Elisa Pieri | CV

Postdoctoral Fellow at Stanford University

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Fields: Theoretical/Computational Chemistry, Photochemistry and Photobiology

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Education and Training

PostDoc in Theoretical Chemistry - Stanford University — Current

- Supervisor: Todd J. Martínez
- Projects: Development of the NonAdiabatic Nanoreactor, computational study of red fluorescent proteins, photochemistry of thymine analogues and other small molecules

PhD in Computational Photochemistry - Aix-Marseille University — 2018

- Supervisors: Nicolas Ferré and Vincent Ledentu
- Dissertation: Investigating the pH-Dependency of Biomolecules Photoactivity Using a Multiscale CpHMD-then-QM/MM Approach
- Committee: Ursula Röthlisberger, Matthias Ullmann, Elise Dumont and Frédéric Biaso

M.Sc. in Chemistry - University of Siena — 2014

- Supervisor: Massimo Olivucci
- Master thesis: Force Fields and Non-Adiabatic Dynamics of Biomimetic Molecular Motors
- Final grade: 110/110 magna cum laude

B.Sc in Chemical Sciences - University of Siena — 2012

- Supervisors: Massimo Olivucci and Sandeep Handa
- Bachelor thesis (redacted during ERASMUS stay): Synthesis progress on Epibatidine Analogues
- Final grade: 110/110 magna cum laude

Peer reviewed Publications

10. "The Non-Adiabatic Nanoreactor: Towards the Automated Discovery of Photochemistry.", **E. Pieri**, D. Lahana, A.M. Chang, C.R. Aldaz, K.C. Thompson and T.J. Martínez, *Chemical Science, **2021**, 12, 7294-7307*, DOI:10.1039/D1SC00775K.

9. "ChemVox: Voice-Controlled Quantum Chemistry.", U. Raucci, A. Valentini, **E. Pieri**, H. Weir, S. Seritan and T.J. Martínez, *Nature Computational Science, **2021**, 1, 42-45* DOI:10.1038/s43588-020-00012-9.

8. "Frontiers in Multiscale Modelling of Photoreceptor Proteins", M. Mroginski, S. Adam, G. Amoyal, A. Barnoy, A. Bondar, V. Borin, J. Church, T. Domratcheva, B. Ensing, F. Fanelli, N. Ferré, O. Filiba, L. González, R. González, C. González-Espinoza, R. Kar, L. Kemmler, S. Kim, J. Kongsted, A. Krylov, Y. Lahav, M. Lazaratos, Q. Eddin, I. Navizet, A. Nemukhin, Ma. Olivucci, J. Olsen, A. Pérez de Alba Ortíz, **E. Pieri**, A. Rao, Y. Rhee, N. Ricardi, S. Sen, I. Solov'yov, L. De Vico, T. Wesolowski, C. Wiebeler, X. Yang and I. Schapiro, *Photochem. Photobiol., Invited Review, **2020*** DOI:10.1111/php.13372.

7. "Relaxation Dynamics of Hydrated Thymine, Thymidine, and Thymidine Monophosphate Probed by Liquid Jet Time-Resolved Photoelectron Spectroscopy.", B.A. Erickson, Z.N. Heim, **E. Pieri**, E. Liu, T.J. Martínez and D.M. Neumark, *J. Phys. Chem. A **2019**, 123, 50, 10676-10684*, DOI:10.1021/acs.jpca.9b08258.

6. "CpHMD-Then-QM/MM 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, M. Olivucci and N. Ferré, *J. Chem. Theory Comput. **2019**, 15, 8, 4535-4546*, DOI:10.1021/acs.jctc.9b00221.

5. "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, *Phys. Chem. Chem. Phys., **2018**, 20, 30159-30173*, DOI:10.1039/c8cp05469j.

4. "Sampling the protonation states: pH-dependent UV absorption spectrum of a polypeptide dyad.", **E. Pieri**, V. Ledentu, M. Huix-Rotllant and N. Ferré, *Phys. Chem. Chem. Phys., **2018**, 20, 23252-23261*, DOI:10.1039/c8cp03557a.

3. "pH-Dependent absorption spectrum of a protein: a minimal electrostatic model of Anabaena Sensory Rhodopsin.", M. Stenrup, **E. Pieri**, V. Ledentu and N. Ferré, *Phys. Chem. Chem. Phys., **2017**, 19, 14073-14084*, DOI:10.1039/c7cp00991g.

2. "Design, synthesis and dynamics of a Green Fluorescent Protein 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, *J. Am. Chem. Soc. **2016**, 138, 31, 9807-9825*, DOI:10.1021/jacs.5b10812.

1. "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, *J. Phys. Chem. Lett. **2015**, 6, 4, 599-604*, DOI:10.1021/jz502644h.

- "Predicting and Understanding Fluorescent Quantum Yield in RFP Variants.", **E. Pieri**, A.R. Walker, N. Zhu and T.J. Martínez, *In preparation*.
- "Modeling pH-Dependent Biomolecular Photochemistry", **E. Pieri**, O. Weingart, M. Garavelli, and N. Ferré, *In preparation*.
- "TCPB: Accessing TeraChem as an External Library for Faster QM or QM/MM Simulations.", V. W. D. Cruzeiro, Y. Wang, **E. Pieri**, E. G. Hohenstein, T.J. Martínez, *In preparation*.
- "From Chemical Reaction Discovery to Kinetic Modeling: The Ab Initio Nanoreactor.", R. Xu, A. M. Chang, **E. Pieri** and T.J. Martínez, *In preparation*.

Academic Service and Leadership

Journal reviewer (J. Phys. Chem., J. Chem. Theory Comput. and Comput. Phys. Comm.)	2020-present
Leader of the Proteins Subgroup in the Martínez group	2022, Stanford
Member of the organizing team for mentoring programs in the Martínez group	2021, Stanford
Member of the organizing team for Bay Area Theoretical Chemistry (BATChem) 2021	2021, Stanford
Member of the organizing team for Virtual Conference of Theoretical Chemistry 2020	2020, Stanford
Invited Speaker at the University Open Day as successful alumna	2019, Siena
Member of the organizing team for the MOLCAS Developer Workshop	2015, Siena
Member of the organizing team for the Emory@Unisi Summer School	2011, Siena

Teaching and Mentoring Experience

Mentoring Activity - Master and Graduate level 2014-present

Master level: one student in Siena (2014-2015), one student in Marseille (2017)
Graduate level: two students in Stanford (2020-present)

Quantum Molecular Design Summer School - Lecturer 2019/21, Stanford

Modules: Classical Molecular Dynamics, Force Field and QM/MM Simulations of Proteins

Pedagogy for Higher Education - Diploma 2018, Marseille

Activities:
- Seminars, graded classes and workshops (120 hours)
- On the field training and experience (144 hours)

Teaching Assistant - Undergraduate and Master Courses 2017-18, Marseille

Courses: Organic Chemistry, Thermodynamics, Analytical Chemistry,
Analytical Chemistry II, Physical Chemistry II

Research Experience

Stanford University - Todd J. Martínez's Group 2019-current

- Conceiving and implementing a NonAdiabatic Nanoreactor for the automatic exploration of photochemistry, initially testing on benzene.
- Mapping the ground and excited states potential energy surfaces of five Red Fluorescent Protein mutants to study the effect of mutations on the quantum yield.
- Simulating the excited state behavior of thymine and its derivatives in gas phase using the *Ab Initio* Multiple Spawning method, in order to elucidate and compare the photorelaxation mechanisms.
- Developing ChemVox, an Alexa skill to request quantum calculations and receive the results in real time.

Aix-Marseille University - Nicolas Ferré's Group 2015-2018

- Conceived and implemented a protocol to incorporate CpHMD within a QM/MM framework to study the pH-dependent photochemical properties of biological macromolecules.
- Tested the protocol in the reproduction of Peptide M's absorption spectrum at various pH values.
- Applied the protocol to Anabaena Sensory Rhodopsin (ASR), making use of homology modeling techniques and embedding the protein in a membrane, in order to study the pH-dependence of its absorption spectrum.
- Simulated the pH-dependent excited state dynamics of ASR using the CpHMD information in a massive QM/MM study.

University of Siena - Massimo Olivucci's Group 2013-2015

- Designed retinal-inspired molecular photoswitches and motors and investigated their photochemical properties through potential energy surface mapping and semi-classical nonadiabatic molecular dynamics.

University of Leicester - Sandeep Handa's Group 2012

- Verified and improved organic synthetic routes to fluorinated epibatidine analogues.

Presentations

- "Understanding Fluorescent Quantum Yield in RFP variants", ACTC 2022, Tahoe, **Poster**.
- "The NonAdiabatic NanoReactor: Towards the Automated Discovery of Photochemistry", BASF Fall Meeting 2022, Berkeley, **Poster**.
- "The NonAdiabatic NanoReactor: Towards the Automated Discovery of Photochemistry", ACS Fall 2021, virtual, **Conference Talk**.
- "Predicting and Understanding Fluorescent Quantum Yield in RFP Variants", BATChem 2021, virtual, **Poster, honorable mention in the Lightning Talk competition**.
- "The NonAdiabatic NanoReactor: Towards the Automated Discovery of Photochemistry", 2021, Marseille, **Invited Talk**.
- "The NonAdiabatic NanoReactor: Towards the Automated Discovery of Photochemistry", VCTC2020, virtual, **Conference Talk, awarded in the Lightning Talk competition**.
- "Investigating the pH-Dependency of the Anabaena Sensory Rhodopsin Photoactivity Using a Multiscale CpHMD-then-QM/MM Approach", 2018, Jyväskylä, **Invited Talk**.
- "Computationally Assessing the pH Impact on the Anabaena Sensory Rhodopsin Photochemistry", 2018, Montpellier, **Invited Talk**.
- "Computationally Assessing the pH Impact on the Anabaena Sensory Rhodopsin Excited State Dynamics", ICRP2018, Toronto, **Poster**.
- "Modulation of the Peptide M Absorption Spectrum with the pH", QMMM2017, Manchester, **Conference Talk**.
- "Modulation of the Peptide M Absorption Spectrum with the pH", ECPC2017, Borgo, **Poster**.
- "Modulation of the Peptide M Absorption Spectrum with the pH", ICP2017, Strasbourg, **Conference Talk**.
- "Modulation of the Peptide M Absorption Spectrum with the pH", SCF-PACA2017, Marseille, **Conference Talk**.
- "Modulation of the Peptide M Absorption Spectrum with the pH", ESBS2016, Marseille, **Poster**.
- "Titration Curves Calculation using CpHMD in Anabaena Sensory Rhodopsin", MQM2016, Uppsala, **Poster**.

Spoken Languages

- Italian (mother-tongue)
- English
- French