Curriculum Vitae

PERSONAL INFORMATION

de la LANDE Aurélien
Research ID: P-5656 2016
ORCID : 0000-0003-0745-4171
Date of birth: July 21st 1979
Nationality: French
URL for web site: *http://hebergement.universite-paris-saclay.fr/adelalandecnrs/*

EDUCATION & DIPLOMA

2015 **Habilitation à Diriger les Recherches**. Université Paris-Sud. *How molecular modelling can help to understand charge transfers mechanisms in biological media.*

2015 Participant to the program "*CNRS Jeunes Talents*". During this highly selective formation (20 people selected by CNRS annually) I was trained to ***modern team management technics*** (12 days).

2007-2009 **Post-doctoral fellow** in Prof. D.R. Salahub's group (University of Calgary, Canada). *1) Development and implementation of constrained DFT for modelling electron transfers in proteins. 2) Multiscale simulations of the catalytic mechanisms of RNA polymerases.*

2007 **Joint PhD** from Université Pierre et Marie Curie (Paris, France) and Universidad Jaime I (Castelló, Spain) Supervision: Dr. O. Parisel and Prof. V. Moliner. *Multi-scale modelling of non-coupled copper monooxygenases: from dioxygen activation to long-range-electron transfer.*

1997-2003 **Chemistry engineer diploma** from the higher school of education ESCOM (*Ecole Supérieure de Chimie Organique et Minérale*, Cergy Pontoise, France)

2004 **Master 2** (*Diplôme d'études approfondies) Chimie Informatique et Théorique. Université Pierre et Marie Curie (Paris, France)*

PERMANENT RESEARCH POSITIONS

Since 2020 Directeur de Recherche CNRS (senior staff researcher).
2010 - 2020 Chargé de Recherche CNRS (staff researcher).
Laboratoire de Chimie Physique, Université Paris Sud, CNRS. France

SCIENTIFIC PRODUCTION

75 articles in peer-reviewed articles, 4 book chapters. h-index =22 (google scholar) 5 representative publications:

1) A. Parise, A. Alvarez-Ibarra, X. Wu, X. Zhao, J. Pilmé, **A. de la Lande**, *J. Phys. Chem. Lett.* **2018**. *9*, 844. DOI: 10.1021/acs.jpclett.7b03379 2) J. Řezáč*, **A. de la Lande**, *J. Chem. Theor. Comput*. **2015**, *11*, 528. DOI: 10.1021/ct501115m 3) F. Cailliez, P. Müller, Th. Firmino, P. Pernot, **A. de la Lande**, *J. Am. Chem. Soc*. **2016**, *138*, 1904. DOI: 10.1021/jacs.5b10938;4) C. Narth, N. Gillet, F. Cailliez, B. Lévy, **A. de la Lande** *Acc. Chem. Res*. **2015**, *48*, 1090. DOI: 10.1021/ar5002796 **; 5) A. de la Lande**, D. R. Salahub* *J. Mol. Struct.* **2010**, 943, 115.DOI : doi.org/10.1016/j.theochem.2009.11.012

RESEARCH GRANTS

2024-2028 **PI, BIRD** *BIrth, Relaxation and Diffusion of Low Energy Electrons in Condensed Phase*. Funded by the French National Agency for Research (ANR).

2022-2026 **Partner**. **ELECTROPHYLLE** *Understanding charge separation in photosynthetic reaction center II by a novel spectroscopy of gas phase chlorophyll constructions*.(PI: Dr. N Shafizadeh,

ISMO, Univ. Paris Saclay). Funded by the French National Agency for Research (ANR).

2022-2026 **Partner Super-ET** *Superoxide Production by Transmembrane Electron Transfer*. (PI: Dr. F Cailliez, ICP, Univ. Paris Saclay). Funded by the French National Agency for Research (ANR).

2020-2024 **PI, RUBI project** Ultrafast Reactivity of Biomolecules Subjected to Ionizing Irradiations. Funded by the French National Agency for Research (ANR).

2013-2015 **PI**. *Photo-induced ligand dissociations within metallo-porphyrins: Synergistic experimental and computational approaches*. Funded by the Laboratory of Excellence PALM.

2014-2017 **PI**. *Intertwined Electron and Proton Hopping: Synergistic experimental and theoretical approaches*. Funded by the French National Agency for Research (ANR).

2015 **PI**. *Mechanism of ultrafast proton transfer in the cryptochrome photosensor protein*. Funded by the Laboratory of Excellence PALM (Physics, Atom, Light, Matter).

2014-2018 **Partner** *Quantum COntrol of large molecular systems : application to CONical IntersectionS (CoCONIC)*. ANR funds.

2016-2019 **Partner** *Probing the ultrashort-lived and powerful oxidizing radical cation $H_2O^{\bullet+}$.* ANR funds.

SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2013 - 2015 Shufeng Chen, **postdoc**, *Photoinduced ligand dissociation within metalloporphyrins. Synergistic experimental and computational approaches*. 2 articles.

2014-2016 Thiago Firmino, **postdoc**, *Simulations of ultrafast electron and proton transfers in cryptochromes and the role of quantum coherences*. 3 articles.

2016 Daniel Mejia-Rodriguez, **postdoc**, *Development and implementation of multi-component Density Functional Theory in deMon2k.* 1 article in preparation.

Since 2017 Aurelio Alvarez-Ibarra, **postdoc**, *Development of electron-nuclear dynamics in the framework of auxiliary DFT.* 2 article + 2 in preparation.

2012-2014 Natacha Gillet, **PhD** (co-advisor with Prof. Demachy and Prof. Moliner). *Numerical simulations of interdependent electron and protons in proteins*. 6 articles.

2016-2018 Xiaojing Wu, **PhD**. *Investigation of electron transfers in flavohemoglobins, application of innovative computational approaches*.

ORGANISATION OF INTERNATIONAL SCIENTIFIC MEETINGS

2014 Flagship CECAM Workshop: *Investigating fine quantum effects in biological systems: toward a synergy between experimental and theoretical approaches*. 28th-30th May 2014, Paris France. **Initiator and Coordinator** of the organizing committee. 55 participants.

2015 deMon developers' meeting. Sofia, Bulgaria. **Member** of the organizing committee. 30 participants

2015 CECAM tutorial *deMon2k and deMon-nano tutorial*. 15th-20th June 2015, Orsay, France. **Initiator and Coordinator** of the organizing committee. 16 (organizers, lecturers) + 30 participants.

2017 CFCAM Discussion meeting:

COMMISSIONS OF TRUST

Since 2022 Member of the

2016-2021 Elected member of National Committee of CNRS in charge of recruitments, promotion and evaluation of permanent staff CNRS researchers. Section physical, theoretical and analytical chemistry (13th). Scientific secretary of the section.

2011-2016	Member of the panel "Ultrafast Dynamics: from radiation source to multiscale responses" of the Laboratory of Excellence PALM. Selection of projects to be funded in laboratories pertaining to University Paris-Saclay
2015-2022	Panel member for GENCI (thematic committee Molecular Modelling applied to Biology) for the allocation of national supercomputer resources to academic research groups in France.
since 2014	Scientific expert for PRACE, the European research infrastructure for High Performance Computing, as external project reviewer or as panel member for Tier-0 calls for proposals.

SCIENTIFIC NETWORK

Advanced numerical simulations technics. I am active ***co-author*** of deMon2k which is a highly efficient computer code for Density Functional Theory calculations. It is an open-source software developed by several academic research groups worldwide. I have also established a solid collaboration with **J. Řezáč** (Czech Acad. of Sci.; Czech Republic) for developing innovative set-ups (e.g. QM/MM) for the simulation of physicochemical processes in complex molecular systems.

Collaborations with experimental groups. The investigation of physicochemical processes in complex biological systems greatly benefit from combined experimental and theoretical approaches.

COMPLETE LIST OF PUBLICATIONS
(UP TO 2022)

Peer-reviewed articles (69)

Corresponding authors are marked by a star *

69 Derivation of flavin hyperfine interactions for the protein magnetosensor cryptochrome.
J. Deviers, F. Cailliez, B. Zúñiga Gutiérrez, D. Kattnig, **A. de la Lande***. *Physical Chemistry Chemical Physics*, under review.

68 Insights on the effect of distal histidine and water hydrogen bonding on NO ligation to the Ferrous and Ferric Heme: a DFT study.
F. Fateminasab, Fatemeh; R. Omidyan*, **A. de la Lande,** RSC Advances. **2022** i*n press.*

67 Anisotropic magnetic field effects in the re-oxidation of cryptochrome in the presence of scavenger radicals.
J Deviers, F Cailliez, **A de la Lande**, DR Kattnig*, *J. Chem. Phys*. **2022**, 156, 025101. doi.org/10.1063/5.0078115

66 Theoretical insights on the effect of environments on binding of CO to the Heme: Ferrous and Ferric systems
F Fateminasab, M Aarabi, **A de la Lande**, R Omidyan*, J. Mol. Liquids **2021** , *344*, 117961. doi.org/10.1016/j.molliq.2021.117961

65 The mystery of sub-picosecond charge transfer following irradiation of hydrated uridine monophosphate
A. de la Lande*, S.A. Denisov, M. Mostafavi*, Physical Chemistry Chemical Physics*, **2021,** 23, 21148-21162. doi.org/10.1039/D0CP06482C

64 Reliability and performances of real-time time-dependent auxiliary density functional theory
R. Tandiana, C. Clavaguéra, K. Hasnaoui, J. N. Pedroza-Montero, **A. de la Lande***, *Theor. Chem. Acc.* **2021**, 140, 1-12. Numéro special "20th deMon developers Workshop". doi.org/10.1007/s00214-021-02819-9

63 Heme ligation in the gas phase
N. Shafizadeh, M. E. Crestoni, **A. de la Lande**, B Soep*
Inter. Rev. Phys. Chem. **2021**, 40, 365-404, doi.org/10.1080/0144235X.2021.1952006

62 Femtosecond responses of hydrated DNA irradiated by ionizing rays focus on the sugar-phosphate part.
A. de la Lande*, *Theor. Chem. Acc*. **2021**, 140, 1. Special isue in honor of F. Spiegelemann. doi.org/10.1007/s00214-021-02778-1

61 Mechanistic Insights on Heme-to-Heme Transmembrane Electron Transfer Within NADPH Oxydases From Atomistic Simulations

X. Wu, J. Hénin, L. Baciou, M. Baaden, F. Cailliez*, **A. de la Lande***, *Front Chem.* **2021**, 9, 271. doi.org/10.3389/fchem.2021.650651

60 First-Principles Simulations of Biological Molecules Subjected to Ionizing Radiation
K. A. Omar, K. Hasnaoui, **A de la Lande***, *Ann. Rev. Phys. Chem*, **2021**, 72, 445-465. invited article. doi.org/10.1146/annurev-physchem-101419-013639

59 Elucidating the electronic structure of a delayed fluorescence emitter via orbital interactions, excitation energy components, charge-transfer numbers, and vibrational reorganization energy.
Z. Pein, Q. Ou*, Y. Mao*, J. Yang, **A. de la Lande**, F. Plasser*, W. Liang*, Z. Shuai* Y. Shao*, *J. Phys. Chem. Lett*. **2021**, 12, 11, 2712. doi.org/10.1021/acs.jpclett.1c00094

58 The physical stage of radiolysis of solvated DNA by high-energy-transfer particles: insights from new first principles simulations
A. Alvarez-Ibarra, A. Parise, K. Hasnaoui, **A. de la Lande***, *Physical Chemistry Chemical Physics* **2020**, 22, 7747-7758 doi.org/10.1039/D0CP00165A

57 Attosecond dynamics simulations of glycine irradiated by alpha particle
A. Parise, **A. de la Lande**, T. Marino, N. Russo*, Commentary in *Phys. Life Rev*., **2019**, DOI. doi.org/10.1016/j.plrev.2019.08.012

56 Molecular Simulations with the in−deMon2k QM/MM, a Tutorial−Review
A. de la Lande*, A. Alvarez−Ibarra, K. Hasnaoui, F. Cailliez, X. Wu, T. Mineva, J. Cuny, P. Calaminici, L. López−Sosa, G. Geudtner, I. Navizet, C. Garcia Iriepa, D.R. Salahub, A. M. Köster*, Molecules **2019**, *24*, 1653. DOI: doi.org/10.3390/molecules24091653

55 Multicomponent density functional theory with density fitting
D. Mejia−Rodriguez, **A. de la Lande***, *J. Chem. Phys*. **2019**, 150, 174115. DOI 10.1063/1.5078596

54 Water binding to Fe III Hemes studied in a cooled ion trap, characterization of a strong 'weak' ligand
M. Aarabi, S. Soorkia, G. Grégoire, M. Broquier, **A. de la Lande**, B. Soep, R. Omidyan , N. Shafizadeh*. *Phys. Chem. Chem. Phys*. **2019**, 21, 21329−21340 DOI: 10.1039/C9CP03608C

53 The Dramatic Effect of N-methylimidazole on Trans Axial Ligand Binding to Ferric Heme: Experiment and Theory
M. Aarabi, R. Omidyan*, S. Soorkia, G. Gregoire, M. Broquier, M. E. Crestoni, **A. de la Lande**, B. Soep, N. Shafizadeh*. *Phys. Chem. Chem. Phys*. **2019**. sous presses DOI: 10.1039/C8CP06210B

52 Retardation in electron dynamics simulations based on time-dependent density functional theory.
X. Wu, A. Alvarez-Ibarra, D. R. Salahub, **A. de la Lande***, *Eur. J. Phys. D*. **2018**, *72*, 206. DOI: 10.1140/epjd/e2018-90219-3

51 Gating the Electron Transfer at a Monocopper Centre through the Supramolecular Coordination of Water Molecules within a Protein Chamber Mimic.

N. Le Poul, B. Colasson, G. Thiabaud, D. Jeanne Dit Fouque, C. Iacobucci, A. Memboeuf, B. Douziech, J. Řezáč, Th. Prangé, **A. de la Lande**, O. Reinaud* , Y. Le Mest*. *Chem. Sci*., **2018**, ***9***, 8282. DOI: 10.1039/C8SC03124J

50 The Surprisingly High Ligation Energy of CO to Ruthenium Porphyrins.
N. Shafizadeh*, S. Boyé-Péronne, S. Soorkia, B. K. Cunha de Miranda, G. A. Garcia, L. Nahon, S. Chen, **A. de la Lande**, L. Poisson, B. Soep, *Phys. Chem. Chem. Phys*. **2018**, *20*, 11730. DOI: 10.1039/C8CP01190G

49 Quantum Chemical topology of the Electron Localization Function in the Field of Attosecond Electron Dynamics.
A. Parise, A. Alvarez-Ibarra, X. Wu, X. Zhao, J. Pilmé, **A. de la Lande***, *J. Phys. Chem. Lett.* **2018**, *9*, 844. DOI: 10.1021/acs.jpclett.7b03379

48 AMOEBA Polarizable Force Field Parameters of the Heme Cofactor in its Ferrous and Ferric Forms
X. Wu, C Clavaguéra*, L. Lagardère, J. -P. Piquemal, **A. de la Lande***, *J. Chem. Theor. Comput*. **2018**, *14*, 2705. DOI: 10.1021/acs.jctc.7b01128

47 Multidimensional Quantum Mechanical Modeling of Electron Transfer and Electronic Coherence in Plant Cryptochromes: The Role of Initial Bath Conditions
D. Mendive-Tapia, E. Mangaud, Th. Firmino, **A. de la Lande**, M. Desouter-Lecomte, H. Dieter-Meyer, F. Gatti*, *J. Phys. Chem. B*. **2018**. DOI: 10.1021/acs.jpcb.7b10412.

46 Ultrafast flavin photoreduction in an oxidized animal (6-4) photolyase through an unconventional tryptophan tetrad
R. Martin, F. Lacomba, A. Espagne, N. Dozov, P. Plaza*, J. Yamamoto, P. Müller, K. Brettel and **A. de la Lande**, *Phys. Chem. Chem. Phys.* **2017**, *19*, 24493-24504 DOI: 10.1039/C7CP04555G

45 Simulating Electron Dynamics in Polarizable Environments
X. Wu, J. -M. Teuler, C. Clavaguéra, F. Cailliez, D. R. Salahub, **A. de la Lande***, *J. Chem. Theor. Comput*. **2017**, *13*, 3985, DOI: 10.1021/acs.jctc.7b00251

44 Theoretical estimation of redox potential of biological quinone cofactors.
N. Gillet*, B. Lévy, V. Moliner, I. Demachy, **A. de la Lande***, *J. Comput. Chem*. **2017**, *38*, 1612. DOI: 10.1002/jcc.24802

43 Ultra-fast Charge Migration Competes with Proton Transfer in the Early Chemistry of $H_2O^{\bullet+}$
F. Wang, U. Schmidhammer, **A. de la Lande**, M. Mostafavi, *Phys. Chem. Chem. Phys*. **2017**, 19, 2894. DOI: 10.1039/C6CP07013B

42 On the accuracy of population analyses based on fitted densities
A. de la Lande*, C. Clavaguéra, A. M. Köster*, J. Mol. Mod*. **2017**, 23, 99, DOI: 10.1007/s00894-017-3264-5. Special issue in honor of H. Chermette.

41 On the role of charge transfer in halogen bonding
J. Řezáč*, **A. de la Lande**, *Phys. Chem. Chem. Phys*. **2017**, *19*, 791. DOI: 10.1039/C6CP07475H

40 Electronic Coupling Calculations for Bridge-Mediated Charge Transfer Using CDFT and Effective Hamiltonian approaches at DFT and FODFTB level
N. Gillet, L. Berstis*, X. Wu, F. Gajdos, A. Heck, **A. de la Lande***, J. Blumberger*, M. Elstner*, *J. Chem. Theor. Comput*. **2016**, *12*, 4793. DOI: 10.1021/acs.jctc.6b00564

39 Ultrafast Scavenging of the Precursor of H• Atom, (e^- , H_3O^+), in Aqueous Solutions.
A. Balcerzyk, U. Schmidhammer, F. Wang, **A. de la Lande**, M. Mostafavi*, *J. Phys. Chem. B*, **2016**, *120*, 9060. DOI: 10.1021/acs.jpcb.6b04944

38 Quantum effects in Ultrafast Electron Transfers within Cryptochromes
Th. Firmino, E. Mangaud, F. Cailliez, A. Devolder, D. Mendive-Tapia, F. Gatti, C. Meier*, M. Desouter-Lecomte*, **A. de la Lande***, *Phys. Chem. Chem. Phys*. **2016**, *18*, 21442. DOI: 10.1039/C6CP02809H

37 Structure of the Cobalt Protoporphyrin Chloride and its Dimer, Observation and DFT Modeling
A. de la Lande*, M. -H Ha Thi, S. Chen, B. Soep, N. Shafizadeh*, *Phys. Chem. Chem. Phys*. **2016**, *18*, 16700. DOI: 10.1039/C6CP02304E

36 QM/MM Study of L-Lactate Oxidation by Flavocytochrome b2
N. Gillet*, J. J. Ruiz-Pernía, **A. de la Lande**, B. Lévy, F. Lederer, I. Demachy, V. Moliner* *Phys. Chem. Chem. Phys*. **2016**, *18*, 15609. DOI: 10.1039/C6CP00395H

35 Energetics of Photoinduced Charge Migration within the Tryptophan Tetrad of an Animal (6-4) Photolyase
F. Cailliez, P. Müller*, Th. Firmino, P. Pernot, **A. de la Lande***, *J. Am. Chem. Soc*. **2016**, *138*, 1904. Article selected by the editor to appear as a "Spotlight article" of issue 6. DOI: 10.1021/jacs.5b10938

34 Unexpected Ultrafast Silver Ion Reduction: Dynamics Driven by the Solvent Structure
A. Balcerzyk, U. Schmidhammer, G. Horne, F. Wang, J. Ma, S. M. Pimblot, **A. de la Lande**, M. Mostafavi* *J. Phys. Chem. B* **2015**, *119*, 10096. DOI: 10.1021/acs.jpcb.5b04907

33 Progress and Challenges in Simulating and Understanding Electron Transfer in Proteins
A. de la Lande*, N. Gillet, S. Chen, D. R. Salahub*, *Arch. Biochem. Biophys*. **2015**, *582*, 28. Special issue in computational modeling on biological systems. DOI: 10.1016/j.abb.2015.06.016

32 Electron Transfer within a Reaction Path Model Calibrated by Constrained DFT calculations: Application to Mixed-Valence Organic Compounds
E. Mangaud, **A. de la Lande**, C. Meier, M. Desouter-Lecomte*, *Phys. Chem. Chem. Phys*. **2015**, 17, 30889. DOI: 10.1039/C5CP01194A

31 Electron Transfer, Decoherence, and Protein Dynamics: Insights from Atomistic Simulations
C. Narth, N. Gillet, F. Cailliez, B. Lévy, **A. de la Lande*** *Acc. Chem. Res*. **2015**, *48*, 1090. Published as part of the *Accounts of Chemical Research* special issue “Protein Motion in Catalysis”.DOI: 10.1021/ar5002796

30 QM/MM Calculations with deMon2k
D R. Salahub*, S. Y. Noskov, B. Lev, R. Zhang, V. Ngo, A. Goursot, P. Calaminici, A. M. Köster, A. Alvarez-Ibarra, D. Mejía-Rodríguez, J. Řezáč, F Cailliez**, A. de la Lande** *Molecules* **2015**, *20*, 4780. DOI: 10.3390/molecules20034780

29 Robust, Basis-Set Independent Method for the Evaluation of Charge-Transfer Energy in Noncovalent Complexes
J. Řezáč*, **A. de la Lande**, *J. Chem. Theor. Comput*. **2015**, *11*, 528. DOI: 10.1021/ct501115m

28 Electron and Hydrogen Atom Transfers in the Hydride Carrier Protein EmoB
N. Gillet*, B. Lévy, V. Moliner, I. Demachy, **A. de la Lande*** *J. Chem. Theor. Comput.* **2014**, *10*, 5036.

27 ATP Binding and Aspartate Protonation Enhance Photoinduced Electron Transfer in Plant Cryptochrome
F. Cailliez*, P. Müller, M. Gallois, **A. de la Lande***, *J. Am. Chem. Soc*. **2014**, *136*, 12974. DOI: 10.1021/ja506084f

26 Selective Recognition of Fluoride Anion in Water by a Copper(II) Center Embedded in a Hydrophobic Cavity
A. Brugnara, F. Topić, K. Rissanen, **A. de la Lande**, B. Colasson, O. Reinaud*. *Chem. Sci*. **2014**, 5, 5897. DOI: 10.1039/C4SC01457J

25 Topological Analyses of Time-Dependent Electronic Structures: Application to Electron-Transfers in Methionine Enkephalin
J. Pilmé*, Ea. Luppi, J. Bergès*, C. Houée-Levin, **A. de la Lande*** *J. Mol. Mod.* **2014***, 20,* 2368. DOI: 10.1007/s00894-014-2368-4

24 Investigation of the Hydroxylation Mechanism of Non-Coupled Copper Oxygenases by *ab initio* Molecular Dynamics Simulations.
C. Melia, S. Ferrer, J. Řezáč, O. Parisel, O. Reinaud, V. Moliner**, A. de la Lande*** *Chem. Eur. J*. **2013**, *19*, 17328. DOI: 10.1002/chem.201301000

23 Investigation of the Molecular Mechanisms of Electronic Decoherence within a Quinone Cofactor
C. Narth, N. Gillet, B. Lévy, I. Demachy, **A. de la Lande*** *Can. J. Chem*. **2013**, 91, 628.DOI: 10.1139/cjc-2012-0529

22 *New insights into the mechanism of electron transfer within flavohemoglobins: tunnelling pathways, packing density, thermodynamic and kinetic analyses.*
E. El Hammi, C. Houée-Lévin, J. Řezáč, B. Lévy, I. Demachy, L. Baciou*, **A. de la Lande*** *Phys. Chem. Chem. Phys*. **2012**. *14,* 13872. Invited article for the special issue "*Electron Transfer Theory*" edited by D. N Beratan et J. N. Onuchic.

21 *Robust and efficient constrained DFT molecular dynamics approach for biochemical modeling*.
J. Řezáč, B. Lévy, I. Demachy, **A. de la Lande*** *J. Chem. Theor. Comput*. **2012**, 8, 418.

20 *Quantum effects in biological electron transfer.*

A. de la Lande, N. Babcock, J. Řezáč, B. Lévy, B. C. Sanders, D. R. Salahub* *Invited Perspective* in *Phys. Chem. Chem. Phys*. **2012**, 14, 5902.

19 *Transmission coefficients for chemical reactions with multiple states: the role of quantum decoherence*.
A. de la Lande*, J. Řezáč, B. Lévy, B. C. Sanders, D. R. Salahub, *J. Am. Chem. Soc.* **2011**, 133, 3883.

18 *Competitive ligand/chelate binding in [Cu(TMPA)]$^{(+)}$ and [Cu(tren)]$^{(+)}$ based complexes.*
L. Bonniard, **A. de la Lande**, S. Ulmer, J.-P. Piquemal, O. Parisel, H. Gérard*, *Catalysis Today*, **2011**, 177, 79.

17 *Spin-driven activation of dioxygen in various metalloenzymes and their inspired models*.
A. de la Lande*, D. R. Salahub, J. Maddaluno, A. Scemama, J. Pilmé, O. Parisel, H. Gérard, M. Caffarel, J. -P. Piquemal*, Communication in *J. Comput. Chem.* **2011**, 32, 1178.

16 *Surface residues dynamically organize water bridges to enhance electron transfer between proteins.*
A. de la Lande, N. Babcock, J. Řezáč, B. C. Sanders, D. R. Salahub* *Proc. Nat. Acad. Soc*. **2010**, 107, 11799.

15 *Derivation of interpretative models for long range electron transfer from constrained density functional theory*.
A. de la Lande, D. R. Salahub* *J. Mol. Struct.* **2010**, 943, 115.

14 *The QM-MM Interface for CHARMM-deMon.*
B. Lev, R. Zhang, **A. de la Lande**, D. R. Salahub, S. Y. Noskov* *J. Comput. Chem*. **2010**, 21, 1015.

13 *Study of the docking of competitive inhibitors at a model of tyrosinase active site: insights from joint broken-symmetry/Spin-Flip DFT computations and ELF topological analysis.*
A. de la Lande, J. Maddaluno, O. Parisel, T.A. Darden, J.-P. Piquemal* *Inter. Sci. Comput. Life Sci*. **2010**, 2, 3.

12 Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their Cu-M Coordination Sphere
A. de la Lande*, D. R. Salahub, V. Moliner, H. Gérard, J. -P. Piquemal, O. Parisel. Inorg. Chem. **2009**, 48, 7033.

11 Multipoint molecular recognition within a calix[6]arene funnel complex.
D. Coquière, **A. de la Lande**, S. Martí, O. Parisel, T. Prangé, O. Reinaud*, *Proc. Nat. Acad. Soc*. **2009**, 106, 10449.

10 Replacement of a Nitrogen by a Phosphorus Donor in Biomimetic Copper Complexes: a Surprising and Informative Case Study with Calix[6]arene-Based Cryptands.
D. Over, **A. de la Lande***, Zeng, X.S. O. Parisel, O. Reinaud*, *Inorg. Chem*. **2009**, 48, 4317.

9 Exploring the molecular origin of the high selectivity of multisubunit RNA polymerases by stochastic kinetic models.
R. Zhu, **A. de la Lande**, R. Zhang, D. R. Salahub*, *Interdiscip. Sci Comput. Life Sci*. **2009**, 1, 91.

8 Shuffling lithiated mixed aggregates: NMR and Car-Parrinello molecular dynamics reveal an unexpected associative pathway.
F. Paté, H. Gérard, H. Oulyadi, A. de la Lande, A. Harrison-Marchand, O. Parisel, J. Maddaluno*. *Chem. Comm*. 2009, 319.

7 Directional Control and Supramolecular Protection Allowing the Chemo- and Regioselective Transformation of a Triamine.
D. Coquière, **A. de la Lande**, O. Parisel, Th. Prangé, O. Reinaud*, *Chem. Eur. J.* **2009**, 15, 11912.

6 Theoretical exploration of the oxidative properties of a $[(tren(Me_1))CuO_2]^+$ adduct relevant to copper monooxygenase enzymes: Insights into competitive dehydrogenation versus hydroxylation reaction pathways.
A. de la Lande, O. Parisel*, H. Gérard, V. Moliner, O. Reinaud, *Chem. Eur. J*. **2008**, 14, 6465.

5 Long distance electron-transfer mechanism in peptidylglycine alpha-hydroxylating monooxygenase: A perfect fitting for a water bridge.
A. de la Lande, O. Parisel, S. Martí, V. Moliner*, *J. Am. Chem. Soc*. **2007**, 129, 11700.

4 Singlet-triplet gaps in large multireference systems: Spin-flip-driven alternatives for bioinorganic modeling
A. de la Lande, V. Moliner, O. Parisel*, *J. Chem. Phys*. **2007**, 126, 035102.

3 First-principles molecular dynamics evaluation of thermal effects on the NMR (1)J(Li,C) spin-spin coupling
A. de la Lande, C. Fressigné, H. Gérard, J. Maddaluno, O. Parisel*, *Chem. Eur. J*. **2007**, *13*, 3459.

2 Theoretical modelling of tripodal CuN_3 and CuN_4 cuprous complexes interacting with O_2, CO or CH_3CN
A. de la Lande, H. Gérard, V. Moliner, G. Izzet, O. Reinaud, O. Parisel*. *J. Biol. Inrog. Chem.* **2006**, 11, 593.

1 Revisiting the structure of (LiCH3)(n) aggregates using Car-Parrinello molecular dynamics
H. Gérard*, **A. de la Lande**, J. Maddaluno, O. Parisel, M.E. Tuckerman *J. Phys. Chem. A*, **2006**, 110, 4787.

Book Chapters (6)

6 *Electron and Molecular Dynamics Simulations with Polarizable Embedding,*
A. Alvarez-Ibarra, K. A. Omar, K. Hasnaoui, A. de la Lande, dans *Multiscale Dynamics Simulations: Nano and Nano-bio Systems in Complex Environments. RSC editions.* Ed. Wei, D.; Salahub, *D.R.* **2021**.

5 *QM/MM with Auxiliary DFT in deMon2k*
J. D. Samaniego-Rojas, L.-I. Hernández-Segura, L. López-Sosa, R. I. Delgado-Venegas, B. Gomez, J.-C. Lambry, A. de la Lande, T. Mineva, J. Alejandre, B. A. Zúñiga-Gutiérrez, R. Flores-Moreno, P. Calaminici, G. Geudtner, A. M. Köster*, dans dans *Multiscale Dynamics Simulations: Nano and Nano-bio Systems in Complex Environments. RSC editions*. Ed. Wei, D.; Salahub, D.R. **2021.**

4 *Electron Transfer Reactions in Enzymes: Seven Things that Might Break Down in Vanilla Marcus Theory and How to Fix Them if They Do.*
A. de la Lande*, F. Cailliez*, D. R. Salahub* dans *Simulating Enzyme Reactivity: Computational Methods in Enzyme Catalysis*. (Eds.: V. Moliner and I Tuñon). Royal Chemical Society, **2017**.

3 *A Mixed Quantum-Classical View to the Kinetics of Chemical Reactions Involving Multiple Electronic States.*
A. de la Lande,* B. Lévy, I. Demachy dans *Reaction Rate Constant Computations; Theories and Applications*. (Eds.: T. Chu). RCS, **2013**.

2 *Recent Progress in Density Functional Methodology for Biomolecular Modeling.*
D. R. Salahub*, **A. de la Lande**, A. Goursot, R. Zhang, Y. Zhang dans *Applications of Density Functional Theory to Biological and Bioinorganic Chemistry, Structure and Bonding* (Eds.: M. V. Putz, D. Mingos, P. Micheal). Springer. **2013**, Vol. 150, pp 1-64.

1 *Extending the DoMain of Application of Constrained Density Functional theory to Large Molecular Systems.*
A. de la Lande, D. R. Salahub*, A. M. Köster. soumis en March **2012** dans "*Concepts and Methods in Modern Theoretical Chemistry, Volume 1; Electronic structure and Reactivity*". (Eds.: S. K. Ghosh, P. K. Chattaraj). Taylor and Francis. **2012**, Vol. pp. 201-219.

Oral communication, invited presentations

Only given by A. de la Lande

16 WATOC reporté à 2022

15 I Congreso Internacional y III Congreso Latinoamericano de Física, Química y Biología Computacional. Arequipa, Perou. Janvier **2020**. *First Principles Simulations of Matter under Ionizing Radiations*. **A. de la Lande**

14 CECAM flagship workshop. Beyond point charges: novel electrostatic developments in force fields. *AMOEBA Polarizable Force Field for the Heme Cofactor in its Ferrous and Ferric States*. **X Wu**, C Clavaguéra, LLagardère, J−P Piquemal, **A de la Lande** (N'ayant pas pu me rendre au workshop en raison de grèves des transports, X Wu a fait la présentation en mon nom)

13 The 11th Xiamen Workshop on Surface Chemistry: Excited-state electronic structure and dynamics theories of complex systems. Xiamen, Chine. Décembre **2019**. (organized by the State Key Laboratory of Physical Chemistry of Solid Surfaces). *Toward First Principles Simulations of Biological Matter under Ionizing Radiations* **A. de la Lande**

12 Quantum BioInorganic Chemistry Conference − QBIC−V. Marseille, France Juillet **2019**. *AMOEBA Polarizable Force Field for the Heme Cofactor in its Ferrous and Ferric States*. X Wu, C Clavaguéra, L Lagardère, J−P Piquemal, **A de la Lande**

11 10th Triennial Congress of the International Society for Theoretical Chemical Physics. Tromsø, Norvège. Juillet **2019**. *Toward First Principles Simulations of Biological Matter under Ionizing Radiations* A. Alvarez−Ibarra, A. Parise, X. Wu, K Hasnaoui, D. R. Salahub, **A de la Lande**

10 14th International Conference of Computational Methods in Sciences and Engineering. Rodes, Grèce. Mai **2019**. *First principles simulations of double strand DNA irradiated by high energy charged particles*. **A de la Lande**

9 44th Congreso Internacional de Químicos Teóricos de Expresión Latina (QUITEL **2018**). Santiago de Chile. Octobre 2018. *First Principles Simulations of Biological Matter under Ionizing Radiations*. **A. de la Lande**, X. Wu, A. Alvarez-Ibarra, A. Parise, F. Cailliez, C. Clavaguéra, D. R. Salahub

8 100th Canadian Chemistry Conference. Toronto,28 mai-1er juin 1 **2017**. *On the role of coherences in ultrafast biological electron transfers*. **Aurélien de la Lande** Etienne Mangaud, Fabien Cailliez, Thiago Firmino, Michelle Desouter, Christoph Meier

7 Current Trends in Theoretical Chemistry. Nha Trang, Vietnam, 25-29 Août **2014**. *Computational Investigation of the hydroxylation mechanism of non-coupled copper oxygenases*. **Aurélien de la Lande**, Conchín Melía, Jan Řezáč, Silvia Ferrer, Olivier Parisel, Olivia Reinaud and Vicent Moliner

6 Forum TERACHEM, 1-2 juillet **2014**. *Decoherence and electron transfers within proteins. Are quantum effects relevant for biology* ? **A de la Lande**, I Demachy, B Lévy, F Cailliez, DR Salahub, B Sanders, Jan Řezáč

5 CECAM workshop. Functional Dynamics of Biomolecules - computational and experimental approaches. Lugano, 28-30 novembre **2012**. *Investigating the multiscale nature of electron transfers within hemo- and flavo-proteins.*

4 Xth Girona Seminar on Theoretical and Computational Chemistry for the Modeling of Biochemical Systems, Espagne; Juillet **2012**.

(http://xgironaseminar.wordpress.com/). *The constrained DFT approach: a versatile tool for the modeling of biochemical processes*". Conférence plénière sur invitation.

3 2nd ENSC (Ecole Normale Supérieure Cachan) -Schrödinger Meeting, Mai **2011**. *Integrating the multiscale aspects of non-adiabatic chemical reactions in biology*. Conférence plénière sur invitation

2 241st ACS National Meeting in Anaheim, California, USA. March **2011**. Symposium "20 Years of Tunnelling Pathways". *Dynamical organization of water mediated electron transfer pathways in biological system.*

1 6th Congress of the International Society for Theoretical Chemical Physics (ISTCP VI). Juillet **2008**. Vancouver, Canada. "L*ong Range Electron Transfer in PHM : Like a Bridge Over Troubled Water*".

Oral presentations

Fev. 2021 virtual	COST ACTION Attochem. *Promises of Auxiliary DFT to Investigate Radiation Chemistry Problems. **A de la Lande,** X Wu, K Hasnaoui, K Ali Omar*
Sept 2021 virtual	20th virtual deMon developers workshop. *Recent Developements and Applications of Real-Time Time Dependent Auxiliary Density Functional Theory*, **A de la Lande**, K Hasnaoui, J N Pedroza-Montero, K Ali Omar.
Juin 2021	5ème e-meeting du GDR NOX. *Mechanistic Insights on Heme-to-Heme Transmembrane Electron Transfer within NADPH Oxydases from Atomistic Simulations*. X Wu, J Hénin, M Baaden, L Baciou, F Cailliez, **A de la Lande**
Mars 2021	Journées Scientifiques de l'ICP. Computer Simulations of Transmembrane Electron Transfers within NADPH Oxydase X Wu, J Hénin, M Baaden, L Baciou, F Cailliez, **A de la Lande**
Mars 2021	ModSim conference of RCTF. Fisrt Principles Simulations of Ionizing Radiation with Matter at ICP. Karwan A Omar, Damien Tolu, Angela Parise, Aurelio Alvarez, Fabien Cailliez, Carine Clavaguéra, Karim Hasnaoui, **Aurélien de la Lande**
36) Juin 2019	Rencontres Prospectives "Modélisation Multiéchelle" du réseau français de chimie théorique. Nantes, France. *Quelles approches pour modéliser l'interaction rayonnement ionisant / matière biologique à partir des premiers principes?* A Alvarez−Ibarra, A Parise, X Wu, K Hasnaoui, J Pilmé, D R Salahub, F Cailliez, **A de la Lande**

35) Mai 2019	19th deMon Developers workshop. Fréjus, France *Multicomponent density functional theory with density fitting*. **A de la Lande**, D. Mejia Rodriguez
34) Mai 2018	18th deMon developers meeting. Overview of the recent developments from Orsay in deMon2k. **A de la Lande**, X Wu, D Mejia-Rodriguez, A Alvarez-Ibarra, J -M Teuler, DR Salahub.
33) Jan. 2018	CFCAM discussion meeting. Orsay France Numerical Approaches for Simulating the Ultrafast Reactivity of Complex Biomolecules under Irradiation. **A de la Lande**, A Alvarez-Ibarra, X Wu, A Parise, X Zhao, J Pilmé, C Clavaguéra, F Cailliez, D Salahub
32) Nov. 2017	*DNA Damages and Repair Workshop The Lorentz Center, Leiden, Netherland . Oct 30th-Nov 3rd 2017* "Numerical Approaches for Simulating the Ultrafast Reactivity of Complex Biomolecules under Irradiation". **A de la Lande**,
31) Août 2017	UK Biochemical Society Focused Meeting. Extracellular electron Transfer. Norwich, UK, 21-23 aout 2017. "Photoinduced electron transfer mechanisms in animal (6-4) photolyases". **Aurélien de la Lande**, Fabien Cailliez, Thiago Firmino, Pascal Pernot
30) Juillet 2017	XLIIIème Congrès des Chimistes Théoriciens d'Expression Latine. Paris 3-7 juillet 2017. "simulating electron dynamics in polarizable environments". **Aurélien de la Lande**, Xiaojing Wu, Fabien Cailliez, Jean-Marie Teuler, Carine Clavaguera, Dennis Salahub
29) Mai 2017	Rencontres franco-chinoises des chimistes théoriciens. Xiamen, Chine. "Numerical simulations of ultrafast photoinduced electron transfers in plant cryptochromes". Aurélien de la Lande
28) Sept 2016	Conférence d'ouverture du GDR Ultrafast. Paris 28-30 septembre, Paris. "Compétition entre Migration de Charge et Transfert de Proton Ultrarapide Impliquant l'Espèce $H_2O^{\circ+}$". **Aurélien de la Lande**, Karwan Ali Omar, Shufeng Chen, Mehran Mostafavi
27) Mai 2016	deMon developers' workshop Zhengzhou, China, Mai 4th-7th 2016, "Photoinduced electron transfer mechanisms in animal (6-4) photolyases". **Aurélien de la Lande**, Fabien Cailliez, Pascal Pernot, Thiago Firmino, Pavel Müller.

26) Avril 2016	Atelier de Modélisation des Molécules d'Intérêt Biologique (AMMIB) de Paris-Saclay. April 12th 2016, Châtenait-Malabry. "Mécanismes de transferts d'électrons picosecondes dans les photolyases d'animaux", **Aurélien de la Lande**, Fabien Cailliez, Pascal Pernot, Thiago Firmino, Pavel Müller.
25) Oct 2015	Workshop "Chemical Concept", UMPC, Paris. *"Robust, basis-set independent method for the evaluation of charge-transfer energy in noncovalent complexes*". **Aurélien de la Lande**, Jan Řezáč. https://wiki.lct.jussieu.fr/workshop/index.php/Program_hdr
24) Mai 2015	deMon developers' workshop Sofia, Bulgaria, Mai 28th-31st 2015. "*Robust, basis-set independent method for the evaluation of charge-transfer energy in noncovalent complexes*". **Aurélien de la Lande**, Jan Řezáč.
23) Avril 2015	Modeling Photoactive Molecules Conference, April 21-24 2015 Nantes. "*Enhancement of electron transfer in plant cryptochrome by D396 protonation and ATP-binding: experiment and theory*", **Aurélien de la Lande**, Fabien Cailliez, Pavel Müller.
22) Mars 2015	*Colloque* Développement de codes de chimie théorique dans un environnement HPC, IDRIS, Orsay 12, &" mars 2015. *"Atouts et limitations actuels du programme DFT deMon2k"*. **Aurélien de la Lande.**
21) Janvier 2015	Colloque Spectroscopies Ultrarapides pour les Systèmes d'Intérêt Biologique" SUSBIS2015. http://iramis.cea.fr/meetings/SUSIB2015/index.php "*Stratégies pour la simulation numérique des transferts d'électrons ultra-rapides photoinduits*" **Aurélien de la Lande**, Fabien Cailliez, Pavel Müller
20) Juillet 2014	Forum TERATECH 2014, Palaiseau, France "*Decoherence and electron transfers within proteins. Are quantum effects relevant for biology* ? " **Aurélien de la Lande**, Isabelle Demachy, Bernard Lévy, Fabien Cailliez, Dennis Salahub, Barry Sanders, Jan Řezáč
19) Mai 2014	CECAM Workshop "Fine quantum effects in biology", Paris, France "*Development of atomistic simulation algorithms for investigating biological electron transfers*", **Aurélien de la Lande** , Jan Řezáč, Dennis Salahub, Bernard Lévy, Natacha Gillet, Christophe Narth, Fabien Cailliez, Isabelle Demachy.

18) Avril 2014	13th deMon developers Workshop, Los Cabos, Mexico "*Computational investigation of the hydroxylation mechanism of noncoupled copper oxygenases*", Conchín Melía, Silvia Ferrer, Jan Řezáč, Olivier Parisel, Olivia Reinaud, Vicent Moliner, **Aurélien de la Lande**.
17) Mars 2014	Journées de chimie biologiques et théoriques. Marseille, France "*Computational investigation of the hydroxylation mechanism of noncoupled copper oxygenases*", Conchín Melía, Silvia Ferrer, Jan Řezáč, Olivier Parisel, Olivia Reinaud, Vicent Moliner, **Aurélien de la Lande**.
16) Nov 2013	LABEX PALM *" Effets Quantiques en Biologie"*, **Aurélien de la Lande**, Isabelle Demachy, Bernard Lévy, Natacha Gillet, Dennis Salahub, Jan Řezáč.
15) Août 2013	Workshop on prophyrins and phtalocyanins. Minsk, Belaruss. "*Theoretical investigation of metalled porphyrin systems from the gas phase to the protein environment*". **Aurélien de la Lande**.
14) Juillet 2013	QUITEL 2013 (Quimicos teoricos de esprecion latina), Grenade, Espagne. "*Investigation of the molecular mechanisms of electronic decoherence within biological systems*" **Aurélien de la Lande**, Jan Řezáč, Dennis Salahub, Bernard Lévy, Natacha Gillet, Christophe Narth, Isabelle Demachy.
13) Juin 2013	13th deMon developers Workshop, Toulouse, France. *"Electronic population analysis with deMon2k".***Aurélien de la Lande**.
12) Juin 2013	TheoBio 2013, Göteborg, Suède. "*Mechanism of Hydride transfer between two flavins*". **Natacha Gillet**, Bernard Lévy, Vicent Moliner, Isabelle Demachy, Aurélien de la Lande.
11) Juin 2013	Journées de modélisation ENS-ENSCP de Paris. **Natacha Gillet**, Bernard Lévy, Vicent Moliner, Isabelle Demachy, Aurélien de la Lande.
10) Avril 2013	Journées de modélisation du sud parisien. Orsay, "*Quelques résultats sur l'analyse du couplage entre changements de structure électronique et dynamique multi-échelle des biomolécules*",

	Aurélien de la Lande, Natacha Gillet, Fabien Cailliez, Bernard Lévy, Jacqueline Ridard, Isabelle Demachy
9) Février 2013	Colloque de la fédération de Chimie Physique Paris Saclay. Orsay *"Modélisation multi-échelle des transferts d'électrons en biologie : succès et limitations actuelles des simulations numériques"*. **Aurélien de la Lande.**
8) Juin 2012	Journées de modélisation ENS ENSCP de Paris. *"Principes, applications et limitations de l'approche DFT dite sous contrainte*", **Aurélien de la Lande**, Isabelle Demachy, Bernard Lévy.
7) Juillet 2011	deMon developers' Workshop. Brême, Germany. "*Investigating charge transfer processes with the deMon2k constrained DFT modules*", **Aurélien de la Lande**.
6) Juin 2010	"ELF twenty years" - Workshop Paris. "*An innovating tool to analyze electronic structures: constrained DFT and ELF analysis*", A**urélien de la Lande**.
5) Juin 2010	Journées de modélisation ENS-ENSCP in Paris. *Modélisation des réactions de transferts d'électrons*", **Aurélien de la Lande**, Isabelle Demachy, Jacqueline Ridard, Bernard Lévy.
4) Février 2009	9th deMon developers Meeting, Pune, India "*Philosophy of Constrained DFT. A Central Tool for the Multiscale Modeling of Electron Transfer Reactions*". **Aurélien de la Lande**, Dennis Salahub.
3) Juin 2007	8th deMon developers Meeting, Paris, France. *"Long Range Electron Transfer in PHM. A perfect Fitting for a Water Bridge*" **Aurélien de la Lande**.
2) Juin 2007	Conférence internationale TheoBio 07, Cetraro, Italy. "Long Range Electron Transfer in PHM. A perfect Fitting for a Water Bridge" **Aurélien de la Lande**

1) Mai 2007	Journées de Modélisation ENS-ENSCP, Pari, France. "*Transfert Electronique dans la PHM. Récit de Voyage d'un électron*" **Aurélien de la Lande**

Séminaires de laboratoires en France et à l'étranger (32)

(je n'indique que les séminaires pour lesquels j'étais l'orateur)

32)	Séminaire à l'Institut Lumière Matière (Univ. Lyon 1). Toward first principles numerical simulations of the early stages of radiolysis of matter. A de la Lande
31) Sept. 2019	Séminaire dans le groupe de J. Blumberger (UCL, Londres). *Toward First Principles Simulations of Biological Matter under Ionizing Radiations.* **A. de la Lande**
30) Sept 2019	Séminaire au CEA de Marcoule. *Toward First Principles Simulations of Biological Matter under Ionizing Radiations*. **A. de la Lande**
29) Juillet 2019	Séminaire au Synchrotron SOLEIL (Eq. L. Nanhon, Orsay). *Toward First Principles Simulations of Biological Matter under Ionizing Radiations.* **A. de la Lande**
28) Fev. 2019	Séminaire à l'hôpital universitaire de Sherbrook (Eq. De L. Sanche, Canada). Séminaire à l'Université de Calgary (Canada) *Toward First Principles Simulations of Biological Matter under Ionizing Radiations.* **A. de la Lande**
27) Fev. 2019	Séminaire à l'Université de Calgary (Eq. De DR Salahub, Canada). *Toward First Principles Simulations of Biological Matter under Ionizing Radiations*. A. de la Lande
26) Dec. 2018	Séminaire Marne la Vallée. *First Principles Simulations of Biological Matter under Ionizing Radiations*. **Aurélien de la Lande**, Xiaojing Wu, Angela Parise, Aurelio Alvarez
25) Juin 2018	Séminaire à l'ITODYS. *Transferts d'électrons dans les protéines, la théorie de Marcus poussée dans ses retranchements*. **Aurélien de la Lande**, Etienne Mangaud, Fabien Cailliez, Thiago Firmino, Michelle Desouster, Christoph Meier
24) Dec. 2017	Séminaire à l'université d'Ispahan (Iran). *Numerical Approaches for Simulating the Ultrafast Reactivity of Complex Biomolecules under Irradiation*. **Aurélien de la Lande.**
23) Sept 2017	Séminaire Université de Castello (Spain). Numerical Approaches for Simulating the Early Chemical Reactivity Following Irradiation of Complex Biomolecules

22) Jul. 2017	Séminaire invité par P. ungwirth (Prague). Reactivity of the $H_2O^{\circ+}$ species in solution. **Aurélien de la Lande**, Karwan Ali Omar, Xiaojing Wu, Shufeng Chen, Mehran Mostafavi
21) Oct. 2016	Séminaire du Laboratoire de Chimie Théorique (UPMC). Réactivité de l'Espèce $H_2O^{\circ+}$ en Solution. **Aurélien de la Lande**, Karwan Ali Omar, Xiaojing Wu, Shufeng Chen, Mehran Mostafavi
20) Mars 2015	Séminaire de l'IBPC, Paris, France. "*Simulations numériques des transferts d'électrons dans les protéines*". **Aurélien de la Lande**
19) Janvier 2015	Soutenance d'Habilitation à Diriger des Recherches. "*Quelques apports de la modélisation moléculaire a la compréhension des processus de transferts de charges en milieu biologique*". **Aurélien de la Lande**
18) Dec 2014	Séminaire de l'équipe CTMM - Institut Charles Gerhardt, Montpellier, France. "Effet tunnel, decoherence électronique et dynamique des protéines", **Aurélien de la Lande**, Natacha Gillet, Bernard Lévy, Fabien Cailliez, Michèle Desouter, Isabelle Demachy.
17) Dec 2014	Séminaire de l'ISMO, Université Paris Sud. "*Structure, dynamique et réactivité des porphyrines metallées: de la phase gazeuse à l'environnement protéique*", **Aurélien de la Lande**, Shufeng Chen, Natacha Gillet, Bernard Lévy, Isabelle Demachy
16) Mars 2014	Séminaire à l'université de Calgary, Canada, "*Investigating the relationships between electron transfer and protein dynamics*", **Aurélien de la Lande**, Natacha Gillet, Isabelle Demachy, Bernard Lévy, Jan Řezáč, Conchín Melia, Silvia Ferrer, Vicent Moliner
15) Mai 2013	Séminaire à l'Université Libre de Berlin (groupe de Petra Imhof) *"Investigation of the molecular mechanisms of electronic decoherence within biological system*s", **Aurélien de la Lande**, Natacha Gillet, Bernard Lévy, Isabelle Demachy.
14) Avril 2013	Séminaire du groupe "théorie" ENS Paris. "*Modeling the multiscale aspects of biological electron transfers short-range vs. long range processes"*. **Aurélien de la Lande,** Natacha Gillet, Bernard Lévy, Isabelle Demachy.
13) Jan 2013	Séminaire interne du groupe TheoSim. "*Mécanismes de transferts d'électrons en biologie ».*
12) Mai 2011	Séminaire du département Química física i analítica, Universitat Jaume I "*Integrating the multiscale aspects of non-adiabatic chemical reactions in biology"*
11) Avril 2009	Séminaire du département Química física i analítica, Universitat Jaume I "*Long Range Electron Transfers in Biology"*.

10) Fev 2009	Séminaire du Laboratoire de Chimie Physique. Université Paris-Sud 11 "*Réactions de Transferts d'Electrons dans les Milieux Biologiques*".
9) Dec 2008	Séminaire "Chimie théorique". Université de Calgary, Canada. "*Non-adiabatic Reactions in Biological Media, the Case of Long-Range Electron Transfers*".
8) Nov 2008	Séminaire du département de Physique, Jacobs University, Brême, Allemagne. "*Non-adiabatic Reactions in Biological Media, the Case of Long-Range Electron Transfers*".
7) Oct. 2008	Séminaire de l'équipe Chimie et Biochimie Théorique, Université Nancy 1, France. *"Réactions Non-Adiabatiques dans les Milieux Biologiques. L'Exemple des Transferts Electroniques à Longue Distance".*
6) Oct. 2008	Séminaire de l'équipe CTMM - Institut Charles Gerhardt, Montpellier, France. *"Une Description Théorique des Transferts Electroniques Intra- et Inter-protéines : l'Exemple d'une Neuroenzyme et d'un Couple de la Chaîne Respiratoire"*
5) Nov. 2007	IBI Meetings, Université de Calgary, Canada. *"A Multiscale Approach to Investigate the Catalytic Cycle of a Copper Monooxygenase. What Can we Learn from Theoretical Chemistry?*"
4) Sept 2007	Soutenance de thèse, Université Paris VI, France. *"Modélisation Multiéchelle de Monooxygénases à Centres Cuivreux non Couplés : de l'activation du dioxygène au transfert électronique à longue distance"*
3) Mai 2007	Université Paris V Descartes, France. "*Approche Multiéchelle de l'Hydroxylation dans une Monooxygénase à Cuivre. Activation du Dioxygène et Transferts d'Electrons »*
Juanary 2007	Séminaire Laboratoire de Chimie Théorique, Université Paris VI, France. "*Approche Multiéchelle de l'Hydroxylation dans une Monooxygénase à Cuivre. Transferts d'électron et d'hydrogène"*
2) Fev 2006	Séminaire de l'Université Jaume I, Castellon, Espagne. "*Evaluación de la constante de acoplamiento* $^{1}J_{(Li,C)}$ *en los agregados de metil litio".*
1) Sept 2004	Séminaire Laboratoire de Chimie Théorique, Université Paris VI, France. "*Evaluation de la constante de couplage spin-spin dans les agrégats de méthyllithium, une étude DFT statique et dynamique*".