

M^a DEL CARMEN MARÍN PÉREZ



Ph.D. Chemical Sciences and Pharmacy

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WORK EXPERIENCE

JSPS Postdoctoral Fellowship

University of Tokyo (ISSP)

📅 Nov 2020 – 📍 Kashiwano-ha, Kashiwa, Japan

- Physicochemical study on the molecular mechanism of microbial rhodopsins and other photo-receptive proteins.

Laboratory Analyst

La Bética Aceitera S.C.A.

📅 Nov 2019 – Mar 2020 📍 Quesada, Jaén, Spain

- Analysis of olive and pomace yields by Soxhlet method and NIR and NMR spectroscopy.

MIUR Fondation Postdoctoral Scholarship

University of Siena (UNISI)

📅 Nov 2018 – Oct 2019 📍 Siena, Italy

- Computational research of fluorescent mutants for Optogenetic applications.

Ph.D. Internship

Institute of Physics and Chemistry of Materials (CNRS)

📅 Nov 2017 – Feb 2018 📍 Strasbourg, France

- Development and applications of computational QM/MM models to discover/understanding the high fluorescence observed in some mutants in microbial rhodopsins.

Ph.D. Internship

Laboratory of Computational Photochemistry and Photobiology (BGSU)

📅 Mar – Aug 2016 📍 Bowling Green, Ohio, EEUU

- Computational investigation of the “Primary event” observed in biological photoreceptors. Development of a computational protocol for the automatic construction of congruous sets of QM/MM models of rhodopsin-like photoreceptors.

MSc. Internship

MINYANOTECH. University of Alcalá (UAH)

📅 Jan – Jul 2015 📍 Madrid, Spain

- Development of new material modified with nanomaterials for electrochemical sensing and (bio)sensing.

BSc. Internship

Nutrientes Foliars S.A.

📅 Jul – Sep 2013 📍 Quesada, Jaén, Spain

- Development and analysis of new fertilizers for treatment of olive, vineyard and fruit trees.

EDUCATION

Ph.D. Chemical Sciences and Pharmacy

University of Siena

📅 Nov 2015–Mar2019 📍 Siena, Italy

- GPA: *Cum Laude*

MSc. Characterization of Chemical Systems

University of Alcalá

📅 Sep 2014 – Jul 2015 📍 Madrid, Spain

- GPA: 7.8/10

BSc. Chemistry

University of Jaén

📅 Sep 2010 – Jul 2014 📍 Jaén, Spain

- Specialty: Oil technology
- GPA: 7.5/10




SCIENTIFIC SKILLS

- Extensive knowledge of the most advanced computational chemistry methods (level of theory), including but not limit to:
 - Wave function-based methods, such as C(R)ASSCF/MS-C(R)ASPT2
 - DFT and TD-DFT
 - Semi-empirical methods (MP2)
 - Embedding methodologies, such as QM/MM and solvation models
- Highly skilled in the description of chemical and photochemical reaction paths, though the location of:
 - Stationary structures
 - Conical intersections
 - Minimum energy paths
- Description and rationalization of chemical reactions.
- Experienced in the retrieval of physical chemical properties of molecules, with particular emphasis on photoactive compounds.
- Excellent interpersonal skills, demonstrated by communicating with supervised students, colleagues and non-technical professionals on a daily basis.
- Able to work individually without direct supervision and also as a dedicated member of a technical team whenever required.

STRENGTHS

- Leadership and team work
- Fast learner
- Critical thinking
- Good communication skills
- Data analysis and numerical reasoning

PROGRAMMING

Fortran, Python, Bash 
Molcas, Propka, Office package, Latex 
Avogadro, Gaussian, Molden, VMD, PyMol 

PUBLICATIONS

- L. Pedraza-González, M.d.C. Marín, A. N. Jorge, T. D. Ruck, X. Yang, A. Valentini, M. Olivucci and L. De Vico (2020) "Web-ARM: a Web-Based Interface for the Automatic Construction of QM/MM Models of Rhodopsins" *J. Chem. Inf. Model.* 60(3): 1481-1493.
- K. Inoue, M.d.C. Marín, S. Tomida, R. Nakamura, Y. Nakajima, M. Olivucci, and H. Kandori (2019) "Red-shifting Mutation of Light-driven Sodium Pump Rhodopsin" *Nature Comm.* 10(1): 1993-2004.
- L. Pedraza-González, L. De Vico, M.d.C. Marín, F. Fanelli and M. Olivucci (2019) "*a*-ARM: Automatic Rhodopsin Modeling with Chromophore Cavity Generation, Ionization State Selection and External Counter-ion Placement" *J. Chem. Theory Comput.*, 15(5): 3134-3152.
- M.d.C. Marín, L. De Vico, S.S. Dong, L. Gagliardi, D.G. Truhlar and M. Olivucci (2019) "Assessment of MC-PDFT excitation energies for a set of QM/MM models of rhodopsins" *J. Chem. Theory Comput.* 15(3): 1915-1923.
- M.d.C. Marín, D. Agathangelou, Y. Orozco-Gonzalez, A. Valentini, Y. Kato, R. Abe-Yoshizumi, H. Kandori, A. Choi, K-H. Jung, S. Haacke, and M. Olivucci (2019) "Fluorescence Enhancement of a Microbial Rhodopsin via Electronic Reprogramming" *J. Am. Chem. Soc.* 141(1): 262-271.
- D. Agathangelou, Y. Orozco-Gonzalez, M.d.C. Marín, P.P. Roy, J. Brazard, H. Kandori, K-H. Jung, J. Léonard, T. Backup, N. Ferré, M. Olivucci and S.Haacke (2018) "Effect of point mutations on the ultrafast photo-isomerization of *Anabaena* sensory rhodopsin" *Faraday Discuss.* 207, 55-75.
- D. Smyrnova, M.d.C. Marín, M. Olivucci and A. Ceulemans (2018) "Systematic excited state studies of reversibly switchable fluorescent proteins" *J. Chem. Theory Comput.* 14(6): 3163-3172.
- Y. Orozco-Gonzalez, M. Manathunga, M.d.C. Marín, D. Agathangelou, K-H. Jung, F. Melaccio, N. Ferré, S. Haacke, K. Coutinho, S. Canuto, and M. Olivucci (2017) "An average solvent electrostatic configuration protocol for QM/MM free energy optimization: Implementation and application to rhodopsin systems" *J. Chem. Theory Comput.* 13(12): 6391-6404.
- F. Melaccio, M.d.C. Marín, A. Valentini, F. Montisci, S. Rinaldi, M. Cherubini, X. Yang, Y. Kato, M. Stenrup, Y. Orozco-Gonzalez, N. Ferré, H.L. Luk, H. Kandori, and M. Olivucci (2016) "Toward automatic rhodopsin modeling as a tool for high-throughput computational photobiology" *J. Chem. Theory Comput.* 12(12): 6020-6034.
- M. Moreno-Guzman, A. Martín, M.d.C. Marín, T. Sierra, A. Ansón-Casaos, M.T. Martínez, A. Escarpa (2016) "Electrochemical behavior of hybrid carbon nanomaterials: the chemistry behind electrochemistry" *Electrochimica Acta* 214: 286-294.

LANGUAGES

- Spanish: Mother Tongue
- English: Official Cambridge Certificate (Level B2)
- Italian: Official CILS Certificate (Level B1)

HONORS & AWARDS

- **Primo Levi Award 2019:** Awarded with the **Mention of Merit** by Italian Chemical Society.
- **TEDx Communication Siena 2019** "Our journey, our vision, an excellent project!"
- **Best Ph.D. Thesis Cycle XXXI** awarded by the University of Siena.
- Awarded with **Project of Excellent 2018-2022 Foundation Scholarship** (MIUR, Nov 2018 – Oct 2019). University of Siena (Italy).

REFERENCES

Prof. Keiichi Inoue

@ inoue@issp.u-tokyo.ac.jp

✉ **Associated Professor.**The Institute for Solid State Physics.
University of Tokyo
5-1-5, Kashiwanoha, Kashiwa, 277-0882 Chiba, Japan
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Prof. Massimo Olivucci

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✉ **Full Professor.** Department of Biotechnology, Chemistry and Pharmacy.
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Prof. Luis Manuel Frutos

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✉ **Full Professor.**Department of Analytical Chemistry, Physical Chemistry and Chemical Engineering.
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EXTRA INFORMATION

- **Driving license category B.**
- **Availability to geographic mobility**
- Official certification of prevention of occupational hazards
- Extensive experience in agricultural campaign (olive harvesting)