Elise Dumont

List of Publications by Year in descending order

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Version: 2024-02-01

105 papers	2,072 citations	257450 24 h-index	302126 39 g-index
116 all docs	116 docs citations	116 times ranked	2779 citing authors

#	Article	IF	Citations
1	Synthesis and Electrochemistry of Freeâ€Base Porphyrins Bearing Trifluoromethyl mesoâ€Substituents. ChemElectroChem, 2022, 9, .	3.4	4
2	Reactivity of Singlet Oxygen with DNA, an Update^{â€}. Photochemistry and Photobiology, 2022, 98, 564-571.	2.5	5
3	How Fragile We Are: Influence of Stimulator of Interferon Genes (STING) Variants on Pathogen Recognition and Immune Response Efficiency. Journal of Chemical Information and Modeling, 2022, 62, 3096-3106.	5.4	4
4	Monte Carlo simulation of free radical production under keV photon irradiation of gold nanoparticle aqueous solution. Part II: Local primary chemical boost. Radiation Physics and Chemistry, 2021, 179, 109161.	2.8	3
5	Synthesis and Properties of Higher Nuclearity Polyazanes. Chemistry - A European Journal, 2021, 27, 3670-3674.	3.3	2
6	Recognition of a tandem lesion by DNA bacterial formamidopyrimidine glycosylases explored combining molecular dynamics and machine learning. Computational and Structural Biotechnology Journal, 2021, 19, 2861-2869.	4.1	11
7	Electron-Triggered Metamorphism in Palladium-Driven Self-Assembled Architectures. Inorganic Chemistry, 2021, 60, 3543-3555.	4.0	6
8	Assessing the sequence dependence of pyrimidineâ€“pyrimidone (6â€“4) photoproduct in a duplex double-stranded DNA: A pitfall for microsecond range simulation. Journal of Chemical Physics, 2021, 154, 135103.	3.0	9
9	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Supramolecular Polymers. ECS Meeting Abstracts, 2021, MA2021-01, 778-778.	0.0	0
10	A Dynamic View of the Interaction of Histone Tails with Clustered Abasic Sites in a Nucleosome Core Particle. Journal of Physical Chemistry Letters, 2021, 12, 6014-6019.	4.6	10
11	Exploring the Concept of Dimerization-Induced Intersystem Crossing: At the Origins of Spinâ€“Orbit Coupling Selection Rules. Journal of Physical Chemistry B, 2021, 125, 8572-8580.	2.6	8
12	Influence of Divalent Cations in the Protein Crystallization Process Assisted by Lanthanide-Based Additives. Inorganic Chemistry, 2021, 60, 15208-15214.	4.0	3
13	Light-inducedin situchemical activation of a fluorescent probe for monitoring intracellular G-quadruplex structures. Nanoscale, 2021, 13, 13795-13808.	5.6	11
14	Capturing the dynamic association between a tris-dipicolinate lanthanide complex and a decapeptide: a combined paramagnetic NMR and molecular dynamics exploration. Physical Chemistry Chemical Physics, 2021, 23, 11224-11232.	2.8	6
15	The Behavior of Triplet Thymine in a Model Bâ€DNA Strand. Energetics and Spin Density Localization Revealed by ab initio Molecular Dynamics Simulations. Photochemistry and Photobiology, 2021, , .	2.5	1
16	Organoâ€Polyoxometalateâ€Based Hydrogenâ€Bond Catalysis. Chemistry - A European Journal, 2021, 27, 17761-17764.	3.3	5
17	Molecular Mechanisms Associated with Clustered Lesion-Induced Impairment of 8-oxoG Recognition by the Human Glycosylase OGG1. Molecules, 2021, 26, 6465.	3.8	4
18	Polymerization Photoinitiators with Near-Resonance Enhanced Two-Photon Absorption Cross-Section: Toward High-Resolution Photoresist with Improved Sensitivity. Macromolecules, 2020, 53, 9264-9278.	4.8	29

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19	The dark side of disulfide-based dynamic combinatorial chemistry. Chemical Science, 2020, 11, 8151-8156.	7.4	9
20	Nucleosomal embedding reshapes the dynamics of abasic sites. Scientific Reports, 2020, 10, 17314.	3.3	13
21	Impact of the Nucleosome Histone Core on the Structure and Dynamics of DNA-Containing Pyrimidineâ€“Pyrimidone (6â€“4) Photoproduct. Journal of Chemical Theory and Computation, 2020, 16, 5972-5981.	5.3	10
22	Molecular Dynamics Approach for Capturing Calixareneâ€“Protein Interactions: The Case of Cytochrome C. Journal of Physical Chemistry B, 2020, 124, 11371-11378.	2.6	9
23	Effect of the Ligand Binding Strength on the Morphology of Functionalized Gold Nanoparticles. Journal of Physical Chemistry Letters, 2020, 11, 2717-2723.	4.6	11
24	Monte Carlo simulation of free radical production under keV photon irradiation of gold nanoparticle aqueous solution. Part I: Global primary chemical boost. Radiation Physics and Chemistry, 2020, 172, 108790.	2.8	6
25	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Supramolecular Polymers. ECS Meeting Abstracts, 2020, MA2020-01, 932-932.	0.0	0
26	A Halogenâ€Bond Donor Catalyst for Templated Macrocyclization. Angewandte Chemie - International Edition, 2019, 58, 14940-14943.	13.8	13
27	A Halogenâ€Bond Donor Catalyst for Templated Macrocyclization. Angewandte Chemie, 2019, 131, 15082-15085.	2.0	0
28	Tuning Protein Frameworks via Auxiliary Supramolecular Interactions. ACS Nano, 2019, 13, 10343-10350.	14.6	40
29	Wetting the lock and key enthalpically favours polyelectrolyte binding. Chemical Science, 2019, 10, 277-283.	7.4	8
30	A Water Solvation Shell Can Transform Gold Metastable Nanoparticles in the Fluxional Regime. Journal of Physical Chemistry Letters, 2019, 10, 1092-1098.	4.6	14
31	Photo/redox-responsive 2D-Supramolecular assembly involving Cucurbit[8]uril and a star-shaped porphyrin tecton. Electrochimica Acta, 2019, 316, 79-92.	5.2	14
32	A biomimetic strategy for the selective recognition of organophosphates in 100% water: synergies of electrostatic interactions, cavity embedment and metal coordination. Organic Chemistry Frontiers, 2019, 6, 1627-1636.	4.5	7
33	Probing interaction of a trilysine peptide with DNA underlying formation of guanineâ€“lysine cross-links: insights from molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 23418-23424.	2.8	10
34	Dynamic Molecular Metamorphism Involving Palladiumâ€Assisted Dimerization of Ïâ€Cation Radicals. Chemistry - A European Journal, 2019, 25, 1573-1580.	3.3	6
35	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 2570-2585.	5.3	16
36	Diastereoselective Synthesis of a Dyn[3]arene with Distinct Binding Behaviors toward Linear Biogenic Polyamines. Organic Letters, 2018, 20, 2420-2423.	4.6	5

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37	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	2.9	10
38	Dynamics of the excited-state hydrogen transfer in a (dG)Â·(dC) homopolymer: intrinsic photostability of DNA. Chemical Science, 2018, 9, 7902-7911.	7.4	29
39	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	3.8	85
40	Unveiling the Binding Modes of the Crystallophore, a Terbiumâ€based Nucleating and Phasing Molecular Agent for Protein Crystallography. Chemistry - A European Journal, 2018, 24, 9739-9746.	3.3	19
41	Interstrand cross-linking implies contrasting structural consequences for DNA: insights from molecular dynamics. Nucleic Acids Research, 2017, 45, gkw1253.	14.5	10
42	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662.	14.5	17
43	Free energy profiles for two ubiquitous damaging agents: methylation and hydroxylation of guanine in B-DNA. Physical Chemistry Chemical Physics, 2017, 19, 14695-14701.	2.8	3
44	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	3.3	19
45	Molecular Dynamics Insights into Polyamineâ€“DNA Binding Modes: Implications for Crossâ€Link Selectivity. Chemistry - A European Journal, 2017, 23, 12845-12852.	3.3	34
46	Elucidation of the Conformation of Polyglycine Organoâ€Polyoxotungstates: Evidence for Zipper Folding. Chemistry - A European Journal, 2017, 23, 13323-13327.	3.3	12
47	Grafting of Secondary Diolamides onto [P₂W₁₅V₃O₆₂]^{9â^'} Generates Hybrid Heteropoly Acids. Angewandte Chemie - International Edition, 2016, 55, 5961-5965.	13.8	16
48	Grafting of Secondary Diolamides onto [P₂W₁₅V₃O₆₂]^{9â^'} Generates Hybrid Heteropoly Acids. Angewandte Chemie, 2016, 128, 6065-6069.	2.0	4
49	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	2.8	10
50	Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity. Journal of Physical Chemistry Letters, 2016, 7, 3760-3765.	4.6	30
51	Radical-induced purine lesion formation is dependent on DNA helical topology. Free Radical Research, 2016, 50, S91-S101.	3.3	11
52	Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA helix distortion. Nucleic Acids Research, 2016, 44, 8588-8599.	14.5	37
53	Singlet Oxygen Attack on Guanine: Reactivity and Structural Signature within the Bâ€DNA Helix. Chemistry - A European Journal, 2016, 22, 12358-12362.	3.3	34
54	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Coordination Polymers. Journal of the American Chemical Society, 2016, 138, 15234-15242.	13.7	25

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55	Two-photon-absorption DNA sensitization via solvated electron production: unraveling photochemical pathways by molecular modeling and simulation. Physical Chemistry Chemical Physics, 2016, 18, 18598-18606.	2.8	20
56	Probing the reactivity of singlet oxygen with purines. Nucleic Acids Research, 2016, 44, 56-62.	14.5	57
57	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. Physical Chemistry Chemical Physics, 2016, 18, 7829-7836.	2.8	24
58	DNA Photosensitization by an â€œInsiderâ€• Photophysics and Triplet Energy Transfer of 5â€Methylâ€2â€pyrimidone Deoxyribonucleoside. Chemistry - A European Journal, 2015, 21, 11509-11516.	3.3	19
59	Understanding DNA under oxidative stress and sensitization: the role of molecular modeling. Frontiers in Chemistry, 2015, 3, 43.	3.6	48
60	Editorial: Radiation-induced and oxidative DNA damages. Frontiers in Chemistry, 2015, 3, 54.	3.6	7
61	Spectral lineshapes in nonlinear electronic spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 30925-30936.	2.8	39
62	Optical properties of prodigiosin and obatoclax: action spectroscopy and theoretical calculations. Physical Chemistry Chemical Physics, 2015, 17, 25946-25955.	2.8	15
63	Insights into the Structure of Intrastrand Cross-Link DNA Lesion-Containing Oligonucleotides: G[8â€“5m]T and G[8â€“5]C from Molecular Dynamics Simulations. Biochemistry, 2015, 54, 1259-1267.	2.5	11
64	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. Journal of Physical Chemistry Letters, 2015, 6, 576-580.	4.6	48
65	Photophysics of Acetophenone Interacting with <scp>DNA</scp>: Why the Road to Photosensitization is Open. Photochemistry and Photobiology, 2015, 91, 323-330.	2.5	15
66	Interaction of Palmatine with DNA: An Environmentally Controlled Phototherapy Drug. Journal of Physical Chemistry B, 2015, 119, 410-419.	2.6	39
67	Excited state evolution of DNA stacked adenines resolved at the CASPT2//CASSCF/Amber level: from the bright to the excimer state and back. Physical Chemistry Chemical Physics, 2015, 17, 7291-7302.	2.8	35
68	DFT investigation of the formation of linear aminols as the first step toward the induction of oxidatively generated interstrand cross-link DNA lesions. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	1
69	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. Faraday Discussions, 2015, 177, 345-362.	3.2	29
70	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	20
71	Stability of the Guanine Endoperoxide Intermediate: A Computational Challenge for Density Functional Theory. Journal of Physical Chemistry A, 2014, 118, 11612-11619.	2.5	16
72	Are Dinucleoside Monophosphates Relevant Models for the Study of DNA Intrastrand Cross-Link Lesions? The Example of G[8â€“5m]T. Chemical Research in Toxicology, 2014, 27, 1133-1141.	3.3	5

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73	A multidimensional approach to the analysis of chemical shift titration experiments in the frame of a multiple reaction scheme. Magnetic Resonance in Chemistry, 2013, 51, 641-648.	1.9	4
74	Structure, Dynamics, and Interactions of a C4â€²-Oxidized Abasic Site in DNA: A Concomitant Strand Scission Reverses Affinities. Biochemistry, 2013, 52, 8115-8125.	2.5	6
75	Exploration of the supramolecular interactions involving tris-dipicolinate lanthanide complexes in protein crystals by a combined biostructural, computational and NMR study. Physical Chemistry Chemical Physics, 2013, 15, 18235.	2.8	13
76	Benzophenone and DNA: Evidence for a Double Insertion Mode and Its Spectral Signature. Journal of Physical Chemistry Letters, 2013, 4, 4119-4124.	4.6	42
77	Towards an accurate treatment of Ïƒâˆ—â†Ïƒ transitions: Moving onto. Chemical Physics Letters, 2013, 580, 14-20.	2.6	0
78	Addressing the competitive formation of tandem DNA lesions by a nucleobase peroxyl radical: a DFT-D screening. Organic and Biomolecular Chemistry, 2013, 11, 3038.	2.8	26
79	What Singles Out the G[8â€“5]C Intrastrand DNA Cross-Link? Mechanistic and Structural Insights from Quantum Mechanics/Molecular Mechanics Simulations. Biochemistry, 2013, 52, 425-431.	2.5	22
80	Impact of DNA Environment on the Intrastrand Cross-Link Lesions: Hydrogen Atom Release as the Last Step of Formation of G[8-5m]T. Journal of Physical Chemistry B, 2013, 117, 16397-16404.	2.6	5
81	Insights into Intrastrand Cross-Link Lesions of DNA from QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2012, 134, 2111-2119.	13.7	61
82	Superior Performance of Range-Separated Hybrid Functionals for Describing Ïƒ* â†•Ïƒ UVâ€“Vis Signatures of Three-Electron Two-Center Anions. Journal of Physical Chemistry A, 2012, 116, 3237-3246.	2.5	10
83	Oneâ€electron addition on shortâ€loop selenylsulfide and diselenideâ€linked biomolecules: From diethyldichalcogens to Grx3â€like selenopeptides. International Journal of Quantum Chemistry, 2012, 112, 2018-2029.	2.0	0
84	Improved DFT Description of Intrastrand Cross-Link Formation by Inclusion of London Dispersion Corrections. Journal of Physical Chemistry B, 2011, 115, 15138-15144.	2.6	22
85	Geometrical Embedding Governs a Dramatic Variation of Electron Paramagnetic Resonance Hyperfine Coupling Constants of Disulfide Radical Anions. Journal of Physical Chemistry B, 2011, 115, 6776-6783.	2.6	5
86	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. Chemical Physics Letters, 2011, 501, 245-251.	2.6	19
87	Unraveling Gold(I)â€Specific Action Towards Peptidic Disulfide Cleavage: A DFT Investigation. ChemPhysChem, 2011, 12, 2596-2603.	2.1	2
88	Electronic effects and ring strain influences on the electron uptake by seleniumâ€containing bonds. International Journal of Quantum Chemistry, 2010, 110, 513-523.	2.0	6
89	Intersulfur Distance Is a Key Factor in Tuning Disulfide Radical Anion Vertical UVâ^'Visible Absorption. Journal of Physical Chemistry Letters, 2010, 1, 581-586.	4.6	6
90	How does microhydration impact on structure, spectroscopy and formation of disulfide radical anions? An ab initio investigation on dimethyldisulfide. Chemical Physics Letters, 2009, 481, 173-179.	2.6	8

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91	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. Chemical Physics Letters, 2009, 475, 120-123.	2.6	35
92	Inductive Effects on Proton Affinity of Benzene Derivatives: Analysis Using Fictitious Hydrogen Atoms. Journal of Physical Chemistry A, 2009, 113, 2990-2994.	2.5	9
93	Analyzing the Selectivity and Successiveness of a Two-Electron Capture on a Multiply Disulfide-Linked Protein. Journal of Chemical Theory and Computation, 2009, 5, 1700-1708.	5.3	11
94	Effect of ring strain on disulfide electron attachment. Chemical Physics Letters, 2008, 458, 276-280.	2.6	25
95	Huge Disulfide-Linkageâ€™S Electron Capture Variation Induced by Î±-Helix Orientation. Journal of Chemical Theory and Computation, 2008, 4, 1171-1173.	5.3	13
96	Factors Governing Electron Capture by Small Disulfide Loops in Two-Cysteine Peptides. Journal of Physical Chemistry B, 2008, 112, 13661-13669.	2.6	11
97	Intracule functional models. II. Analytically integrable kernels. Journal of Chemical Physics, 2007, 127, 141103.	3.0	27
98	Intracule functional models: I. Angle-corrected correlation kernels. Physical Chemistry Chemical Physics, 2007, 9, 5340.	2.8	21
99	Comparison of Charge Models for Fixed-Charge Force Fields:Â Small-Molecule Hydration Free Energies in Explicit Solvent. Journal of Physical Chemistry B, 2007, 111, 2242-2254.	2.6	245
100	Investigation of pure inductive effects on benzene ring by 13C NMR chemical shifts: A theoretical study using fictitious nuclear charges of hydrogen atoms (â€˜Hâ^— methodâ€™). Chemical Physics Letters, 2007, 435, 354-357.	2.6	16
101	FTIR and ab Initio Study of the 1/1 Complex between Water and Carbon Dioxide in Solid Nitrogen. Journal of Physical Chemistry A, 2006, 110, 51-56.	2.5	23
102	Dielsâ€“Alder reaction: A theoretical comprehensive study of substituent effects using the â€˜H* methodâ€™. Computational and Theoretical Chemistry, 2006, 758, 161-167.	1.5	14
103	The Hâ^— method: hydrogen atoms with a fictitious nuclear charge. A versatile theoretical tool for study of atom and group properties as substituents: electronegativity and partition of Ïƒ and Ï€ contributions. Computational and Theoretical Chemistry, 2004, 680, 99-106.	1.5	23
104	Neutron and X-ray Diffraction Studies and DFT Calculations of Asymmetric Bis(silyl) Niobocene Hydrides. Organometallics, 2004, 23, 2845-2847.	2.3	24
105	Confinement of molecular liquids: Consequences on thermodynamic, static and dynamical properties of benzene and toluene. European Physical Journal E, 2003, 12, 19-28.	1.6	132