

# ELISA PIERI

## PERSONAL INFORMATION

Born in Siena (Italy), 14 July 1990

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## ACADEMICS

2019 Stanford University, United States of America

*Postdoctoral  
Fellowship*

TOPICS: *Study of photoreactions by means of excited state dynamics, potential energy surfaces mapping and QM/MM techniques; nanoreactor on the excited state.*

2015-2018 University of Aix-Marseille, France

*PhD in  
Computational  
Photochemistry*

THESIS: *Investigating the pH-Dependency of Biomolecules Photoactivity Using a Multiscale CpHMD-then-QM/MM Approach*

SUPERVISORS: Pr. Nicolas FERRÉ & Dr. Vincent LEDENTU

COMMITTEE: Pr. Ursula RÖTHLISBERGER, Pr. Matthias ULLMANN, Pr. Elise DUMONT & Dr. Frédéric Biaso

2012-2014 University of Siena, Italy

*M.Sc. in  
Chemistry*

FINAL GRADE: 110/110 cum laude

THESIS: *Force Fields and Non-Adiabatic Dynamics of Biomimetic Molecular Motors*

SUPERVISOR: Pr. Massimo OLIVUCCI

2009-2012 University of Siena, Italy

*B.Sc in Chemical  
Sciences*

FINAL GRADE: 110/110 cum laude

THESIS: *Synthesis progress on Epibatidine Analogues*

SUPERVISORS: Pr. Massimo OLIVUCCI & Dr. Sandeep HANDA

## PROJECTS & COLLABORATIONS

2015-2018 ANR/DFG Co-Funded Project "FEMTO-ASR".

2016 Pr. François DEHEZ & Pr. Christophe CHIPOT (*University of Lorraine*).

2018 Pr. Massimo OLIVUCCI (*University of Siena*).

2018 Pr. Tiago BUCKUP (*University of Heidelberg*).

2018-2019 Dr. Oliver WEINGART (*University of Düsseldorf*).

2019 Pr. Dan NEUMARK & Blake ERICKSON (*University of California, Berkeley*).

2019 Pr. Steven A. LOPEZ & Jordan COX (*Northeastern University*).

## PUBLICATIONS

- JCTC  
2018  
*In Preparation* A Computational Study on the pH Impact on the Anabaena Sensory Rhodopsin Excited State Dynamics.  
E. Pieri, V. Ledentu, O. Weingart, M. Garavelli and N. Ferré
- JCTC  
2018  
Submitted *In-silico identification of the amino-acids responsible for the Anabaena Sensory Rhodopsin pH-dependent electronic absorption spectrum*  
E. Pieri, V. Ledentu, M. Sahlin, F. Dehez, C. Chipot and N. Ferré
- PCCP  
2018, 20  
30159-30173 *Mapping the Ultrafast Vibrational Dynamics of all-Trans and 13-Cis Retinal Isomerization in Anabaena Sensory Rhodopsin*  
P. P. Roy, Y. Kato, R. Abe-Yoshizumi, E. Pieri, N. Ferré, H. Kandori and T. Buckup
- PCCP  
2018, 20  
23252-23261 *Sampling the protonation states: pH-dependent UV absorption spectrum of a*

*polypeptide dyad*

E. Pieri, V. Ledentu, M. Huix-Rotllant and N. Ferré

PCCP

2017, 19

14073-14084

*pH-Dependent absorption spectrum of a protein: a minimal electrostatic model of Anabaena sensory rhodopsin*

M. Stenrup, E. Pieri, V. Ledentu and N. Ferré

JACS

2016, 138 (31)

9807-9825

*Design, Synthesis and Dynamics of a GFP Fluorophore Mimic with an Ultrafast Switching Function*

M. Paolino, M. Gueye, E. Pieri, M. Manathunga, S. Fusi, L. Latterini, D. Pannacci, M. Filatov, J. Léonard, M. Olivucci and A. Cappelli

JPC Letters

2015, 6 (4)

599-604

*Directionality of Double-Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center*

G. Marchand, J. Eng, I. Schapiro, A. Valentini, L. M. Frutos, E. Pieri, M. Olivucci, J. Léonard and E. Gindensperger

## OTHER COMMUNICATIONS

*Invited Speaker*

Stanford

ORAL: *Investigating the pH-Dependency of the Anabaena Sensory Rhodopsin Photoactivity Using a Multiscale CpHMD-then-QM/MM Approach**Invited Speaker*

Jyväskylä

ORAL: *Investigating the pH-Dependency of the Anabaena Sensory Rhodopsin Photoactivity Using a Multiscale CpHMD-then-QM/MM Approach**Invited Speaker*

Montpellier

ORAL: *Computationally Assessing the pH Impact on the Anabaena Sensory Rhodopsin Photochemistry*

ICRP2018

POSTER: *Computationally Assessing the pH Impact on the Anabaena Sensory Rhodopsin Excited State Dynamics*

E. Pieri, V. Ledentu, O. Weingart and N. Ferré

QMMM2017

ICP2017

SCF-PACA2017

ORAL: *Modulation of the Peptide M Absorption Spectrum with the pH*

E. Pieri, V. Ledentu and N. Ferré

ESBS2016

ECPC2017

POSTER: *Modulation of the Peptide M Absorption Spectrum with the pH*

E. Pieri, V. Ledentu and N. Ferré

MQM2016

POSTER: *Titration Curves Calculation using CpHMD in Anabaena Sensory Rhodopsin*

E. Pieri, V. Ledentu, M. Stenrup and N. Ferré

## COMPUTER SKILLS

*Miscellaneous*Fortran, Python, Bash, ViM, L<sup>A</sup>T<sub>E</sub>X, OpenOffice, C*Scientific*

MOLCAS, AMBER, Terachem, FMS90, GAUSSIAN, Tinker, PropKa, H++, MCCE, Chimera, Molden, VMD, PyMOL, Avogadro, Sparky, PSPP

## TEACHING ACTIVITY

2016-2018

Organic Chemistry, Thermodynamics, Analytical Chemistry

2016-2018

University Graduate Degree in *Pedagogy for higher education*

## OTHER INFORMATION

*Scholarships*MARCH-AUGUST 2012 · *"European Union Erasmus Exchange Program"* spent in University of Leicester (Department of Chemistry), United Kingdom.*Schools & Courses*JUNE-JULY 2011 · *"Emory@Unisi Summer School 2011"* spent in University of Siena (Department of Chemistry), Italy.1-4 APRIL 2014 · *"Introduction to Fortran 90"*, SCAI-CINECA, Segrate, Milan, Italy.5-6 MAY 2014 · *"Introduction to Scientific and Technical Computing in C"*, SCAI-CINECA, Segrate, Milan, Italy.18-20 NOVEMBER 2015 · *"High Performance Molecular Dynamics"*, SCAI-CINECA, Casalecchio di Reno, Bologna, Italy.NOVEMBER-DECEMBER 2015 · *"Cours du label chimie thorique"*, RCTF, ENS, Lyon, France.

23-27 MAY 2016 · "*Dynamol 2016*", Société Chimique de France & Société Française de Physique, Chimie ParisTech, Paris, France.

31 JANUARY-2 FEBRUARY 2018 · "*Virtual Winterschool 2018*".

*Languages*

ENGLISH · Fluent (IELTS 2015 Overall Band Score 7.5 - Listening 7.5, Reading 8.0, Writing 6.5, Speaking 7.0)

FRENCH · Fluent

ITALIAN · Mothertongue

May 14, 2019