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
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(under maintenance)

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

COMMISSIONS OF TRUST

Since 2024 President of the "*commission de spécialistes de l'Université Paris-Saclay*" for chemistry (CNU divisions 31-32-33, vice-president in 2023, member since 2022). This committee is responsible for assessing the career development of teaching and research staff at *Université Paris Saclay* (setting up recruitment committees, assessing requests for promotion, etc.).

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- Panel member for GENCI (thematic committee Molecular Modelling applied to Biology) for the

2022 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 PRODUCTION

85 articles in peer-reviewed articles, 4 book chapters. h-index =28 (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.* 2 articles

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*.

2019-2022 Angela Paris, **PhD**. *Approches multi-échelles pour aider à clarifier les mécanismes impliqués dans les processus d'activation/inhibition de systèmes biologiques importants*. » Co-supervision with Prof. T. Marino, Universita della Calabria, Italy

2020-2023 Jean Deviers, **PhD**, *Magnetic field effects in the reoxidation of avian cryptochrome: a computational exploration. Co-supervision with Prof. D. Kattnig,* University of Exeter, UK.

2020-2023 Damien Tolu, **PhD**. *Simulations moléculaires aux temps courts de l'irradiation ionisante de solutions d'extractant du plutonium*. Co-supervision with Dr. D. Guillaumont, CEA Marcoule.

2020-2023 Karwan Ali Omar, **PhD**, *First-Principles Simulations of BiologicalMolecules Subjected to Ionizing Radiation.*

2020-2023 Feven Alemu Korsaye, **PhD**, Descripteurs basés sur la densité pour la dynamique électronique des états excités utilisant la RT-TDDFT. Co-supervision with Dr. I. Ciofini, CNRS Chimie Paris Tech.

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:

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.