

Dr. Romain BERRAUD-PACHE

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Maître de conférences (Assistant Professor) LAMS (UMR8220) Sorbonne-Université, Paris, France

Formations:

2014-2017: PhD in theoretical chemistry, Université Gustave Eiffel, Marne-la-Vallée, France

“QM/MM study of bioluminescent systems”

Keywords: Bioluminescence, Theoretical Chemistry, QM/MM calculations, Classical Molecular Dynamics, Excited States, Reactivity

PhD supervisor: Pr. NAVIZET Isabelle. Email: isabelle.navizet@univ-eiffel.fr

2009-2014: Bachelor's and Master's degree, University of Rennes 1, Rennes, France

Master's degree in Molecular Chemistry, option Theoretical Chemistry with honours

Positions:

Nov 2020-now: Maître de conférences LAMS (UMR8220), Sorbonne-Université, Paris, France

Modelling molecular interactions, physical and chemical properties in lake pigments

2018-2020: Postdoc researcher Max-Planck-Institut für Kohlenforschung, Mülheim, Germany

“Excited state studies of large molecules”

Keywords: Excited states, Theoretical chemistry, Coupled Clusters methods, Molecular Dynamics, QM/MM calculations, Fluorescent dyes, Photochemical reactions, Modelling photophysical properties

Supervisor: Dr. IZSAK Róbert. Email : robert.izsak@kofo.mpg.de

Teaching activities:

At Sorbonne-Université:

LU1Ci002: Tutorials and Practicals

LU2Ci002: Practicals

4Ci102: Supervision of bibliographic projects

2015-2017: “Monitorat”, Université Gustave Eiffel, Marne-la-Vallée, France

Tutorials in organic chemistry (2nd year), practical in kinetics (1st year), practical in coordination chemistry (3rd year), and supervision of several bibliographic projects in chemistry

2021: Supervision of a Master M1 Student: Dune André, “Theoretical study of carminic acid in water”, 3 months

2016: Co-supervision of a Master M1 Student: Sephora Mondesir, “Theoretical studies of organic molecule possibly responsible for Parkinson disease”, 2 months

Prize/Grants:

November 2018: PhD prize from Doctoral School SIE of Université Paris-Est.

June 2016: Congress Grant to attend a conference from French Chemical Society (SCF)

November 2015: Research Grant - Short-Term Grant from the DAAD for an internship in a German Lab.

July 2015: Grant from GDRI RFCCT 0808 (International Research Grouping) for a conference in Beijing, China

Computer information

Softwares: Orca (expert), xTB (expert), Molcas (expert), Gaussian (expert), AMBER (expert), Tinker (advanced), VMD (expert), Chemdraw (advanced), shell (advanced), Fortran 90 (average), Python (average), C (notions)

Systems: Linux, Mac OS X, Windows

Scientifics Communication:

Publications

- 1) Berraud-Pache, R.; Santamaría-Aranda, E.; de Souza, B.; Bistoni, G.; Neese, F.; Sampedro, D.; Izsák, R., Redesigning donor–acceptor Stenhouse adduct photoswitches through a joint experimental and computational study. *Chemical Science* **2021**, *12* (8), 2916-2924.
- 2) Ghosh, S.; Kumar Dutta, A.; de Souza, B.; Berraud-Pache, R.; Izsák, R., A new density for transition properties within the similarity transformed equation of motion approach. *Molecular Physics* **2020**, *118* (19-20).
- 3) Kozma, B.; Berraud-Pache, R.; Tajti, A.; Szalay, P. G., Potential energy surfaces of charge transfer states. *Molecular Physics* **2020**, *118* (19-20), e1776903.
- 4) Sirohiwal, A.; Berraud-Pache, R.; Neese, F.; Izsak, R.; Pantazis, D. A., Accurate Computation of the Absorption Spectrum of Chlorophyll a with Pair Natural Orbital Coupled Cluster Methods. *J Phys Chem B* **2020**, *124* (40), 8761-8771.
- 5) Berraud-Pache R., Bistoni G., Neese F. and Izsák R.; Unveiling the photophysical properties of Boron-dipyrrromethene dyes using a new accurate excited state coupled cluster method, *Journal of Chemical Theory and Computation*, **2020**, *1*, 564 DOI: 10.1021/acs.jctc.9b00559
- 6) Berraud-Pache R., Bistoni G., Neese F. and Izsák R.; Computational Design of Near-Infrared Fluorescent Organic Dyes Using An Accurate New Wavefunction Approach, *J. Phys. Chem. Lett.*, **2019**, *10*, 17, 4822-4828, DOI: 10.1021/acs.jpcclett.9b02240
- 7) Carrasco-López, C.; C Ferreira, J.C.; Lui, N.; Schramm, S.; Berraud-Pache, R.; Navizet, I.; Panjikar, S.; Naumov, P. and Rabeh, W.; Color emission mechanism for beetle luciferases, *Life Science Alliance*, **2018**, *1* (4) e201800072
- 8) Berraud-Pache R.; Lindh R. and Navizet I.; QM/MM study of the formation of the dioxetanone ring in fireflies through a superoxide ion, *The Journal of Physical Chemistry B*, **2018**, *122*, 20, 5173-5182b DOI: 10.1021/acs.jpcc.8b00642
- 9) Berraud-Pache, R.; Garcia-Iriepa, C.; Navizet, I. Modelling chemical reactions by QM/MM calculations: the case of the tautomerization in fireflies bioluminescent systems, *Frontiers in Chemistry*, **2018**, *6*, 116 DOI: 10.3389/fchem.2018.00116
- 10) Garcia-Iriepa, C.; Gosset, P.; Berraud-Pache, R.; Zemmouche, M.; Taupier, G.; Dorkenoo, K.; Didier, P.; Léonard, J.; Ferré, N.; Navizet, I. Simulation and analysis of the spectroscopic properties of oxyluciferin and its analogues in water, *Journal of Chemical Theory and Computation*, **2018**, *14*, 2117-2126 DOI: 10.1021/acs.jctc.7b01240
- 11) Vacher, M.; Fernández Galván, I.; Ding, B.W.; Schramm, S.; Berraud-Pache, R.; Naumov, P.; Ferré, N.; Liu, Y.J.; Navizet, I.; Roca-Sanjuán, D.; Baader, W.; Lindh, R.; Chemi- and Bioluminescence of Cyclic Peroxides, *Chemical Reviews*, **2018**, DOI: 10.1021/acs.chemrev.7b00649
- 12) Berraud-Pache R. and Navizet I. ; QM/MM calculations on a newly synthesised oxyluciferin substrate : new insights into the conformational effect, *Physical Chemistry Chemical Physics*, **2016**, *18*, 27460-27467 DOI: 10.1039/C6CP02585D
- 13) Schramm, S.; Navizet, I.; Naumov, P.; Nath, N. K.; Berraud-Pache, R.; Oesau, P.; Weiss, D.; and Beckert, R.; The Light Emitter of the 2-Coumaranone Chemiluminescence : Theoretical and Experimental Elucidation of a Possible Model for Bioluminescent Systems. *Eur. J. Org. Chem.*, **2016**, 678–681. DOI: 10.1002/ejoc.201501515
- 14) Pointillart, F.; Jung, J.; Berraud-Pache, R.; Le Guennic, B.; Dorcet, V.; Golhen, S.; Cador, O.; Maury, O.; Guyot, Y.; Decurtins, S.; Liu, S. X. and Ouahab, L.; Luminescence and Single-Molecule Magnet Behavior in Lanthanide Complexes Involving a Tetrathiafulvalene-Fused Dipyridophenazine Ligand, *Inorganic Chemistry*, **2015**, *54*, 5384-5397 DOI: 10.1021/acs.inorgchem.5b00441

Books Chapter:

- 1) *Theoretical Study of Chemiluminescence* , Garcia-Iriepa, C.; Berraud-Pache, R.; Navizet, I., A **Comprehensive Guide to Chemiluminescence**, 2019, ISBN: 978-1-53616-170-0

Oral Communications:

- 1) September 2019: STC-2019, Rostock, Germany: “Modelling and predicting photodynamic and spectroscopic properties of fluorescent dyes” <http://www.stc2019.de/programme.html>, (English, 20 min)
- 2) May 2018: ISBC 18, Nantes, France: “Insights into the formation of the dioxetanone cycle in the firefly bioluminescence” <https://isbc-2018.sciencesconf.org/program>, session BL1 (English, 20 min)
- 3) November 2016: ESCS 16 Paris, France: “Theoretical study of excited state in a bioluminescent reaction” <http://escs2016.chimie-paristech.fr/program.html> (English, 25 min)

- 4) October 2016: CPC16 Nancy, France: “Theoretical study of a red-emitter of firefly oxyluciferin”
<http://cpc2016nancy.wixsite.com/website/program> (English, 30 min)
- 5) June 2016: RCTF 2016 Lyon, France: “Calcul QM/MM sur un nouvel émetteur de la luciférine”
<http://rctf2016.univ-lyon1.fr/fr/pages/rctf2016-program> (French, 20 min)

Posters:

- 1) Berraud-Pache R., de Souza, B., Neese F., Bistoni G. and Izsák R.: “Modelling photokinetic properties of organic molecules”
February 2020: MPPM 2020, London, United Kingdom
- 2) Berraud-Pache R., Bistoni G., Neese F. and Izsák R.: “Computational Design of Near-Infrared Fluorescent Organic Dyes Using A Novel Excited State Coupled Cluster Method”
July 2019: MQM 2019 Conference, Heidelberg, Germany
- 3) Berraud-Pache R. and Navizet I.: “Keto-enol tautomerization on the bioluminescence emitter in fireflies”
August 2017: WATOC 2017 Conference, Munich, Germany
- 4) Berraud-Pache R. and Navizet I.: “QM/MM Calculation on a red emitter of firefly oxyluciferin”
August 2015: MOLIM Conference, UPEM, Marne-la-Vallée, France
April 2015: MPM Conference, Université de Nantes, Nantes, France