Adèle D. LAURENT

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Degrees and Academic Positions

- **University of Nantes** — France
  Tenure researcher (CNRS, Chargée de recherche 1) — *10/2016 – present*
- **University of Nantes** — France
  Tenure researcher (CNRS, Chargée de recherche 2) — *10/2012 – 09/2016*
- **University of Southern California** — Los Angeles, USA
  Postdoctoral Fellow — *01/2011 – 09/2012*
  - Advisor: Anna I. Krylov
- **University of Lorraine** — France
  Ph.D. student and teaching assistant in Computational and Theoretical Chemistry — *2007 – 2010*
  - Advisor: Xavier Assfeld
  - PhD thesis: Electronic phenomena of macromolecular systems using QM-MM hybrid methods.
  - French Government Fellowship (*Bourse MRT*)
- **University of Namur** — Belgium
  B.Sc. & M.Sc. Chemistry — *2003 – 2007*
  - Advisors: Éric A. Perpète and Denis Jacquemin
  - Master thesis: Evaluation of absorption spectra of photochromes with the help of *ab initio* methods.

Award and Grants

Projects in which I am involved as member, partner or principal investigator; indicated grant amounts correspond to the part I am in charge of.

- **Tournesol PHC project (travel grant)** — Jan. 2018 – Dec. 2019
  Principal investigator BE, Partner: L. Leherte (Univ. Namur): DoIFad — *2 400 €*
- **Regional project (*Étoile Montante*)** — Jan. 2018 – Dec. 2020
  Principal investigator: MiM-Breg — *140 000 €*
- ***Prime d'Encadrement Doctoral et de Recherche* (PEDR)** — 2016–2021

- ***Institut National du Cancer* (Cancer Health and Biology call)** — Dec. 2016 – Dec. 2019
  Partner, PLBIOL16 coordinated by P. Legembre (OSS INSERM Rennes) — *231 000 €*
- **Regional project (*Dynamique scientifique*)** — Jan. 2016 – Dec. 2021
  Partner[2], *PIRAMID PI: J. Lebreton (CEISAM, Nantes), link* — *175 000 €*
- **Regional project (*Pari scientifique*)** — Oct 2014 – Sept. 2018
  Principal investigator: MES-TransMed — *200 000 €*
- **Regional project (*Pari scientifique*)** — Oct 2013 – Jun. 2017
  Member, ECRIN PI: J.-Y. Le Questel (CEISAM, Nantes)

- **Regional project (*Pari scientifique*)** Oct 2013 – Jun. 2017
  Member, SAPOMAP PI D. Jacquemin (CEISAM, Nantes)
- **ERC Starting** Oct 2012 – Feb. 2017
  Member, MARCHES PI: D. Jacquemin (CEISAM, Nantes), link
- **HPC-Europa Grant** Oct. 2010 – Nov. 2010

Responsabilities

- **Member of the scientific committee** 2018
  RFCT 2018 – Toulouse
- **Member of the scientific committee** 2017-2018
  Journes "Thorie, Modlisation et Simulations"
- **Coordinator** Jan. 2017 – present
  Pôle Ouest du Réseau Français de Chimie Théorique, *link*
- **Elected member** Sept. 2016 – Jul. 2021
  Section 13 National Committee at CNRS, link
- **Co-coordinator** Jan. 2015 – Dec. 2016
  Pôle ouest du Réseau Français de Chimie Théorique
- **International conference co-organizer** April, 25-28 2016
  Multi-Responsive Photochrome conference (Nantes),link
- **Member of the pilot and scientific committees** Jan. 2016 – Dec. 2021
  Regional project (Dynamique scientifique): PIRAMID
- **International conference co-organizer** April, 21 – 25 2015
  Modeling Photoactive Molecules conference (Nantes), link
- **Q-Chem *ab initio* quantum chemistry developer** 2012 – now
  Effective Fragment Potential part
- **Reviewer for several international journals**
  J. Am. Chem. Soc., J. Chem. Theory Comput., Chem. Sci., Phys. Chem. Chem. Phys., ...
- **Responsible of ModES team website**
  link

Appearance in press articles

- Jan. 31st, 2018: Press confrence within the framework of the "Rising Star" call.
  Ouest France, Pays de la Loire Region, RFI LUMOMAT, Telenantes
- June 3rd, 2019: Press release on new photochrome.
  EurekAlert, Phys.org.

Scientific production (recent articles are listed at http://www.univ-nantes.fr/laurent-a-3)

Patents (2)

2. European Patent, EPO n^o 14306182.8-1452
   Title: *Emetteur Dual à Base d'Hydroxybenzazoles Substitués*
   Authors: K. Benelhadj, J. Massue, G. Ulrich, R. Ziessel, D. Jacquemin, A.D. Laurent
   Date: 21.07.2014

1. European Patent, EPO n^o 18306468.2-1110
   Titre : New competitve modulators of insect nicotinic acetylcholine receptors
   Auteurs : J.-Y. Le Questel, J. Graton, A. D. Laurent, B. Selvam, J. Lebreton, M. Mathe-Allainmat, E. Landagaray, S. THany, A. Cartereau
   Date: 13.03.2019

Book chapter (1)

1. D. Escudero-Masa,* A. D. Laurent* and D. Jacquemin*
   Ed.: J. Leszczynski
   Time-Dependent Density Functional Theory: A Tool to Explore Excited States
   Handbook of Computational Chemistry, Springer Netherlands, 1–35 (2016) doi.

Articles published in popularization/industry-related journals (2)

2. A. D. Laurent*
   Évaluation des propriétés photochimiques de chromophores d'interêt technologique et/ou biologique à l'aide d'outils théoriques
   Revue des Questions Scientifiques (FI=NA), **182**, 275–302 (2011) link. Front Cover

1. A. D. Laurent*, V. Wathelet, M. Bouhy, D. Jacquemin and E. A. Perpète
   Simulation de la Perception des Couleurs de Colorants Organiques
   Techniques de l'Ingénieur (FI=NA), **AF6** n^{o}810 (23 p.) (2010) link.

Proceedings Articles (1)

1. I. Vetrivel, L. Hoffmann, S. Guegan, B. Offmann and A. D. Laurent
   PBmapclust: Mapping and Clustering the Protein Conformational Space Using a Structural Alphabet EUROVIS 2019, Editors: J. Byka, M. Krone, and B. Sommer link.

Articles published in peer-reviewed journals (72)

Sum of the Times Cited: 2516
Sum of Times Cited without self-citations: 2410
Citing Articles: 2109
Citing Articles without self-citations: 2062
Average Citations per Item: 33.55
H-index: 20
M-index[a]: 1.67

[a]Computed as H/career length=20/(2019-2007), 2007 being the first year of the PhD.

77. D. Velic, C. Charlier, M. Popova1, T. Jaunet-Lahary, Z. Bouchouireb, S. Henry, P. Weigel, J.-Y. Masson, A. D. Laurent, I. Nabiev, F. Fleury*
Interactions of the Rad51 Inhibitor DIDS with Human and Bovine Serum Albumins: Optical Spectroscopy and IsoThermal Calorimetry Approaches
Biochimie (IF= 3.188) **to be submitted**, – (2019) doi.

76. A. Qumner, R. Sousa, S. Morisseau, K. Trillet, M. Maillasson, I. Leray, J. Dion, I. Barbieux, M. Frutoso, A.D. Laurent, Le Questel J.Y. and E. Mortier*
Anchorage of IL-15Rα to the cell membrane either in cis and in trans is essential to stabilize IL-15 within the IL-2Rβ/γc receptor for an optimal activation.
Proc. Natl. Acad. Sci. USA (IF= 9.580) **under review**, – (2019) doi.

75. R. Sousa, A. D. Laurent, A. Qumner, E. Mortier, J.-Y. Le Questel*
Mechanistic and structural insights on the IL-15 system through molecular dynamic simulations
Molecules (IF= 3.060) **under review**, – (2019) doi.

74. Z. Alamiddine, B. Selvam, J. Graton, A. D. Laurent, E. Landagaray, J. Lebreton, M. Math-Allainmat, S. Thany, J.Y. Le Questel*
Binding of sulfoxaflor to Aplysia californica-AChBP: computational insights from multiscale approaches
J. Chem. Inf. Model. (IF= 3.966) **under review**, – (2019) doi.

73. M. W. H. Hoorens, M. Medved, A. D. Laurent, M. Di Donato, S. Fanetti, L. Slappendel, M. Hilbers, B. L. Feringa*, W. J. Buma,* W. Szymańnski,*
Iminothioindoxyl (ITI): a new molecular photoswitch with 100 nm band separation in the visible range
Nat. Commun. (IF= 11.878) **10**, 2390(1–) (2019) doi.

72. J. Boucard, R. Boudjemaa, K. Steenkeste, C. Jacqueline, N. Stephant, F.-X. Lefvre, A. D. Laurent, L. Lartigue, P. Hulin, S. Nedellec, M.-P. Fontaine-Aupart and and E. Ishow
Phosphonic Acid Fluorescent Organic Nanoparticles for High-Contrast and Selective Staining of Gram-Positive Bacteria
ACS Omega (IF= 2.584) **3**, 17392–21740 (2018) doi.

71. L. Leherte,* A. Petit, D. Jacquemin, D.V. Vercauteren, A. D. Laurent
Investigating Cyclic Peptides Inhibiting CD2-CD58 Interactions Through Molecular Dynamics and Molecular Docking Methods
J. Comput. Aid. Mol. Des. (IF= 3.250) **32**, 1295–1313 (2018) doi.

70. B. Jedrzejewska, A. Skotnicka, A. D. Laurent, M. Pietrzak, D. Jacquemin,* and B. Osmialowski*
The Influence of the Nature of the Amino Group in Highly Fluorescent Difluoroborates Exhibiting Intramolecular Charge Transfer
J. Org. Chem. (IF= 4.745) **83**, 7779–7788 (2018) doi.

69. T. Jaunet-Lahary, Daniel P. Vercauteren, D. Jacquemin, A. D. Laurent*
Computational Simulations Determining Disulfonic Stilbene Derivatives Biodisponibility Within Human Serum Albumin
Phys. Chem. Chem. Phys. (IF= 3.906) **20**, 18020–18030 (2018) doi.

68. M. M. Lerch, M. Di Donato, A. D. Laurent, M. Medved, A. Iagatti, L. Bussotti, A. Lapini, W. J. Buma, P. Foggi, W. Szymańnski,* B. L. Feringa*
Solvent Effects on the Actinic Step of Donor-Acceptor Stenhouse Adduct Photoswitching
Angew. Chem. Int. Ed. (IF= 12.257) **57**, 8063–8068 (2018) doi.

67. M. M. Lerch, M. Medved, A. Lapini, A. D. Laurent, A. Iagatti, L. Bussotti, W. Szymański, W. J. Buma, P. Foggi, M. Di Donato,⋆ B. L. Feringa⋆
Tailoring Photoisomerization Pathways in Donor-Acceptor Stenhouse Adducts: The Role of the Hydroxyl Group
J. Phys. Chem. A (IF= 2.641) **122**, 955–964 (2018) doi. Special Issue: Time-Resolved Vibrational Spectroscopy

66. M. Di Donato, M. M. Lerch, A. Lapini, A. D. Laurent, A. Iagatti, L. Bussotti, S. P. Ihrig, M. Medved, D. Jacquemin, W. Szymański, W. J. Buma, P. Foggi, B. L. Feringa ⋆
Shedding Light on the Photo-Isomerization Pathway of DonorAcceptor Stenhouse Adducts
J. Am. Chem. Soc. (IF= 13.858) **139**, 15596–15599 (2017) doi. ACS AuthorChoice

65. B. Le Guennic, G. Scalmani, M.J. Frish, A. D. Laurent and D. Jacquemin⋆
Investigating the optical properties of BOIMPY dyes using ab initio tools
Phys. Chem. Chem. Phys. (IF= 4.123) **138**, 169–175 (2017) doi.

64. Š. Budzák, T. Jaunet-Lahary, A. D. Laurent, C. Laurence, M. Medved and D. Jacquemin⋆
Exploring the Solvatochromism of Betaine 30 with Ab Initio Tools: From Accurate Gas-Phase Calculations to Implicit and Explicit Solvation Models
Chem. Eur. J. (IF= 5.317) **23**, 4108–4119 (2017) doi.

63. A. M. Grabarz, B. Jedrzejewska, A. Zakrzewska, R. Zaleśny, A. D. Laurent, D. Jacquemin⋆ and B. Ośmiałowski⋆
Photophysical Properties of Phenacylphenantridine Difluoroboranyls: Effect of Substituent and Double Benzannulation
J. Org. Chem. (IF= 4.849) **82**, 1529–1537 (2017) doi.

62. F. Bassal, A. D. Laurent, B. Le Guennic and D. Jacquemin⋆
Exploring the Excited-States of Squaraine Dyes with TD-DFT, SOS-CIS(D) and ADC(2)
Dyes and Pigments (IF= 3.473) **138**, 169–175 (2017) doi.

61. J. Bosson, G.M. Labrador, S. Pascal, F.-A. Miannay, O. Yushchenko, H. Li, L. Bouffier, N. Sojic, R. C. Tovar, G. Muller, D. Jacquemin, A. D. Laurent, B. Le Guennic, E. Vauthey⋆ and J. Lacour⋆
Physicochemical and Electronic Properties of Cationic [6]Helicenes, from Chemical and Electrochemical Stabilities to Far-Red (Polarized) Luminescence
Chem. Eur. J. (IF= 5.317) **22**, 1–11 (2016) doi. Hot Paper

60. A. D. Laurent, E. Otten, B. Le Guennic and D. Jacquemin⋆
Formazanate Boron Difluoride Dyes: Discrepancies Between TD-DFT and Wavefunction Descriptions
J. Mol. Mod. (IF= 1.425) **22**, 263 (2016) doi.

59. A. D. Laurent, B. Le Guennic and D. Jacquemin⋆
Theoretical Spectroscopy of BASHY Dyes
Theor. Chem. Acc. (IF= 1.890) **135**, 173 (8 pages) (2016). doi.

58. T. Jaunet-Lahary, A. Goupille, D. Jacquemin, F. Fleury, J. Graton and A. D. Laurent⋆
A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives
ChemPhysChem (IF= 3.075) **17**, 2434–2445 (2016). doi.

57. S. Budzák, A. D. Laurent, C. Laurence, M. Medved and D. Jacquemin⋆
on March 11, 2016 *Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide*
J. Chem. Theory Comput. (IF= 5.245) **12**, 1919–1929 (2016). doi.

56. C. Azarias, S. Budzák, A. D. Laurent, G. Ulrich and D. Jacquemin*
February 2016 *Tuning ESIPT Fluorophores into Dual Emitters*
Chem. Sci. (IF= 8.668) **7**, 3763–3774 (2016). doi.

55. A. M. Grabarz, A. D. Laurent, B. Jedrzejewska, A. Zakrzewska, D. Jacquemin*, and B. Ośmiałowski*
The Influence of the Π*-Conjugated Spacer on Photophysical Properties of Difluoroboranyls Derived from Amides Carrying a Donor Group*
J. Org. Chem. (IF= 4.849) **81**, 2280–2292 (2016) doi.

54. A. D. Laurent, M. Medved and D. Jacquemin*
Using TD-DFT to Probe the Nature of Donor-Acceptor Stenhouse Adduct (DASA) Photochromes
ChemPhysChem (IF= 3.075) **17**, 1846–1851 (2016). doi. Very Important Paper, Front Cover, Special issue: Molecular Machines.

53. K. J. Chen, A. D. Laurent, F. Boucher, F. Odobel and D. Jacquemin*
Determining the Most Promising Anchors for CuSCN: Ab Initio Insights towards p-Type DSSCs
J. Mater. Chem. A (IF= 8.867) **4**, 2217–2227 (2016) doi.

52. J.P. Cerón-Carrasco,* D. Jacquemin* and A. D. Laurent*
*First Computational Step Towards the Understanding of the Antioxidant Activity of the Phycocyanobilin:Ferredoxin Oxidoreductase in Complex with Biliverdin IX*α
Comput. Theor. Chem. (IF = 1.549) **1077**, 58–64 (2016) doi.

51. S. H. Thany,* C. M. Bourdin, J. Graton, A. D. Laurent, M. Mathé-Allainmat, J. Lebreton and J.-Y. Le Questel
Similar Comparative Low and High Doses of Deltamethrin and Acetamiprid Differently Impair Retrieval of the Proboscis Extension Reflex in the Forager Honey Bee (Apis Mellifera)
Insects (open access) **6**, 805–814 (2015) doi.

50. Z. Alamiddine, B. Selvam, J.P. Cerón-Carrasco, M. Mathé-Allainmat, J. Lebreton, S. H. Thany, A. D. Laurent, J. Graton and J.-Y. Le Questel*
Molecular recognition of thiaclopride by Aplysia californica AChBP: new insights from a computational investigation
J. Comput. Aided Mol. Des. (IF=2.990) **29**, 1151–1167 (2015) doi.

49. S. Maione, A. M. Gil, G. Fabregat, L. J. del Valle, J. Triguero, A. Laurent, D. Jacquemin, F. Estrany, A. I. Jiménez, D. Zanuy, C. Cativiela and C. Alemàn*
Electroactive Polymer-Peptide Conjugates for Adhesive Biointerfaces
Biomater. Sci. (IF= 3.614) **3**, 1395-1405 (2015) doi.

48. A. D. Laurent, A. Blondel and D. Jacquemin*
Choosing an Atomic Basis Set for TD-DFT, soPPA, ADC(2), CIS(D), CC2 and EOM-CCSD Calculations of Low-Lying Excited-States of Organic Dyes.
Theor. Chem. Acc. (IF= 1.806) **134**, 76(1-11) (2015) doi.

47. E. Taillebois, Z. Alamiddine, C. Brazier, J. Graton, A. D. Laurent, S. H. Thany* and J.-Y. Le Questel*
Molecular Features and Toxicological Properties of Four Common Pesticides, Acetamiprid, Deltamethrin, Chlorpyriphos and Fipronil
Bioorg. Med. Chem. (IF=2.951) **23**, 1540–1550 (2015) doi.

46. M. Medved,* S. Budzak, A. D. Laurent and D. Jacquemin

Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes
J. Phys. Chem. A (IF= 3.187) **119**, 3112–3124 (2015) doi.

45. K. J. Chen, A. Charaf-Eddin, B. Selvam, F. Boucher, A. D. Laurent and D. Jacquemin*
Interplay Between TiO2 Surface and Organic Photochromes: A DFT Study of Adsorbed Azobenzenes and Diarylethenes
J. Phys. Chem. C (IF=3.187) **119**, 3684–3696 (2015) doi.

44. S. Chibani, A. D. Laurent, B. Le Guennic* and D. Jacquemin*
Excited States of Ladder-Type π Conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach
J. Phys. Chem. A (IF= 2.883) **119**, 5417–5425 (2015) doi.

43. Y. Houari, S. Chibani, D. Jacquemin and A. D. Laurent*
A TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in HydroxyphenylBenzImidazole (HBI) Dyes
J. Phys. Chem. B (IF= 3.187) **119**, 2180–2192 (2015) doi.

42. B. Selvam, J. Graton, A. D. Laurent, Z. Alamiddine, J. Lebreton*, M. Mathé-Allainmat, O. Coqueret, C. Olivier, S. H. Thanyand J.-Y. Le Questel*
Imidacloprid and Thiacloprid Neonicotinoids Bind More Favourably to Cockroach than to Honeybee α6 Nicotinic Acetylcholine Receptor: Insights from Computational Studies
J. Mol. Graph. Model. (IF=2.022) **55**, 1–12 (2015) doi.

41. Shao, Y.; Gan, Z.; Epifanovsky, E.; Gilbert, A. T.; Wormit, M.; Kussmann, J.; Lange, A. W.; Behn, A.; Deng, J.; Feng, X.; Ghosh, D.; Goldey, M.; Horn, P. R.; Jacobson, L. D.; Kaliman, I.; Khaliullin, R. Z.; Ku, T.; Landau, A.; Liu, J.; Proynov, E. I.; Rhee, Y. M.; Richard, R. M.; Rohrdanz, M. A.; Steele, R. P.; Sundstrom, E. J.; Woodcock, H. L.; Zimmerman, P. M.; Zuev, D.; Albrecht, B.; Alguire, E.; Austin, B.; Beran, G. J. O.; Bernard, Y. A.; Berquist, E.; Brandhorst, K.; Bravaya, K. B.; Brown, S. T.; Casanova, D.; Chang, C.-M.; Chen, Y.; Chien, S. H.; Closser, K. D.; Crittenden, D. L.; Diedenhofen, M.; DiStasio, R. A.; Do, H.; Dutoi, A. D.; Edgar, R. G.; Fatehi, S.; Fusti-Molnar, L.; Ghysels, A.; Golubeva-Zadorozhnaya, A.; Gomes, J.; Hanson-Heine, M. W.; Harbach, P. H.; Hauser, A. W.; Hohenstein, E. G.; Holden, Z. C.; Jagau, T.-C.; Ji, H.; Kaduk, B.; Khistyaev, K.; Kim, J.; Kim, J.; King, R. A.; Klunzinger, P.; Kosenkov, D.; Kowalczyk, T.; Krauter, C. M.; Lao, K. U.; Laurent, A. D.; Lawler, K. V.; Levchenko, S. V.; Lin, C. Y.; Liu, F.; Livshits, E.; Lochan, R. C.; Luenser, A.; Manohar, P.; Manzer, S. F.; Mao, S.-P.; Mardirossian, N.; Marenich, A. V.; Maurer, S. A.; Mayhall, N. J.; Neuscamman, E.; Oana, C. M.; Olivares-Amaya, R.; ONeill, D. P.; Parkhill, J. A.; Perrine, T. M.; Peverati, R.; Prociuk, A.; Rehn, D. R.; Rosta, E.; Russ, N. J.; Sharada, S. M.; Sharma, S.; Small, D. W.; Sodt, A.; Stein, T.; Stack, D.; Su, Y.-C.; Thom, A.J.; Tsuchimochi, T.; Vanovschi, V.; Vogt, L.; Vydrov, O.; Wang, T.; Watson, M. A.; Wenzel, J.; White, A.; Williams, C. F.; Yang, J.; Yeganeh, S.; Yost, S. R.; You, Z.-Q.; Zhang, I. Y.; Zhang, X.; Zhao, Y.; Brooks, B. R.; Chan, G. K.; Chipman, D. M.; Cramer, C. J.; Goddard, W. A.; Gordon, M. S.; Hehre, W. J.; Klamt, A.; Schaefer, H. F.; Schmidt, M. W.; Sherrill, C. D.; Truhlar, D. G.; Warshel, A.; Xu, X.; Aspuru-Guzik, A.; Baer, R.; Bell, A. T.; Besley, N. A.; Chai, J.-D.; Dreuw, A.; Dunietz, B. D.; Furlani, T. R.; Gwaltney, S. R.; Hsu, C.-P.; Jung, Y.; Kong, J.; Lambrecht, D. S.; Liang, W.; Ochsenfeld, C.; Rassolov, V. A.; Slipchenko, L. V.; Subotnik, J. E.; Van Voorhis, T.; Herbert, J. M.; Krylov, A. I.; Gill, P. M. and Head-Gordon, M
Advances in Molecular Quantum Chemistry Contained in the Q-Chem 4 Program Package
Mol. Phys (IF = 1.837) **113**, 184–215 (2015) doi. Web of Science Highly Cited in Field.

40. T. Jaunet-Lahary, A. Chantzis*, K. J. Chen, A. D. Laurent and D. Jacquemin*
Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes

J. Phys. Chem. C (IF= 4.772) **118**, 28831–28841 (2014) doi.

39. P. O. Hubin⋆, A. D. Laurent, D. P. Vercauteren and D. Jacquemin⋆
Investigation of ESIPT in a Panel of Chromophores Presenting N-H···N Intramolecular Hydrogen Bonds
Phys. Chem. Chem. Phys. (IF= 4.493) **16**, 25288–25295 (2014) doi.

38. S. Chibani, A. D. Laurent⋆, B. Le Guennic⋆ and D. Jacquemin⋆
Improving the Accuracy of Excited-State Simulations of BODIPY and Aza-BODIPY Dyes with a Joint SOS-CIS(D) and TD-DFT Approach
J. Chem. Theory Comput. (IF = 5.498) **10**, 4574–4582 (2014) doi.

37. G. Marchand⋆, A. D. Laurent, Z. Chen, O. Siri and D. Jacquemin⋆
Exceptional Stability of Azacalixphyrin and its Dianion
J. Phys. Chem. A (IF = 2.693) **118**, 8883–8888 (2014) doi.

36. K. Benelhadj, W. Muzuzu, J. Massue⋆, P. Retailleau, A. Charaf-Eddin, A. D. Laurent, D Jacquemin⋆, G. Ulrich⋆ and R. Ziessel⋆
White Emitters by Tuning the Excited-State Intramolecular Proton-Transfer Fluorescence Emission in 2-(2'-Hydroxybenzofuran)benzoxazole Dyes
Chem. Eur. J. (IF = 5.731) **20**, 12843–12857 (2014) doi.

35. A. D. Laurent and D. Jacquemin⋆
Analyzing Excited-State Processes and Optical Signatures of a Ratiomeric Fluorine Anion Sensor: a Quantum Look
Sci. China Chem. (IF= 1.695) **57**, 1363–1368 (2014) doi.

34. S. Chibani, D. Jacquemin⋆ and A. D. Laurent
Modelling Solvent Effects on the Absorption and Emission Spectra of Constrained Cyanines with both Implicit and Explicit MQ/EFP Models
Comput. Theor. Chem. (IF = 1.545) **1040–1041**, 321–327 (2014) doi. Elsevier TOP25 + Hottest Articles

33. A. D. Laurent, C. Adamo and D. Jacquemin⋆
Dye Chemistry with Time-Dependent Density Functional Theory
Phys. Chem. Chem. Phys. (IF = 4.493) **16**, 14334–14356 (2014) doi. RSC Most Read articles

32. A. D. Laurent⋆, V. N. Glushkov, T. Very and X. Assfeld
Toward the Understanding of the Environmental Effects on Core Ionizations
J. Comput. Chem. (IF = 3.589) **35**, 1131–1139 (2014) doi.

31. S. Chibani, A. D. Laurent, A. Blondel, B. Mennucci⋆ and D. Jacquemin⋆
Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model
J. Chem. Theory Comput. (IF = 5.498) **10**, 1848–1851 (2014) doi. ACS Most Read articles

30. J. P. Cerón-Carrasco, H. M. Roy, J. Cerezo, D. Jacquemin and A. D. Laurent⋆
Theoretical Insights on the Antioxidant Activity of Edaravone Free Radical Scavengers Derivatives
Chem. Phys. Lett. (IF = 1.897) **599**, 73–79 (2014) doi.

29. A. D. Laurent⋆, Y. Houari, P. H. P. R. Carvalho, B. A. D. Neto and D. Jacquemin⋆
ESIPT or not ESIPT? Revisiting Recent Results on 2,1,3-Benzothiadiazole under the TD-DFT Light
RSC Adv. (IF = 3.840) **4**, 14189–14192 (2014) doi.

28. K. J. Chen, A. D. Laurent and D. Jacquemin*
Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches
J. Phys. Chem. C (IF = 4.772) **118**, 4334–4345 (2014) doi.

27. Y. Houari, A. Charaf-Eddin, A. D. Laurent, J. Massue, R. Ziessel, G. Ulrich and D. Jacquemin*
Modeling Optical Signatures and Excited-State Reactivities of Substituted HydroxyphenylBenzOxazole (HBO) ESIPT Dyes
Phys. Chem. Chem. Phys. (IF = 4.493) **16**, 1319–1321 (2014) doi.

26. Y. Houari, A. D. Laurent and D. Jacquemin*
Spectral Signatures of Perylene Diimide Derivatives: Insights From Theory
J. Phys. Chem. C (IF = 4.835) **117**, 21682–21691 (2013) doi.

25. A. Chantzis, A. D. Laurent, C. Adamo and D. Jacquemin*
Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?
J. Chem. Theory Comput. (IF = 5.310), **9**, 4517–4525 (2013) doi. ACS Most Read articles

24. Y. Houari, D. Jacquemin and A. D. Laurent*
TD-DFT Study of pKa For Coumarins*
Chem. Phys. Lett. (IF = 1.991) **583**, 218–221 (2013) doi.

23. G. Fabregat, G. Ballano, J. Casanovas, A. D. Laurent, E. Armelin, L.J. del Valle, C. Cativiela, D. Jacquemin and C. Alemán*
Design of Hybrid Conjugates Based on Chemical Similarity
RSC Adv. (IF = 3.708) **3**, 21069–21083 (2013) doi.

22. S. Naseem[+], A. D. Laurent[+], E. C. Carroll, M. Vengris, M. Kumauchi, W. D. Hoff, A. I. Krylov and D. S. Larsen*
Photo-Isomerization Upshifts the pKa of the Photoactive Yellow Protein Chromophore to Contribute to Photocycle Propagation
J. PhotoChem. PhotoBiol. A: Chem. (IF = 2.625), **270**, 43–52 (2013) doi.
[+]These authors contributed equally to this manuscript.

21. Y. Houari, D. Jacquemin and A. D. Laurent*
Methodological Keys For Accurate pKa Simulations*
Phys. Chem. Chem. Phys. (IF = 4.189), **15**, 11875–11882 (2013) doi.

20. A. D. Laurent and D. Jacquemin*
TD-DFT Benchmarks: a Review
Int. J. Quant. Chem. (IF = 1.166), **113**, 2019–2039 (2013) doi. Wiley Most Accessed and Most Cited, Web of Science Highly Cited in Field

19. S. Chibani, B. Le Guennic, A. Charaf-Eddin, A. D. Laurent and D. Jacquemin*
Revisiting the Optical Signatures of BODIPY with Ab Initio Tools
Chem. Sci. (IF = 8.601), **4**, 13941–13952 (2013) doi. Front Cover

18. N. Haspel, A. D. Laurent, D. Zanuy, R. Nussinov, C. Alemán and G. Revilla-López*
Conformational Exploration of Two Peptides and Their Hybrid Polymer Conjugates: Potentialities As Self-Aggregating Materials
J. Phys. Chem. B (IF = 3.607), **116**, 12426–12440 (2012) doi.

17. A. D. Laurent, V. A. Mironov, P. P. Chapagain, A. V. Nemukhin and A. I. Krylov*
Exploring Structural and Optical Properties of Fluorescent Proteins by Squeezing: Modeling High-Pressure Effects on the mStrawberry and mCherry Red Fluorescent Proteins

J. Phys. Chem. B (IF = 3.607) **116**, 12426–12440 (2012) doi.

16. E. Dumont⋆, A. D. Laurent, X. Assfeld and D. Jacquemin
Performances of Recently-Proposed Functionals for Describing Disulfide Radical Anions and Similar Systems
Chem. Phys. Lett. (IF = 2.337), **501**, 245–251 (2011) doi.

15. G. Revilla-López, A. D. Laurent, E. A. Perpète, D. Jacquemin⋆, J. Torras, X. Assfeld⋆ and C. Alemán⋆
Key Building Block of Photoresponsive Biomimetic Systems
J. Phys. Chem. B (IF = 3.696), **115**, 1232–1242 (2011) doi. Front Cover

14. E. Dumont⋆, A. D. Laurent and X. Assfeld
Intersulfur Distance is a Key Factor in Tuning Disulfide Radical Anion Vertical UV-Visible Absorption.
J. Phys. Chem. Lett. (IF = 6.213[1]), **1**, 581–586 (2010) doi.

13. A. D. Laurent and X. Assfeld⋆
Effect of the Enhanced Cyan Fluorescent Proteinic Framework on the UV/visible Absorption Spectra of Some Chromophores
Interdisp. Sci. Comput. Life Sci. (FI=0.672), **2**, 38–47 (2010) doi.

12. E. Dumont⋆, P.-F. Loos, A. D. Laurent and X. Assfeld
Electronic Effects and Ring Strain Influences on the Electron Uptake by Selenium-Containing Bonds
Int. J. Quant. chem. (IF = 1.302), **110**, 513–523 (2010) doi.

11. A. D. Laurent⋆, X. Assfeld, D. Jacquemin, J.-M. André and E. A. Perpète
Substitution Effects on the Optical Spectra of Diarylethene Photochroms: Ab Initio Insights
Mol. Simul. (IF = 1.215), **36** 74–78 (2010) doi.

10. P.-F. Loos, E. Dumont, A. D. Laurent and X. Assfeld⋆
Important Effects of Neighbouring Nucleotides on Electron Induced DNA Single-Strand Breaks
Chem. Phys. Lett. (IF = 2.291), **475**, 120–123 (2009) doi.

9. E. Dumont⋆, A. D. Laurent, P.-F. Loos and X. Assfeld
Analyzing the Selectivity and Successiveness of a Two-Electron Capture on a Multiply Disulfide-Linked Protein
J. Chem. Theory Comput. (IF = 4.804), **5**, 1700–1708 (2009) doi.

8. D. Jacquemin⋆, A. D. Laurent, E. A. Perpète and J.-M. André⋆
An Ab Initio Simulation of the UV/Visible Spectra of N-Benzyildeneaniline Dyes
Int. J. Quantum Chem. (IF = 1.315), **109**, 3506–3515 (2009) doi.

7. D. Jacquemin⋆, E. A. Perpète, A. D. Laurent, X. Assfeld and C. Adamo⋆
Spectral Properties of Self-Assembled Squaraine-Tetralactam: a Theoretical Assessment
Phys. Chem. Chem. Phys. (IF = 4.116), **11**, 1258–1262 (2009) doi. Front Cover

6. J. Preat⋆, A. D. Laurent, C. Michaux, E. A. Perpète and D. Jacquemin
Impact of Tautomers on the Absorption Spectra of Neutral and Anionic Alizarin and Quinizarin Dyes
J. Mol. Struct. (THEOCHEM) (FI= 1.216), **901**, 24–30 (2009) doi.

[1]First IF known in 2011.

5. E. Dumont*, P.-F. Loos, A. D. Laurent and X. Assfeld
Huge Disulfide-Linkage'S Electron Capture Variation Induced by α-Helix Orientation
J. Chem. Theory Comput. (IF = 4.274), **4**, 1171–1173 (2008) doi.

4. C. Simo, A. Salaün, C. Arnarez, L. Delemotte, A. Haegy, A. Kachmar, A. D. Laurent, J. Thomas, B. Jamart-Grégoire, P. Le Grel and A. Hocquet*
The "Hydrazinoturn Hydrogen" Bonding Network in Hydrazinopeptides and Aza-β3-Peptides as Probed by an AIM Topological Analysis of the Electronic Density
J. Mol. Strut. (THEOCHEM) (IF= 1.167), **869**, 41–46 (2008) doi.

3. P.-F. Loos*, J. Preat, A. D. Laurent, C. Michaux, D. Jacquemin, E. A. Perpète and X. Assfeld
Theoretical Investigation of the Geometries and UV/Vis Spectra of Poly(L-Glutamic Acid) Featuring Photochromic Azobenzene Side Chain
J. Chem. Theory Comput. (IF = 4.274), **4** (2008) 637–645 doi.

2. A. D. Laurent, J.-M. André, E. A. Perpète and D. Jacquemin*
Photochromic Properties of Dithienylazoles and Other Conjugated Diarylethenes
J. PhotoChem. PhotoBiol. A: Chem. (IF = 1.911), **192**, 211–219 (2007) doi.

1. A. D. Laurent, J.-M. André, E. A. Perpète and D. Jacquemin*
Hemi-Indigo Photochroms: a Theoretical Investigation
Chem. Phys. Lett. (IF = 2.207), **436**, 84–88 (2007) doi.

Conferences and Seminars

Here are listed only the communications or poster I have presented. The list do not gather the work presented by my students, postdocts or collaborators.

International conferences: 10
French conferences: 5
Invited conferences: 4
Invited seminars: 13

Invited conferences (5)

6. **Avril 2019** 19th DeMon developers workshop (Frejus, France), *Shedding light on new photochrome*

5. **Avril 2019** XXIime Congrs du Groupe de Graphisme et Modlisation Molculaire (Nice, France), *Modlisation d'interaction protine-protine l'aide d'approches de simulations multi-chelles*

4. **May 2017** VIth Chinese-French Workshop in Theoretical Chemistry (Xiamen, China), *Exploring solvatochromism effects of molecular probes*

3. **Nov 2016** Excited States in Complex Systems (Paris, France), *Multiscale method to deal with challenging excited state properties*

2. **Jul. 2014** ACS meeting, Photoinduced Proton Transfer symposium (San Francisco, USA), *Modeling Excited-State Intramolecular Proton Transfer with TD-DFT*

1. **June 2014** Fem-EX (Oslo, Norway), *Multiscale Modeling of a New Promising Class of Fluorescent Protein Bilirubin*

Oral communications (8) in conferences

8. **Avril 2019** XXIe Congrs du Groupe de Graphisme et Modlisation Molculaire (Nice, France), *Modlisation d'interaction protine-protine l'aide d'approches de simulations multi-chelles*

7. **Jun. 2018** Journée Scientifique de l'Université de Nantes, symposium "Travaux scientifiques bass sur le calcul intensif (HPC) dans la rgion des Pays de la Loire" (Nantes, France), *Modlisation des interactions entre l'interleukine 15 et de ses rcepteurs: vers la conception d'inhibiteurs*

6. **Jun. 2016** Journée Scientifique de l'Université de Nantes, symposium PIRAMID (Nantes, France), *Fighting against triple negative breast cancer: simulation and design of new mTOR inhibitors*

5. **Jun. 2015** TheoBio 2015 (Sardaigne, Italy), *Modeling Modelling new covalent mTOR inhibitors against Triple Negative Breast Cancer*

4. **Jul. 2014** 14$^{\text{ime}}$ RCTF (Paris, France), *From pressure effects on fluorescent protein to ligand-induced fluorescent proteins*

3. **June 2014** 4$^{\text{ime}}$ Journée Inter-Régionale de Chimie Moléculaire et Thérapeutique (Nantes), *Modélisation des propriétés structurales et spectrales d'une nouvelle classe de protéine fluorescente originale et prometteuse.*

2. **July 2012** ACS (Philadelphia, USA), *Extension of the Effective Fragment Potential Method to Model Proteins*

1. **June 2008** 2nd International Conference for Young Chemists (Penang, Malaisia), *Proteinic Electronic Response to UV/visible Chromophore Absorption.*

Invited seminars (14)

14. **Feb. 4 2016** Centre Eugène Marquis (Rennes), *Modeling ligand-induced fluorescent proteins*

13. **Dec. 2014** University of Montpellier (France), *Modeling HBI ESIPT dyes and towards reactivity into mTOR kinase*

12. **May 2014** University of Namur, *Multiscale Approach to Model the Recently Discovered Bilirubin-Induced Fluorescent Protein.*

11. **Sept. 2013** University of Southern California (Tuesday's seminar by Krylov, Wittig and Reisler), *Extension of the Effective Fragment Potential Method to Model Proteins.*

10. **Jan. 2012** University of Nantes (France), *Modeling High-Pressure on mStrawberry and mCherry Red Fluorescent Proteins.*

9. **Dec. 2010** Aix-Marseille Université (Marseille, France), *Electronic Phenomena in Biomolecules: Core ionization.*

8. **Nov. 2010** Universitat Politecnica de Catalunya (Barcelona, Spain), *Electronic Phenomena in Biomolecules with the Help of QM/MM Methodology.*

7. **Oct. 2010** ENS Lyon (France), *Electronic Phenomena in Biomolecules: Core ionization.*

6. **Sept. 2010** University of Southern California (Los Angeles, USA), *Electronic Phenomena in Biomolecules: Green Fluorescent Protein.*

5. **Jul. 2010** Scuola Internazionale Superiore di Studi Avanzati di Trieste– SISSA (Trieste, Italie), *Core Ionization Study with the Asymptotic Projection Approach: Environment Effects.*

4. **Jun. 2010** Max Planck Institute (Goettingen, Germany), *Electronic Properties of Macromolecules: Surrounding Effects.*

3. **Sept. 2009** University of Namur (Belgium), *Photochemical Properties of Fluorescent Proteins: Mutations of Chromophores.*

2. **Sept. 2008** University of Namur (Belgium), *Surroundings Effect on Chromophores Inside Proteins.*

1. **Sept. 2008** Universitat Politecnica de Catalunya (Barcelona, Spain), *Proteinic Influence on Absorption Spectra of Chromophore.*

Posters (9)

9. **Jul. 2016** XVth French-speaking Theoretical Chemists Meeting (Lyon, France), *Properties of Rad51 inhibitors embedded in transport protein.*

8. **Jun. 2013** VII Molecular Quantum Mechanics (Lugano, Swizterland), *Extension of the Effective Fragment Potential Method to Proteins.*

7. **Apr. 2013** TD-DFT Conference (Nantes, France), *Modelling the pressure effects on optical properties of mStrawberry.*

6. **Jan. 2012** 59th Annual Western Spectroscopy Conference (Pacific Grove, USA), *Modelling the Pressure Effects on Optical Properties of Fluorescent Proteins from the mFruit Family.*

5. **Jul. 2011** Ninth World Association of Theoretical and Computational Chemists – WATOC (Santiago de Compostela, Spain), *Characterization of Coupled trans-cis Isomerization and Proton Transfer in the Photoactive Yellow Protein Chromophore.*

4. **Jul. 2010** XIIth French-speaking Theoretical Chemists Meeting (Namur, Belgium), *Core Ionization Study with the Asymptotic Projection Approach: Environment Effects*

3. **Jul. 2009** 3rd Methods and Applications of Computational Chemistry – MACC (Odessa, Ukraine), *Importance of the Electronic Response of the Surrounding to UV/visible Chromophore Absorption* and *Core and Valence Hole States from Orthogonality Constrains Techniques.*

2. **Jul. 2008** XIth French-speaking Theoretical Chemists Meeting (Dinard, France), *Proteinic Electronic Response to UV/visible Chromophore Absorption: QM/MM Results.*

1. **Feb. 2008** 1st Theoretical Tools for in-silico Spectroscopy – THETIS (Paris, France), *Proteinic Electronic Response to UV/visible Chromophore Absorption: QM/MM Results.*

Participation in workshops and conferences (9)

- **Jun. 2017** Journée Scientifique de l'Université de Nantes, Symposium ECRIN, Nantes (France)
- **Fev. 2017** Macrocycle Symposium, Nantes (France)
- **Ap. 2016** Multi-Responsive Photochromes, Nantes (France)
- **Ap. 2015** Modelling Photoactive Molecules, Nantes (France)
- **Ap. 2013** TD-DFT conference, Nantes (France)
- **Aug. 2014** QChem developer meeting, San Francisco (USA)

- **Jun. 2014** ACS Conference, San Francisco (USA)
- **Sept. 2013** ACS Conference, Indianapolis (USA)
- **Sept. 2013** QChem developer meeting, Indianapolis, (USA)
- **July. 2011** QChem developer meeting, Anaheim (USA)
- **2007** Cheminformatics and chemogenomics in drug discovery, University of Namur (Belgium)

Teaching activities

- **Poly-electronic systems (X7LU091, 9h/year),** University of Nantes
  Teaching Assistant (TP), level: Master 1 students (M1 LUMOMAT) *Fall 2014-2016*
- **Poly-electronic systems (X7LU020, 6h/year),** University of Nantes
  Teaching Assistant (TP), level: Master 1 students (M1 A3M) *Fall 2013-2016*
- **Informatic tools for physics and chemistry (X5PC070, 20h/year),** University of Nantes
  Teaching Assistant (TP), level: License students 3 (L3 PC) *Fall 2013-2016*
- **QM-MM hybrid methods (3h),** University of Rennes
  Lecturer, level: Master 2, Gradstudents ('RFCT' session) *Spring 2015-2017*
- **Chemometrics (X7CA130, 8.5h),** University of Nantes
  Lecturer, level: Master 1 students (M1 A3M) *Fall 2013-2015*
- **Introduction to Molecular Dynamics (3h+3h),** University of Angers
  Lecture and Practical session, level: Master 2 students (M2 LUMOMAT) *Fall 2015*
- **Excited states for organic molecules (3h)** University of Rennes
  Lecturer, level: Master 2, Grad students ('RFCT' session) *Spring 2014*
- **Biomathematics (64h/year)** Faculty of Pharmacy, Nancy
  Teaching Assistant, level: Grad students *2007–2010*