

Complete list of publications of Marco Marazzi

Publications with peer review process

1. Runčevski, T.; Blanco-Lomas, M.; Marazzi, M.; Cejuela, M.; Sampedro, D.; Dinnebier, R.E.
Following a Reconstructive Phase Transformation: Photo-Induced Dimerization of a GFP Chromophore Derivative.
Angew. Chem. Int. Ed., **2014**, 53, DOI: 10.1002/anie.201402515.
2. Zapata, F.; Fernández-González, M.A.; Rivero, D.; Álvarez, Á.; Marazzi, M.; Frutos, L.M.
Toward an Optomechanical Control of Photoswitches by Tuning Their Spectroscopical Properties: Structural and Dynamical Insights into Azobenzene.
Journal of Chemical Theory and Computation, **2014**, 10, 312-323.
3. Zapata, F.; Marazzi, M.; Castaño, O.; Acuña, U.; Frutos, L.M.
Definition and Determination of the Triplet-Triplet Energy Transfer Reaction Coordinate.
Journal of Chemical Physics, **2014**, 140, 034102.
4. García-Iriepa, C.; Marazzi, M.; Frutos, L. M.; Sampedro, D.
E/Z photochemical switches: synthesis, properties and applications.
RSC Advances **2013**, 3, 6241-6266.
5. 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.
7. Marazzi, M.; López-Delgado, A.; Fernández-González, M. A.; 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.
8. Marazzi, M.; Navizet, I.; Lindh, R.; Frutos, L. M.
Photostability mechanisms in human γ 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.
9. 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.

10. 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, 7805-781
11. 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 without peer review process

(PO: poster; OC: oral communication; L: lecture; IL: invited lecture; PL: plenary lecture)

12. Torcal, B.; Moron, V.; Marazzi, M.; Wanko, M.; Rubio, A.
Glimpse of the photo-physics in fluorescent proteins
6th International Workshop on Time-Dependent Density-Functional Theory: Prospects and Applications, Benasque, Spain, January 2014.
13. Marazzi, M.; Watanabe, H.C.; Welke, K.; Torcal, B.; Wanko, M.; Elstner, M.
Proteins activated by light as single-component tools for optogenetics and fluorescence imaging.
Humboldt Network Meeting, Jena, Germany, November 2013.
14. Sampedro, D.; García-Iriepa, C.; Marazzi, M.; Zapata, F.; Valentini, A.; Frutos, L.M.
Chiral hydrogen bond environment providing unidirectional rotation in photoactive molecular motors.
26th International Conference on Photochemistry, Leuven, Belgium, July 2013.
15. Marazzi, M.; Fernández-González, M. A.; Zapata, F.; García-Iriepa, C.; Rivero, D.; Castaño, O.; Temprado, M.; Frutos, L. M.
Tuning the absorption spectra of a chromophore by structural effects induced by chemical substitution.
24th IUPAC Symposium on Photochemistry, Coimbra, Portugal, July 2012, PO-135.
16. Valentini, A.; Marazzi, M.; Melaccio, F.; Gozem, S.; Olivucci, M.; Frutos, L. M.
Local CASPT2/CASSCF gradient scaling on QM/MM rhodopsin models.
24th IUPAC Symposium on Photochemistry, Coimbra, Portugal, July 2012, PO-198.
17. García-Iriepa, C.; Marazzi, M.; Zapata, F.; Valentini, A.; Castaño, O.; Sampedro, D.; Frutos, L. M.
Hydrogen bonds in molecular motors as a way to achieve unidirectional rotation: a mechanistic and dynamical study.
24th IUPAC Symposium on Photochemistry, Coimbra, Portugal, July 2012, PO-183.
18. Zapata, F.; Marazzi, M.; Fernández-González, M. A.; Acuña, U.; Frutos, L. M.; Castaño, O.
A quantum chemical approach to the non-vertical triplet-triplet energy transfer.
8th International Voevodsky Conference, Novosibirsk, Russia, July 2012, L-17, p. 45.
19. Marazzi, M.; Frutos, L. M.; Navizet, I.; Lindh, R.
Ultrafast internal conversion as a possible mechanism of photostability in gamma-crystallin.
9th Triennial Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain, July 2011, OC-127.

20. Frutos, L. M.; Zapata, F.; Marazzi, M.; Acuña, A. U.; Castaño, O.
Definition of the triplet energy transfer reaction coordinate.
Simulations in Organic Chemistry 2011, Vigo, Spain, July 2011, IL.
21. Marazzi, M.; Sancho, U.; Castaño, O.; Frutos, L. M.
Effect of the ultraviolet radiation on proteins: a computational study.
Proceedings of the 3rd Young Researchers Conference of the University of Alcalá, Spain, December 2010, p. 319-328.
22. Marazzi, M.; Frutos, L. M.; Castaño, O.; Temprado, M.
Modulating nitric oxide release by nitrosothiols photodecomposition: an ab initio multiconfigurational approach.
23th IUPAC Symposium on Photochemistry, Ferrara, Italy, July 2010, PO-173.
23. Marazzi, M.; Olivucci, O.; Castaño, O.; Frutos, L. M.
New perspectives for "on the fly" excited state dynamics: local scaling of the CASSCF//CASPT2 gradient in a rhodopsin model.
7th Congress on Electronic Structure: Principles and Applications, Oviedo, Spain, July 2010, PO-142, p. 194.
24. Marazzi, M.; Sancho, U.; Acuña, U.; Castaño, O.; Frutos, L.M.
The role of intersection space in energy and charge transfer: new theoretical tools and their application to nonvertical transfer.
7th Congress on Electronic Structure: Principles and Applications, Oviedo, Spain, July 2010, PO-014, p. 64.
25. Castaño, O.; Frutos, L. M.; Sancho, U.; Marazzi, M.; Acuña, U.
Photoinduced energy, electron and proton transfer: a computational approach.
4th Humboldt Conference on Computational Chemistry, Varna, Bulgaria, July 2010, PL-08, p. 13.
26. Marazzi, M.; Sancho, U.; Castaño, O.; Domcke, W.; Frutos, L. M.
A possible mechanism for photostability in polyglycine: description of photoinduced proton transfer reaction paths at the CASSCF//CASPT2 level of theory.
9th Spanish Congress on Photochemistry, Bilbao, Spain, September 2009, p. 45.
27. Castaño, O.; Frutos, L. M.; Sancho, U.; Marazzi, M.; Acuña, U.
Photoinduced energy, electron and proton transfer: a computational approach.
24th International Workshop on Quantum Systems in Chemistry and Physics, San Lorenzo del Escorial, Spain, September 2009, p. 67.
28. Marazzi, M.; Sancho, U.; Castaño, O.; Domcke, W.; Frutos, L. M.
Photoinduced proton transfer reaction paths in a polyglycine model. A CASSCF//CASPT2 study.
24th International Conference on Photochemistry, Toledo, Spain, July 2009, PO-56, p. 581.