
Curriculum Vitae

Elise Dumont

civil status French, 40 years old, civil union, two children (2015, 2018)
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École Normale Supérieure de Lyon
46 allée d'Italie, 69346 Lyon Cedex 07, France

Professor at the École Normale Supérieure de Lyon

Career and academic background

2017-2021

Full Professor, École Normale Supérieure de Lyon, Department of Chemistry

- 2021-... Professeur des Universités 1e classe, awarded by the National Universities Council (CNU)
- 2019-2024 Junior member of the Institut Universitaire de France (IUF), an institution that appoints 2% of French academics in research-intensive chairs.
- 2017-2021 Professeur des Universités (PR2)

Research in computational bio- and supramolecular chemistry, at the Laboratoire de Chimie, ENS de Lyon
DNA damage and repair, QM/MM modeling, classical MD simulations, photo(bio)chemistry, radical chemistry

- 96 research papers, 2 book chapters, complete list of publications [link](#) Google scholar
- ~ 1800 citations (as of Oct. 2021), h-index=23
- 33 oral communications (17 invited lectures), 28 seminars as of May 2021
- Academic stays at UCLA (2011, two weeks), U. Bologna (2013, three weeks), U. Dusseldorf (2013, three weeks), VU Amsterdam (guest scientist 2014-2015, six months in total, U. Valencia (2014, two weeks), U. Tarragona (2015, two weeks), ECNU (2016, invited professor and 2019)

2008-2017

Associate Professor, Maître de Conférences, École Normale Supérieure de Lyon

- 2013 Habilitation à diriger les recherches (HDR, D. Sc. in Chemistry)
Hybrid simulation of biomolecular environment effects: reactivity, structure and spectroscopy
Committee: S. Antonzcak, A. Milet, F. Lankas, R. Vuillemier, J.-L. Ravanat, X. Assfeld, M. Garavelli.
- 2010 six-months stay at EPFL Lausanne, Switzerland, Prof. U. Rothlisberger

2007-2008

Research and teaching assistant (ATER), Université de Nancy, Laboratoire SRSMC

2006-2007

Postdoctoral fellow, Australian National University, Research School of Chemistry, Canberra, P. M. W. Gill

1st sem. 2006

Junior scientist, UCSF, California, group Ken A. Dill

2003-2006

Ph.D. in Theoretical Chemistry, University Paris VI, under the direction of P. Chaquin

Studying electronic substituent effects using fictitious charges: the H^ method.* ([link](#) to the manuscript, in French)

2000-2003

Undergraduate and graduate studies at the Department of Chemistry, École Normale Supérieure Paris

2000-2003: **Magistère in Chemistry**, École Normale Supérieure Paris

2002-2003: **Master 2 in Theoretical and Informatics Chemistry**, University Paris VI

2001-2002: Research stays at Univ. Autònoma Barcelona, U. Paris-Sud, University Paris VI

2000-2001: **Degree and Master 1 in Chemistry**, École Normale Supérieure Paris

Supervision of research projects

PhD students (7, 2 ongoing)

Year(s)	Name	Funding scheme	Publications	Current position
2021-...	Maxime Kerमारrec co-supervision N. Gillet	ANR		— —
2020-...	Laleh Allahkaram co-supervision N. Gillet	ENS fellowship ("bourse présidence")	one submitted	—
2016-2019	Chen-Hui Chan co-supervision D. Loffreda	Labex PRIMES	P60,76,91	Pdoc Korea
2014-2017	Emmanuelle Bignon co-supervision C. Morell	Bourse ED/MESRI	P45,47,48,49,52,53 P60,61,69,80,81	Pdoc U. Lorraine
2014-2017	Debora Vilona	Bourse Région ARA	P52,85	IR XXX
2010-2013	Chandan Patel	Bourse ED/MESRI	P22,26,27,31	
2007-2010	Adèle Laurent	Bourse ED	P12,14,15,17,18,19	CR U. Nantes

Post-doctoral fellowships

Year(s)	Name	Funding scheme	Publications	Current position
2020-2021	Alessio Bartocci	Maison de la Chimie	P89,95	Pdoc U. Strasbourg
2016-2018	Ayad Bellili	ATER ENS	P59	Ass. Prof. U. XXX
2014-2016	Raymond Grüber	Lecturer ENS	P41,67.70,88	Lecturer, U. G. Eiffel
2010-2011	Céline Dupont	Lecturer ENS	P 22,25,26,27	CNRS U. Bourgogne

Visitors and summer internships:

2 L3 internships: David Beroldy (2012), Raphael Finizola (2020) 1 M1 internship: Elsa Fontimpe (M1 ENS, 2009) 5 M2 internships: Inacrist Geronimo (M2 Atosim, 2009, P16), Nils Aronsson (M2 ENSL, 2014), Gilles Touchagues (M2 Atosim, 2014), Victor Claerbout (M2 Atosim, 2017, P80,81), Florence Szczepaniak (M2 ENSL, 2019, P83)

Teaching

2018-2019	Lecture "Introduction to molecular modeling" (M1 Catalysis, La Doua, 15h CM + 15h TD)
2016-2017	Lecture Computational Chemistry (M1, 10h CM). Since 2018,
2015-2018	<i>Chemical bonding</i> (L3, 14h CM)
Since 2008	<i>Molecular modelling hands on</i> (L3, M1, M2), <i>DFT lecture</i>
2012-2014	<i>Computational photochemistry</i>
2011-2017	<i>Spectroscopy L3 : rotation, vibration , rovibration</i> (10h CM)
2008-2014	<i>Electrochemistry practicals</i>
2010-2014	<i>Mathematics L3 : basic notions in algebra and analysis</i>
2008-2013	<i>Computer science for physics: C and python</i>
2008-2014	<i>Teaching in the "Prépa agrégation"</i>

Responsibilities

2021-2024	<i>Elected member of the CoNRS section 16 (Chemistry & Life)</i>
Sept. 2019-	<i>Expert for MESRI/DAEI (European and International Affairs Department, Anses)</i>
Sept. 2019-	<i>Head of Department of Chemistry, ENS de Lyon</i>
2017-	<i>Editorial Board Member for Scientific Reports</i>
2017-	<i>Member of the Council of the Ecole Doctorale in Chemistry of Lyon</i>
2016-2020	<i>Co-animator of the Theory Axis of ENS Lyon (11 permanent members, ~15-20 non permanent researchers), member of the scientific council</i>

2016-2018	Responsible for the teaching program in Chemistry at ENS de Lyon (L3 and M1 Chemistry major) Sciences de la matière ENS de Lyon (~30 students)
2016-2018	Member of the department council
2015-2017	Nominated member at the "Conseil National des Universités", CNU section 31, collège B
2015-2019	Vice-president for the ENSL entrance exam, Chemistry part
2014-2021	Board member of the "Réseau Français de Chimie Theorique" (RCTF); coordinator for the South-East pole
2014	Guest Editor for a Topics " Radiation-induced and oxidative DNA damages " in <i>Frontiers in Chemistry</i>
2014-	Member of 24 PhD committees (13 as referee, 3 in Spain, 1 in Austria, 5 as president) and 4 HDR (2 as referee)
2014	Chair of Session "Radiation-induced DNA damage" – Physics and modeling, 13th International Workshop on Radiation Damage to DNA, MIT
2014-	Member of recruitment committees (5 MCF, 2 PR), AgPr and ATER positions yearly
2013-	Referee for several scientific institutions and funding agencies: ERC, ANR, DAEI/MESRI (10 per year), PRACE (panel member in 2016), NWO, the Slovak Academy of Sciences, the Czech Science Foundation, the Romanian Ministry, the Austrian Academy of Sciences, DAEI, Ville de Paris, NSC Poland, Labex ...
2011	Scientific Board of the workshop "Biophotochem workshop", organized in Marseilles
2010-2015	Elected member of the lab council
2008-	Peer reviewer for journals: publons

Awards & research grants

2020: ANR Nucleomap (partner, PI N. Gillet)
2019: Nomination as IUF (Institut Universitaire de France) junior member, considered equivalent of top 2% of French academics below 40 years
2019: Laureate Fonds Recherche ENSL (30 kE)
2018: Laureate ELAN ERC Idex Lyon (32 kE)
2018: Laureate Fondation de la Maison de la Chimie (50 kE)
2014: Région Rhône-Alpes grant, PhD polyoxometalate-peptide interaction (co-supervisor, E. Lacôte)
ANR funding: Ln23 (2014-2017, grant holder Olivier Maury), Femto2DNA (2015-2019, grant holder Xavier Assfeld), Eco-phos (2017-2020, grant holder Olivier Maury)
2013-2016: member of the COST Action CM 1201, WG "Models of DNA Damage and Consequences"
2012 Member and representant of the lab ("project leader") in the LabEX PRIMES (Physics, Radiobiology, Medical Imaging and Simulation) (2012-2019)
2010 Laureate of a mobility fellowship for a six-months stay at EPFL (2010)
2006 ANU postdoctoral fellowship (2006-2007)

Five selected publications

Title	Journal	Cited
Unveiling the binding modes of the crystallophore, a terbium-based molecular nucleating and phasing agent for protein crystallography	Chem. Eur. J., 2018, 24:9739-9746 doi	14
Insights into the formation of an oxidative intra-strand cross-link DNA lesion from QM/MM molecular dynamics simulations	J. Am. Chem. Soc., 2012, 134:2111-2119 doi	69
Resolving the benzophenone DNA-photosensitization mechanism at QM/MM level	J. Phys. Chem. Lett., 2015, 6:576-580	49
Probing the reactivity of singlet oxygen with purines	Nucl. Acids Res., 2016, 44:56-62, doi	46
Interaction of Palmatine with DNA: An Environmentally Controlled Phototherapy Drug	J. Phys. Chem. B, 2015, 119:410-419	42

Publications

citations: ~1800 (as Sept. 2021) / h-index: 23 / first author: 19 / corresponding author: 19 / co-corresponding-author: 14 / published or in press: 96 + 2 book chapters. Google scholar [Elise Dumont](#), Orcid [0000-0002-2359-111X](#)

*** 2021

[...] Footprinting the binding of crystallophore at protein-protein interfaces : genesis/from a versatile probe to identified crystallization sites, N. Gillet, A. Bartocci,... , E. Girard, E. Dumont

[...] Design of the second generation of crystallophore for protein crystallography, A. Roux, Z. Alsalman, T. Jiang, J.-C. Mulatier, D. Pitrat, [E. Dumont](#), F. Riobé, E. Girard, O. Maury, in preparation

[...] Reactivity of singlet oxygen with DNA, an update, J.-L. Ravanat, [E. Dumont](#), submitted

[...] Molecular mechanisms associated with clustered lesion-induced impairment of 8-oxoG recognition by the human glycosylase OGG1, T. Jiang, E. Dumont, A. Monari, E. Bignon, submitted to *Molecules*. [preprint](#)

[...] Encoding stereochemical molecular information on cyclophanes using non-directional interactions, Y. Zhang, B. Ourri, P.-T. Skowron, E. Jeamet, A. Belenguer, N. Vanthuyne, O. Cala, P. Mandal, C. Duchamp, [E. Dumont](#), F. Perret, L. Vial, I. Huc, J. Leclaire, to be submitted

[...] The behavior of triplet thymine in a model B-DNA strand. Energetics and spin density localization revealed by ab initio molecular dynamics simulations. L. Allahkaram, A. Monari, [E. Dumont](#), submitted

[...] How fragile we are. Influence of STimulator of INterferon Genes, STING, variants on pathogen recognition and immune response efficiency, J. Morere, C. Hognon, T. Miclot, T. Jiang, [E. Dumont](#), G. Barone, E. Bignon, and A. Monari, submitted, [preprint](#)

[P96] Organo-polyoxometalate-based Hydrogen-Bond catalysis, D. Vilona, M. Lelli, [E. Dumont](#), E. Lacôte, *Chem. Eur. J.*, 2021, in press

[P95] Influence of divalent cations in the protein crystallization process assisted by Lanthanide-based additives. A. Roux, R. Talon, Z. Alsalman, S. Engilberge, A. D'Aléo, S. Di Pietro, Adeline Robin, A. Bartocci, G. Pilet, [E. Dumont](#), T. Wagner, S. Shima, F. Riobé, E. Girard, O. Maury, *Inorg. Chem*, 2021, in press [preprint](#)

[P94] Exploring the Concept of Dimerization-Induced Inter System Crossing: at the Origins of Spin-Orbit Coupling Selection Rules, L. Galán, J. Andrés Castán, C. Dalinot, P. Simón Marqués, J. Galiana, P. Blanchard, C. Andraud, [E. Dumont](#), O. Maury, C. Cabanetos, C. Monnereau, T. Le Bahers, *J. Phys. Chem. B*, 2021, in press

[P93] Light-induced in situ chemical activation of a fluorescent probe for monitoring intracellular G-quadruplex structures, M. Mosser, M. Deiana, T. Le Bahers, [E. Dumont](#), M. Dudek, S. Denis-Quanquin, C. Andraud, K. Matczyszyn, L. Guy, C. Monnereau, *Nanoscale*, 2021, accepted

[P92] A dynamic view of histone tails interaction with clustered abasic sites in a nucleosome core particle, E. Bignon, N. Gillet, T. Jiang, C. Morell, [E. Dumont](#), [preprint](#), 2021, *J. Phys. Chem. Lett.*, in press

[P91] Tracing back the Recognition of a Multiply Damaged Site by DNA Bacterial Formamidopyrimidine Glycosylases Through Molecular Dynamics Simulations and a Machine Learning Protocol, E. Bignon, N. Gillet, C.-H. Chan, T. Jiang, A. Monari, [E. Dumont](#), *Comput. Struct. Biotechnol. J.*, accepted

[P90] Low-energy electron transport in gold: mesoscopic potential calculation and its impact on electron emission yields, R. Ramos, F. Poignant, C.-H. Chan, A. Ipatov, B. Gervais, E. Dumont, D. Loffreda, M. Beuve, *Eur. Phys. J. Plus*, 2021, 136:345, [doi](#)

[P89] Capturing the dynamic association between a tris-dipicolinate lanthanide complex and a decapeptide: a combined paramagnetic NMR and molecular dynamics exploration, S. Denis-Quanquin, A. Bartocci, F. Riobé, O. Maury, E. Dumont, N. Giraud, *Phys. Chem. Chem. Phys.*, in press [doi](#)

[P88] Electron-Triggered Metamorphism in Palladium-Driven Self-Assembled Architectures, C. Kahlfuss, S. Chowdhury, A. Fins-Carreira, R. Grüber, E. Dumont, D. Frath, F. Chevallier, E. Saint-Aman, C. Bucher, *Inorg. Chem.*, 2021, 60:3543-3555 [doi](#)

[P87] Radiochimie de l'ADN : études expérimentales et théoriques, J.-L. Ravanat and E. Dumont, *Actualité Chimique*, 2021, [link](#)

[P86] Assessing the sequence dependence of pyrimidine-pyrimidone (6-4) photoproduct in a duplex double-stranded DNA: a challenge for microsecond range simulation, N. Gillet, A. Bartocci, E. Dumont, *J. Chem. Phys.*, 2021, 154:135103 [doi](#)

[P85] Synthesis and properties of higher nuclearity polyazanes, T. Criton, D. Vilona, G. Jacob, M. Médebielle, E. Dumont, L. Joucla, E. Lacôte, *Chem. Eur. J.*, 2021, 27:3670-3674 [doi](#)

[P84] Monte Carlo study of free radical production under keV photon irradiation of gold nanoparticle aqueous solution. Part II: local primary chemical boost. F. Poignant, H. Charfi, C.-H. Chan, E. Dumont, D. Loffreda, E. Testa, B. Gervais, M. Beuve, *Radiation Physics and Chemistry*, 2021, 109161 [doi](#)

*** 2020

[P83] Molecular dynamics approach for capturing calixarenes-proteins interactions: the case of cytochrome c, A. Bartocci, N. Gillet, T. Jiang, F. Szczepaniak, E. Dumont, *J. Phys. Chem. B*, 2020, 124:11371-11378 [doi](#), [preprint](#)

[P82] Polymerization photoinitiators with near-resonance enhanced two-photon absorption cross section towards high-resolution photoresists with enhanced sensitivity, C. Arnoux, Tatsuki, E. A. Poutougnigni, J.-C. Mulatier, D. Pitrat, L. Khrouz, C. Bucher, E. Dumont, K. Kamada, P. Baldeck, C. Andraud, A. Banyasz, C. Monnereau, *Macromolecules*, 2020, [doi](#)

[P81] Impact of the nucleosome histone core on the structure and dynamics of DNA containing pyrimidine-pyrimidone (6-4) photoproduct, E. Matouskova, E. Bignon, V. Claerbout, T. Drsata, N. Gillet, A. Monari, E. Dumont, F. Lankas, *J. Chem. Theor. Comput.*, 2020 [preprint](#)

[P80] Nucleosomal embedding reshapes the dynamics of abasic sites, E. Bignon, V. Claerbout, T. Jiang, C. Morell, N. Gillet, E. Dumont, *Sci. Rep.*, 2020, in press, [preprint](#)

[P79] The Dark Side of Disulfide-based Dynamic Combinatorial Chemistry. M. Dumartin, J. Septavaux, E. Jeamet, E. Dumont, F. Perret, L. Vial, J. Leclaire, *Chem. Sci.*, 2020, [doi](#)

[P78] Effect of the Ligand Binding Strength on the Morphology of Functionalized Gold Nanoparticles, C.-H. Chan, F. Poignant, M. Beuve, E. Dumont, D. Loffreda*, *J. Phys. Chem. Lett.*, 2020, 11, 7, 2717-2723, [doi](#)

[P77] Monte Carlo study of the free radical production under keV photon irradiation in the presence of gold nanoparticles. Part I: global primary chemical boost. F. Poignant, H. Charfi, C.-H. Chan, [E. Dumont](#), D. Loffreda, E. Testa, B. Gervais, M. Beuve, *Radiation Physics and Chemistry*, 2020, accepted [doi](#)

***** 2019**

[P76] Probing interaction of a trilycine peptide with DNA behind formation of guanine-lysine cross-links: insights from molecular dynamics. C.-H. Chan, A. Monari, J.-L. Ravanat, [E. Dumont*](#), *Phys. Chem. Chem. Phys.*, 2019, 21, 23418-23424 (selected as hot paper) [doi](#)

[P75] Tuning Protein Frameworks via Auxiliary Supramolecular Interactions, S. Engilberge, M. L. Rennie, [E. Dumont](#), P. Crowley, *ACS Nano*, 2019, 13:10343-10350 [doi](#)

[P74] A Halogen-Bond Donor Catalyst for Templated Macrocyclization, K. Guillier, E. Caytan, V. Dorcet, F. Mongin, [E. Dumont](#), F. Chevallier, *Angew. Chem. Int. Ed.*, 2019, 58:14940-14943, [doi](#)

[P73] Photo/redox-responsive 2D-Supramolecular assembly involving Cucurbit-[8]-uril and a star-shaped porphyrin tecton, S. Chowdhury, N. Youssef, L. Guy, D. Frath, F. Chevallier, [E. Dumont](#), A. P. Ramos, G. J.-F. Demets, C. Bucher, *Electrochimica Acta*, 2019, 316:79-92 [doi](#)

[P72] Selective and efficient recognition of monophosphoesters in water by a biomimetic resorcinarene Zn(II) complex, S. Collin, N. Giraud, [E. Dumont](#), O. Reinaud, *Org. Chem. Frontiers*, 2019, 6:1627-1636

[P71] A Water Solvation Shell can Transform Gold Metastable Nanoparticles in the Fluxional Regime, C.-H. Chan, F. Poignant, M. Beuve, [E. Dumont](#), D. Loffreda, *J. Phys. Chem. Lett.*, 2019, 10:1092, [doi](#)

[P70] Dynamic Molecular Metamorphism involving Palladium-Assisted Dimerization of π -Cation Radicals. C. Kahlfuss, R. Grüber, [E. Dumont](#), G. Royal, F. Chevallier, E. Saint-Aman, C. Bucher, *Chem. Eur. J.*, 2019, 25:1573-1580 [doi](#)

[P69] Wetting the Lock and Key Enthalpically Favors Polyelectrolytes Binding. E. Jeamet, J. Septavaux, A. Héloin, M. Donnier-Maréchal, M. Dumartin, P. Mandal, I. Huc, E. Bignon, [E. Dumont](#)[†], J.-P. Francoia, F. Perret, L. Vial[†], and J. Leclaire[†], *Chem. Sci.*, 2019, 10, 277 [doi](#) (communiqué: [CNRS news](#))

***** 2018**

[P68] Dynamics of the excited-state hydrogen transfer in a dG-dC homo-polymer: intrinsic photostability of DNA. A. Francés-Monerris, H. Gattuso, D. Roca-Sanjuán, I. Tuñón, M. Marazzi, [E. Dumont](#), and A. Monari, *Chem. Sci.*, 2018, in press (cover)

[P67] Unveiling the binding modes of the crystallophore, a terbium-based molecular nucleating and phasing agent for protein crystallography. S. Engilberge, F. Riobé, S. Di Pietro, T. Wagner, S. Shima, E. Girard, [E. Dumont](#), O. Maury, *Chem. Eur. J.*, 2018, 24:9701-9701 (cover) - [CNRS news](#)

[P66] Diastereoselective Synthesis of a Dyn[3]arene with Distinct Binding Behaviors toward Analogous Biogenic Polyamines. M. Donnier-Maréchal, J. Septavaux, E. Jeamet, A. Héloin, F. Perret, [E. Dumont](#), J.-C. Rossi, F. Ziarelli, J. Leclaire, L. Vial, *Org. Lett.*, 2018, 20:2420-2423 [doi](#)

[P65] Resolving the singlet excited states manifold of benzophenone by first-principles and ultrafast electronic spectroscopy. J. Segarra-Martí, E. Zvereva, M. Marazzi, J. Brazard, [E. Dumont](#), X. Assfeld, S. Haacke, M. Garavelli, A. Monari, J. Léonard, I. Rivalta, *J. Chem. Theor. Comput.*, 2018, 14:2570-2585, [doi](#)

[P64] Accurate estimation of the standard binding free energy of netropsin with DNA. H. Zhang, H. Gattuso, E. Dumont, W. Cai, A. Monari, C. Chipot, F. Dehez, *Molecules*, 2018, 23(2), 228 [doi](#)

[P63] The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. E. A. Zvereva, J. Segarra-Marti, M. Marazzi, J. Brazard, A. Nenov, O. Weingart, J. Léonard, M. Garavelli, I. Rivalta, E. Dumont, X. Assfeld, S. Haacke, A. Monari, *Photochem. Photobiol. Sci.*, 17:323-331 [doi](#)

***** 2017**

[P62] Elucidation of the Conformation of Polyglycine Organo-Polyoxotungstates: Evidence for Zipper Folding, D. Vilona, D. Lachkar, E. Dumont[†], M. Lelli[†], E. Lacôte[†], *Chem. Eur. J.*, 2017, 23, 13323–13327 [doi](#)

[P61] Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process, E. Bignon, M. Marazzi, V. Besancenot, H. Gattuso, C. Morell, L. Eriksson, S. Grandemange[†], E. Dumont[†], A. Monari[†], *Sci. Rep.*, 2017, 7, 8885 [doi](#)

[P60] Molecular dynamics insights into polyamines-DNA binding modes: implications for cross-links selectivity, E. Bignon[†], C.-H. Chan, C. Morell, A. Monari, J.-L. Ravanat, E. Dumont[†], *Chem. Eur. J.*, 2017, 23:12845-12852 [doi](#)

[P59] Free energy profiles for two ubiquitous damaging agents: methylation and hydroxylation of guanine in B-DNA. R. Grüber, J. Aranda, A. Bellili, I. Tuñón, E. Dumont^{*}, *Phys. Chem. Chem. Phys.*, 2017, 19:14695-14701 [doi](#)

[P58] Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. F. Dehez, H. Gattuso, E. Bignon, C. Morell, E. Dumont[†], A. Monari, *Nucl. Acids Res.*, 2017, 45:3654-3662 [doi](#)

[P57] Interstrand cross-linking implies contrasting structural consequences for DNA: insights from molecular dynamics. E. Bignon, T. Drsata, C. Morell, F. Lankas, E. Dumont[†], *Nucl. Acids Res.*, 2017, 45(4):2188-2195 [doi](#)

***** 2016**

[P56] Electron-Triggered Supramolecular Metamorphism in Porphyrin-Based Self-Assembled Materials, C. Kahlfuss, S. Denis-Quanqin, N. Calin, E. Dumont, M. Garavelli, G. Royal, S. Cobo, E. Saint-Aman and C. Bucher, *J. Am. Chem. Soc.*, 2016, 138:15234-15242. [doi](#)

[P55] Thermodynamics of DNA: Sensitizer recognition. Characterizing binding motifs with all-atom simulations, H. Gattuso, E. Dumont[†], C. Chipot, A. Monari, F. Dehez, *Phys. Chem. Chem. Phys.*, 2016, 18:33180-33186. [doi](#)

[P54] Radical-induced purine lesion formation is dependent on DNA helical topology. M. A. Terzidis, A. Priscaru, Z. Molphy, N. Barron, E. Dumont, A. Kellett, and C. Chatgililoglu, *Free Rad. Res.*, 2016, 50:91-101 [doi](#)

[P53] Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity, H. Gattuso, E. Durand, E. Bignon, C. Morell, A. G. Georgakilas, E. Dumont[†], C. Chipot, F. Dehez, A. Monari, *J. Phys. Chem. Lett.*, 2016, 7:3760-3765 [doi](#)

[P52] Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA he-

lix distortion, E. Bignon, H. Gattuso, C. Morell, F. Dehez, A. Georgakilas, A. Monari, E. Dumont[†], *Nucl. Acids Res.*, 2016, 44:8588-8599 [doi](#)

[P52] Grafting of Secondary Diol-Amides onto $[P_2W_{15}V_3O_{62}]^{9-}$ Generates Hybrid Heteropoly Acids. D. Lachkar, D. Vilona, E. Dumont[†], M. Lelli, E. Lacôte *Ang. Chem. Int. Ed.*, 2016, 128:6065-6069 [doi](#)

[P50] Two-photon-absorption DNA sensitization via solvated electrons production: Unraveling the photochemical pathways by molecular modeling and simulation H. Gattuso, M. Marazzi, E. Dumont and A. Monari *Phys. Chem. Chem. Phys.*, 2016, 18:18598-18606 [doi](#)

[P49] Singlet oxygen guanine onto guanine: reactivity and structural signature within the B-DNA helix. E. Dumont^{*}, R. Grüber, E. Bignon, C. Morell, J. Aranda, J.-L. Ravanat, I. Tuñón, *Chem. Eur. J.*, 2016, 22:12358-12362 [doi](#)

[P48] Probing the reactivity of singlet oxygen with purines. E. Dumont[†], R. Grüber, E. Bignon, C. Morell, Y. Moreau, A. Monari, J.-L. Ravanat[†], *Nucl. Acids Res.*, 2016, 44:56-62, [doi](#)

*** 2015

[P47] Insights on the Chemical Meanings of the Reaction Electronic Flux. C. Morell, V. Tognetti, E. Bignon, E. Dumont, N. Hernandez-Haro, B. Herrera, A. Grand, S. Gutiérrez-Oliva, L. Joubert, A. Toro-Labbé, H. Chermette, *Theor. Chem. Acc.*, 2015, 134:133 [doi](#)

[P46] Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. M. Marazzi, M. Wibowo, H. Gattuso, E. Dumont, D. Roca-Sanjuan, A. Monari. *Phys. Chem. Chem. Phys.*, 2015, 18:7829-7836, [doi](#)

[P45] DNA photosensitization by an "insider". Photophysics and triplet energy-transfer of 5-methyl-2-pyrimidone deoxyribonucleoside, E. Bignon, H. Gattuso, C. Morell, E. Dumont[†], A Monari[†]. *Chem. Eur. J.*, 2015, 21:11509-11516 [doi](#)

[P44] Understanding DNA under oxidative stress and sensitization: the role of molecular modeling E. Dumont[†], A. Monari. *Frontiers in Chemistry*, 2015, 3:43, [doi](#)

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Conferences organized

10th ElecMol [link](#)

3rd Workshop on DNA damage and repair [link](#)

15th International Workshop on Radiation Damage to DNA (with Jean-Luc Ravanat) [link](#)

Leiden
Nov. 2017

Lorentz workshop *DNA Damage and Repair: Computations Meet Experiments* [link](#)

Lyon
Nov. 2015

CECAM Workshop *DNA damages: modeling and rationalize structure and reactivity* [link](#), hosted at École Normale Supérieure de Lyon/Centre Blaise Pascal

ENS Lyon
2014–2017

Seminar series of the Department of chemistry

Lyon
2010–2012

Co-organizer of the theoretical chemistry group talks

Lyon
Feb. 2012

CECAM Workshop "New QM/MM opportunities for in silico macromolecular photochemistry" ([link](#)) hosted at École Normale Supérieure de Lyon/Centre Blaise Pascal

Invited presentations

17 invited lectures, 16 oral communications and 28 seminars as of June 2021, including IRWDD 2016 Melbourne, Femex 2017, deMon 2019, Watoc 2020...