

# MARCO MARAZZI

**PERSONAL** Born June 23, 1982 in Colferro (Rome), Italy

## EDUCATION

from 5/2013 Postdoctoral Research Scientist (Humboldt Research Fellowship) at the Karlsruhe Institute of Technology, Institute of Physical Chemistry, Theoretical Chemical Biology, Germany

2/2013 Ph.D. in Fine Chemistry, University of Alcalá, Department of Physical Chemistry, Alcalá de Henares (Madrid), Spain

Doctoral Advisor: Luis Manuel Frutos

Dissertation Topic: *Photochemistry and Photophysics of Chemical and Biologically Relevant Systems: Mechanisms, Dynamics and Methodologies*

2/2009 M.Sc. in Polymer Chemistry, joint program of Humboldt University of Berlin, Technical University of Berlin, Free University of Berlin and Potsdam University, Germany

2/2007 B.Sc. in Chemistry (specialization in Materials Chemistry), Sapienza University of Rome, Italy

## EMPLOYMENT

2/2011-2/2013 Lab assistant in the University of Alcalá, Alcalá de Henares (Madrid), Spain

5/2008-1/2009 Researcher in GKSS, Institute for Polymer Research, Centre for Biomaterial Development, Teltow, Germany

## PARTICIPATION IN GRANTED PROJECTS

1/2013-12/2015 Spanish Ministry for Science and Innovation EUR 84,000

*Control of Optical and Dynamical Properties in Photoactive Proteins and Molecular Devices.*

Chief Researcher: Luis Manuel Frutos

1/2010-12/2012 Spanish Ministry for Science and Innovation EUR 87,000

*Mechanistic and Dynamical Properties of Photoinduced Electron, Proton and Energy Transfer Processes, and its Application to Chemical and Biological Systems.*

Chief Researcher: Luis Manuel Frutos

1/2012-12/2012 District of Madrid and University of Alcalá EUR 10,000

*Development of ab initio Force Fields to Describe Excited States, its Implementation in the Amber Package and Application to the Study of Triplet-Triplet Energy Transfer Processes Within Hydrogen Bonded DNA Base Pairs.*

Chief Researcher: Luis Manuel Frutos

1/2011-12/2011 District of Madrid and University of Alcalá EUR 14,000

*Computational Study of the Substituent Effect in S-nitrosothiols*

Chief Researcher: Manuel Temprado

## PUBLICATIONS

8. García-Iriepa, C.; Marazzi, M.; Frutos, L.M.; Sampedro, D.  
"E/Z Photochemical Switches: Synthesis, Properties and Applications"  
*RSC Advances*, **2013**, 3, 6241-6266.
7. García-Iriepa, C.; Marazzi, M.; Zapata, F.; Valentini A.; Sampedro, D.; Frutos, L.M.  
"Chiral Hydrogen Bond Environment Providing Unidirectional Rotation in Photoactive Molecular Motors"  
*The Journal of Physical Chemistry Letters*, **2013**, 4, 1389-1396.
6. Fernández-González, M.A.; Marazzi, M.; López-Delgado, A.; Zapata, F.; García-Iriepa, C.; Rivero, D.; Castaño, O.; Temprado, M.; Frutos, L.M.  
"Structural Substituent Effect in the Excitation Energy of a Chromophore: Quantitative Determination and Application to S-Nitrosothiols"  
*Journal of Chemical Theory and Computation*, **2012**, 8, 3293-3302.
5. Marazzi, M.; López-Delgado, A.; Fernández-González, M.Á.; Castaño, O.; Frutos, L.M.; Temprado, M.  
"Modulating Nitric Oxide Release by S-Nitrosothiols Photocleavage: Mechanism and Substituent Effects"  
*The Journal of Physical Chemistry A*, **2012**, 116, 7039-7049.
4. Marazzi, M.; Navizet, I.; Lindh, R.; Frutos, L.M.  
"Photostability Mechanisms in Human  $\gamma$ B-Crystallin: Role of the Tyrosine Corner Unveiled by Quantum Mechanics and Hybrid Quantum Mechanics/Molecular Mechanics Methodologies"  
*Journal of Chemical Theory and Computation*, **2012**, 8, 1351-1359.
3. Marazzi, M.; Blanco-Lomas, M.; Rodríguez, M.A.; Campos, P.J.; Castaño, O.; Sampedro, D.; Frutos, L.M.  
"On the Mechanism of the Photocyclization of Azadienes"  
*Tetrahedron*, **2012**, 68, 730-736.
2. Marazzi, M.; Sancho, U.; Castaño, O.; Frutos, L.M.  
"First Principles Study of Photostability Within Hydrogen-Bonded Amino Acids"  
*Physical Chemistry Chemical Physics*, **2011**, 13, 7805-7811.

**ISSUE COVER**

1. Marazzi, M.; Sancho, U.; Castaño, O.; Domcke, W.; Frutos, L.M.  
 "Photoinduced Proton Transfer as a Possible Mechanism for Highly Efficient Excited-State Deactivation in Proteins"  
*The Journal of Physical Chemistry Letters*, **2010**, *1*, 425-428.

**PUBLICATIONS SUBMITTED OR IN PREPARATION**

2. Zapata, F.; Marazzi, M; Sancho, U.; Castaño, O.; Acuña, U.; Frutos, L.M.  
 "Definition and Quantification of the Triplet Energy Transfer Reaction Coordinate"  
 In preparation.
1. Zapata, F.; Fernández-González, M.A.; Marazzi M.; Frutos L.M.  
 "Single Molecule Force Spectroscopy by Classical Dynamics Simulations: Azobenzene Under Stress"  
 In preparation.

**TEACHING**

<i>Quarter</i>	<i>Course</i>	<i>Degree</i>	<i># hours</i>
Winter 2010	General Chemistry Lab	Chemistry	20
Spring 2011	Chemical Physics Lab	Pharmacy	11
Winter 2011	General Chemistry Lab	Chemistry	20
Fall 2012	General Chemistry Lab	Chemistry	20

**MASTER THESIS CO-DIRECTED**

2012 Cristina García-Iriepea (MS in Fine Chemistry, University of Alcalá)  
 Director: Luis Manuel Frutos

2011 Miguel Á. Fernández-González (MS in Fine Chemistry, University of Alcalá)  
 Director: Luis Manuel Frutos

## CONFERENCES

(the presenting author is underlined)

### TALKS

7/18/2012 Felipe, Z.; Marazzi, M.; Fernández-González, M.A.; Acuña, A. U.; Frutos, L.M.; Castaño, O.

8th International Voevodsky Conference, Novosibirsk, Russia

7/21/2011 Marazzi, M.; Frutos, L.M.; Navizet, I.; Lindh, R.

9th Triennial Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain

7/16/2011 Frutos, L.M.; Zapata, F.; Marazzi, M.; Acuña, U.; Castaño, O.

Simulation in Organic Chemistry 2011, Vigo, Spain

7/12/2010 Castaño, O.; Frutos, L.M.; Sancho, U.; Marazzi, M.; Acuña, U.

4th Humboldt Conference on Computational Chemistry, Varna, Bulgaria

9/21/2009 Marazzi, M.; Sancho, U.; Castaño, O.; Domcke, W.; Frutos, L.M.

9th Spanish Congress on Photochemistry, Bilbao, Spain

9/15/2009 Castaño, O.; Frutos, L.M.; Sancho, U.; Marazzi, M.; Acuña, U.

24th International Workshop on Quantum Systems in Chemistry and Physics, San Lorenzo del Escorial, Spain

### POSTERS

7/16/2012 Valentini, A.; Marazzi, M.; Melaccio, F.; Gozem, S.; Olivucci, M.; Frutos, L.M.

24th IUPAC Symposium on Photochemistry, Coimbra, Portugal

7/16/2012 García-Iriepa C.; Marazzi, M.; Zapata, F.; Valentini, A.; Castaño, O.; Sampedro, D.; Frutos, L.M.

24th IUPAC Symposium on Photochemistry, Coimbra, Portugal

7/16/2012 Marazzi, M.; Fernández-González, M.A.; Zapata, F.; García-Iriepa, C.; Rivero, D.; Castaño, O.; Temprado, M.; Frutos, L.M.

24th IUPAC Symposium on Photochemistry, Coimbra, Portugal

7/11/2010 Marazzi, M.; Frutos, L.M.; Castaño, O.; Temprado, M.

23th IUPAC Symposium on Photochemistry, Ferrara, Italy

7/1/2010 Marazzi, M.; Sancho, U.; Acuña, U.; Castaño, O.; Frutos, L.M.

7th Congress on Electronic Structure: Principles and Applications, Oviedo, Spain

7/1/2010 Marazzi, M.; Olivucci, M.; Castaño, O.; Frutos, L.M.

7th Congress on Electronic Structure: Principles and Applications, Oviedo, Spain

7/19/2009 Marazzi, M.; Sancho, U.; Castaño, O.; Domcke, W.; Frutos, L.M.

24th International Conference on Photochemistry, Toledo, Spain

### TALKS IN GROUP AND DEPARTMENTAL SEMINARS

10/17/2012 Mark A. Ratner Group, Department of Chemistry, Northwestern University, Evanston, Illinois

08/05/2011 Laboratory for Computational Photochemistry and Photobiology, Department of Chemistry, Bowling Green State University, Bowling Green, Ohio

10/15/2010 Department of Chemistry – Ångström, The Theoretical Chemistry Program, Uppsala University, Uppsala, Sweden

03/31/2010 Division of Nucleic Acids Chemistry, Belozersky Institute of Physico-Chemical Biology, Lomonosov Moscow State University, Moscow, Russia

## **COURSES AND SCHOOLS ATTENDED**

1/16-1/20/2012 *7th MOLCAS Workshop*, Department of Chemistry – Ångström, The Theoretical Chemistry Program, Uppsala University, Uppsala, Sweden

7/7-7/12/2008 *Mixed Quantum-Classical Dynamics: Foundations and Application to Photo-Biological Questions*, University of Vienna, Vienna, Austria

3/3-3/7/2008 *29th Berlin School on Neutron Scattering*, Hahn-Meitner-Institute, Berlin, Germany

7/24-9/15/2006 *DESY Summer Students Program*, Deutsches Elektronen-Synchrotron, Hamburg, Germany

## **SCHOLARSHIPS**

9/2012-10/2012 *Exchange Program of the University of Alcalá*, spent in Department of Chemistry, Northwestern University, Evanston, Illinois (Prof. Mark A. Ratner)

8/2011-10/2011 *Exchange Program of the University of Alcalá*, spent in Department of Chemistry, Laboratory for Computational Photochemistry and Photobiology, Bowling Green State University, Bowling Green, Ohio (Prof. Massimo Olivucci)

8/2010-10/2010 *Exchange Program of the University of Alcalá*, spent in Department of Chemistry – Ångström, The Theoretical Chemistry Program, Uppsala University, Uppsala, Sweden (Prof. Roland Lindh)

10/2005-2/2006 *European Union Erasmus Exchange Program*, spent in Polytechnic Institute for Materials, Joseph Fourier University, Grenoble, France

## **PROFESSIONAL SOCIETIES**

American Chemical Society, Member  
European Photochemistry Association, Member  
Spanish Chemical Society, Member

## **AWARDS**

Master Distinction promoted by the German Academic Exchange Service (DAAD)