Elisa Pieri

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Research interests: Theoretical/Computational Chemistry, Photochemistry and Photobiology

Education and Training

PhD in Computational Photochemistry - Aix-Marseille University 2015-2018
- Supervisors: Nicolas Ferré and Vincent Ledentu
- Dissertation title: "Investigating the pH-Dependency of Biomolecules Photoactivity Using a Multiscale CpHMD-then-QM/MM Approach"

M.Sc. in Chemistry - University of Siena 2012-2014
- Supervisor: Massimo Olivucci
- Master thesis title: "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 2009-2012
- Supervisors: Massimo Olivucci and Sandeep Handa
- Bachelor thesis (redacted during ERASMUS stay): "Synthesis progress on Epibatidine Analogues"
- Final grade: 110/110 magna cum laude

Professional Experience

PostDoc in Theoretical Chemistry - Stanford University 2019-present
- Supervisor: Todd J. Martínez

Teaching Assistant - Undergraduate and Master Courses 2017-18, Marseille
- Organic Chemistry, Thermodynamics, Analytical Chemistry, Analytical Chemistry II, Physical Chemistry II

Honors and Awards

- Honorable mention in the Lightning Talk competition at Bay Area Theoretical Chemistry (BATChem) 2021
- Winner of the Lightning Talk competition at VCTC 2020
- Bacio Accademico (a highly selective Italian commendation for particularly deserving students) awarded to the undergraduate career for the efforts devoted towards internationality in 2012
- Erasmus Scholarship in 2012 (6 months)

Research Experience

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

- Develop a NonAdiabatic Nanoreactor for the automatic exploration of photochemistry, initially testing on benzene.
- Map the ground and excited states potential energy surfaces of Red Fluorescent Protein to study the relationship between mutations and brightness.
- Simulate the excited state behavior of thymine and its derivatives in gas phase using the *Ab Initio* Multiple Spawning method, to elucidate and compare the photorelaxation mechanisms.
- Develop 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.
- Elucidated pH-dependence of the Anabaena Sensory Rhodopsin (ASR) absorption spectrum in a membrane.
- Simulated the pH-dependent excited state dynamics of ASR using QM/MM and CpHMD.

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

- Improved organic synthetic routes to fluorinated epibatidine analogues.

Publications

16. "Predicting and Understanding Fluorescent Quantum Yield in RFP Variants.", **E. Pieri**, A. R. Walker, N. Zhu and T. J. Martínez (draft available upon request).
15. "Sugar Conformations Affect the Photophysics of the Canonical Nucleoside Thymidine", J. L. Godínez Castellanos, M. Bain, **E. Pieri**, T. J. Martínez and S. Bradforth (in preparation).
14. "Modeling pH-Dependent Biomolecular Photochemistry", **E. Pieri**, O. Weingart, M. Garavelli, and N. Ferré (in preparation).
13. "From Chemical Reaction Discovery to Kinetic Modeling: The Ab Initio Nanoreactor.", R. Xu, A. M. Chang, **E. Pieri** and T. J. Martínez (in preparation).
12. "Conformational Ensembles Reveal Origins of Serine Protease Catalysis", S. Du, R. C. Kretsch, J. Parres-Gold, **E. Pieri**, V. W. D. Cruzeiro, M. Zhu, T. J. Martínez and D. Herschlag (in preparation).
11. "TeraChem Protocol Buffers (TCPB): Accelerating QM and QM/MM Simulations with a Client-Server Model.", V. W. D. Cruzeiro, Y. Wang, **E. Pieri**, E. G. Hohenstein, T. J. Martínez, *J. Chem. Phys.*, **2023**, DOI: 10.1063/5.0130886.
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.

Presentations

- "The NonAdiabatic NanoReactor: Towards the Automated Discovery of Photochemistry", 2022, Los Angeles, **Invited Talk**.
- "Understanding Fluorescent Quantum Yield in RFP variants", ACTC 2022, Palisades 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, **Contributed 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", VCTC 2020, virtual, **Invited Talk as a winner of 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, **Contributred 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, **Contributed Talk**.
- "Modulation of the Peptide M Absorption Spectrum with the pH", SCF-PACA2017, Marseille, **Contributed 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**.

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

Pedagogy for Higher Education - Diploma 2018, Marseille
- Seminars, graded classes, and workshops (120 hours)
- Field training and experience (144 hours)

Teaching Assistant - Undergraduate and Master Courses 2017-18, Marseille
- Organic Chemistry, Thermodynamics, Analytical Chemistry, Analytical Chemistry II, Physical Chemistry II

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 2021-present
- Member of the organizing team for mentoring programs in the Martínez group 2021-present
- 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

Languages

- Italian (mother-tongue)
- English
- French