Olivucci M, Domratcheva T (2015) Role of the Molecular Environment in Flavoprotein Color and Redox Tuning: QM Cluster versus QM/MM Modeling. J Chem Theory Comput 11:3878–3894.

67. Rinaldi S, Melaccio F, Luk H-L, Gozem S, Olivucci M (2016) Comparative Quantum Chemical Studies of the Ultrafast Isomerization of Microbial, Invertebrate and Vertebrate Rhodopsins. International Conference on Ultrafast Phenomena UM4A.1.

68. Paolino M et al. (2016) Design, Synthesis and Dynamics of a GFP Fluorophore Mimic with an Ultrafast Switching Function. J Am Chem Soc 138:9807–9825.

69. Estrada LA, Francés-Monerris A, Schapiro I, Olivucci M, Roca-Sanjuán D (2016) Mechanism of Excited State Deactivation of Indan-1-ylidene and Fluoren-9-ylidene Malononitriles. Phys Chem Chem Phys 18:32786–32795.

70. Luk HL et al. (2016) Modulation of Thermal Noise and Spectral Sensitivity in Lake Baikal Cottoid Fish Rhodopsins. Sci Rep 6:38425.

71. Aquilante F et al. (2016) Molcas8: New Capabilities for Multiconfigurational Quantum Chemical Calculations Across the Periodic Table. J Comput Chem 37:506–541.

72. Manathunga M et al. (2016) Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. J Chem Theory Comput 12:839–850.

73. Melaccio F et al. (2016) Space and Time Evolution of the Electrostatic Potential During the Activation of a Visual Pigment. J Phys Chem Lett 7:2563–2567.

74. Melaccio F et al. (2016) Towards Automatic Rhodopsin Modeling as a Tool for High-throughput Computational Photobiology. J Chem Theory Comput 12:6020–6034.

75. Orozco-Gonzalez Y et al. (2017) An Average Solvent Electrostatic Configuration Protocol for QM/MM Free Energy Optimization: Implementation and Application to Rhodopsin Systems. J Chem Theory Comput 13:6391–6404.

76. Manathunga M, Yang X, Orozco-Gonzalez Y, Olivucci M (2017) Impact of Electronic State Mixing on the Photoisomerization Timescale of the Retinal Chromophore. J Phys Chem Lett 8:5222–5227.

77. Valentini A et al. (2017) Optomechanical Control of Quantum Yield in Trans-Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. Angewandte Chemie, International Edition 56:3842–3846.

78. Gozem S, Luk HL, Schapiro I, Olivucci M (2017) Theory and Simulation of the Ultrafast Double-Bond Isomerization of Biological Chromophores. Chem Rev 117:13502–13565.

79. Nicolaev DM et al. (2018) A Comparative Study of Modern Homology Modeling Algorithms for Rhodopsin Structure Prediction. ACS Omega 3:7555–7566.

80. Agathangelou D et al. (2018) Effect of point mutations on the ultrafast photo-isomerization of Anabaena Sensory Rhodopsin. Faraday Discuss 207:55–75.

81. Manathunga M, Yang X, Olivucci M (2018) Electronic State Mixing Controls the Photoreactivity of a Rhodopsin with All-trans Chromophore Analogues. J Phys Chem Lett 9:6350–6355.

82. Gueye M et al. (2018) Engineering the vibrational coherence of vision into a synthetic molecular device. Nat Commun 9:313.

83. Schnedermann C et al. (2018) Evidence for a vibrational phase-dependent isotope effect on the photochemistry of vision. Nat Chem 10:449–455.

84. El-Tahawy M et al. (2018) Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landau–Zener Model. J Phys Chem Lett 3315–3322.

85. Smirnova D, del Carmen Marin M, Olivucci M, Ceulemans A (2018) Systematic Excited State Studies of Reversibly Switchable Fluorescent Proteins. J Chem Theory Comput 14:3163–3172.

86. Pedraza-González L, De Vico L, Marín MDC, Fanelli F, Olivucci M (2019) a-ARM: Automatic Rhodopsin Modeling with Chromophore Cavity Generation, Ionization State Selection and External Counter-ion Placement. J Chem Theory Comput 15:3134–3152.

87. Marín MDC et al. (2019) Assessment of MC-PDFT excitation energies for a set of QM/MM models of rhodopsins. J Chem Theory Comput 15:1915–1923.

88. Pagano K et al. (2019) Bile Acid Binding Protein Functionalization Leads to a Fully Synthetic Rhodopsin Mimic. J Phys Chem Lett 10:2235–2243.

89. Pieri E et al. (2019) CpHMD-Then-QM/MM Identification of the Amino Acids Responsible for the Anabaena Sensory Rhodopsin pH-Dependent Electronic Absorption Spectrum. Journal of Chemical Theory and Computation J Chem Theory Comput 15:4535–4546.

90. Marín MDC et al. (2019) Fluorescence Enhancement of a Microbial Rhodopsin via Electronic Reprogramming. J Am Chem Soc 141:262–271.

91. Gholami S et al. (2019) Multistate Multiconfiguration Quantum Chemical Computation of the Two-Photon Absorption Spectra of Bovine Rhodopsin. J Phys Chem Lett

92. Fdez. Galván I et al. (2019) OpenMolcas: From Source Code to Insight. J Chem Theory Comput

93. Inoue K et al. (2019) Red-shifting Mutation of Light-driven Sodium Pump Rhodopsin. Nat Commun 1993.

94. Schapiro I et al. (2019) Synthesis, spectroscopy and QM/MM simulations of a biomimetic ultrafast light-driven molecular motor. Photochem Photobiol Sci 18:2259–2269.

95. Marsili E, Farag MH, Xuchun Y, De Vico L, Olivucci M (2019) Two-State Three-Mode Parameterization of the Force Field of a Retinal Chromophore Model. J Phys Chem A 123:1710–1719.

96. Manathunga, M., Jenkins, A. J., Orozco-Gonzalez, Y., Ghanbarpour, A., Borhan, B., Geiger, J. H., Larsen, D. S. and Olivucci, M. (2020) Computational and Spectroscopic Characterization of the Photocycle of an Artificial Rhodopsin. J. Phys. Chem. Lett. 4245-4252

97. Gozem, S., Johnson, P. J. M., Halpin, A., Luk, H. L., Morizumi, T., Prokhorenko, V. I., Ernst, O. P., Olivucci, M. and Miller, R. J. D. (2020) Excited-State Vibronic Dynamics of Bacteriorhodopsin from Two-Dimensional Electronic Photon Echo Spectroscopy and Multiconfigurational Quantum Chemistry. J. Phys. Chem. Lett. 3889-3896

98. Aquilante, F., Autschbach, J., Baiardi, A., Battaglia, S., Borin, V. A., Chibotaru, L. F., Conti, I., De Vico, L., Delcey, M., Fdez. Galván, I., Ferré, N., Freitag, L., Garavelli, M., Gong, X., Knecht, S., Larsson, E. D., Lindh, R., Lundberg, M., Malmqvist, P. Å., Nenov, A., Norell, J., Odelius, M., Olivucci, M., Pedersen, T. B., Pedraza-González, L., Phung, Q. M., Pierloot, K., Reiher, M., Schapiro, I., Segarra-Martí, J., Segatta, F., Seijo, L., Sen, S., Sergentu, D.-C., Stein, C. J., Ungur, L., Vacher, M., Valentini, A. and Veryazov, V. (2020) Modern quantum chemistry with [Open]Molcas. The Journal of Chemical Physics, J. Chem. Phys. 152, 214117

99. Marsili, E., Olivucci, M., Lauvergnat, D. and Agostini, F. (2020) Quantum and quantum-classical studies of the photoisomerization of a retinal chromophore model. Journal of Chemical Theory and Computation, J. Chem. Theory Comput. , in press.

100. Gueye, M., Paolino, M., Gindensperger, E., Haacke, S., Olivucci, M. and Léonard, J. (2020) Vibrational coherence and quantum yield of retinal-chromophore-inspired molecular switches. Faraday Discuss. 221, 299-321

101. Pedraza-González, L., del Carmen Marín, M., Jorge, A. N., Ruck, T. D., Yang, X., Valentini, A., Olivucci, M. and De Vico, L. (2020) Web-ARM: a Web-Based Interface for the Automatic Construction of QM/MM Models of Rhodopsins. J. Chem. Inf. Model. 60, 1481-1493