Elise Dumont

List of Publications by Year in descending order

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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	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
2	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
3	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	3.8	85
4	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
5	Probing the reactivity of singlet oxygen with purines. Nucleic Acids Research, 2016, 44, 56-62.	14.5	57
6	Understanding DNA under oxidative stress and sensitization: the role of molecular modeling. Frontiers in Chemistry, 2015, 3, 43.	3.6	48
7	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. Journal of Physical Chemistry Letters, 2015, 6, 576-580.	4.6	48
8	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
9	Tuning Protein Frameworks via Auxiliary Supramolecular Interactions. ACS Nano, 2019, 13, 10343-10350.	14.6	40
10	Spectral lineshapes in nonlinear electronic spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 30925-30936.	2.8	39
11	Interaction of Palmatine with DNA: An Environmentally Controlled Phototherapy Drug. Journal of Physical Chemistry B, 2015, 119, 410-419.	2.6	39
12	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
13	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. Chemical Physics Letters, 2009, 475, 120-123.	2.6	35
14	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
15	Singlet Oxygen Attack on Guanine: Reactivity and Structural Signature within the Bâ€ÐNA Helix. Chemistry - A European Journal, 2016, 22, 12358-12362.	3.3	34
16	Molecular Dynamics Insights into Polyamineâ€“DNA Binding Modes: Implications for Crossâ€Łink Selectivity. Chemistry - A European Journal, 2017, 23, 12845-12852.	3.3	34
17	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
18	Probing deactivation pathways of DNA nucleobases by two-dimensional electronic spectroscopy: first principles simulations. Faraday Discussions, 2015, 177, 345-362.	3.2	29

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19	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
20	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
21	Intracule functional models. II. Analytically integrable kernels. Journal of Chemical Physics, 2007, 127, 141103.	3.0	27
22	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
23	Effect of ring strain on disulfide electron attachment. Chemical Physics Letters, 2008, 458, 276-280.	2.6	25
24	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Coordination Polymers. Journal of the American Chemical Society, 2016, 138, 15234-15242.	13.7	25
25	Neutron and X-ray Diffraction Studies and DFT Calculations of Asymmetric Bis(silyl) Niobocene Hydrides. Organometallics, 2004, 23, 2845-2847.	2.3	24
26	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. Physical Chemistry Chemical Physics, 2016, 18, 7829-7836.	2.8	24
27	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
28	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
29	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
30	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
31	Intracule functional models: I. Angle-corrected correlation kernels. Physical Chemistry Chemical Physics, 2007, 9, 5340.	2.8	21
32	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	20
33	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
34	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. Chemical Physics Letters, 2011, 501, 245-251.	2.6	19
35	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
36	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	3.3	19

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37	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
38	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662.	14.5	17
39	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
40	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
41	Grafting of Secondary Diolamides onto [P₂W₁₅V₃O₆₂]^{9â€“} Generates Hybrid Heteropoly Acids. Angewandte Chemie - International Edition, 2016, 55, 5961-5965.	13.8	16
42	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
43	Optical properties of prodigiosin and obatoclax: action spectroscopy and theoretical calculations. Physical Chemistry Chemical Physics, 2015, 17, 25946-25955.	2.8	15
44	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
45	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
46	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
47	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
48	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
49	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
50	A Halogenâ€Bond Donor Catalyst for Templated Macrocyclization. Angewandte Chemie - International Edition, 2019, 58, 14940-14943.	13.8	13
51	Nucleosomal embedding reshapes the dynamics of abasic sites. Scientific Reports, 2020, 10, 17314.	3.3	13
52	Elucidation of the Conformation of Polyglycine Organoâ€Polyoxotungstates: Evidence for Zipper Folding. Chemistry - A European Journal, 2017, 23, 13323-13327.	3.3	12
53	Factors Governing Electron Capture by Small Disulfide Loops in Two-Cysteine Peptides. Journal of Physical Chemistry B, 2008, 112, 13661-13669.	2.6	11
54	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

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55	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
56	Radical-induced purine lesion formation is dependent on DNA helical topology. Free Radical Research, 2016, 50, S91-S101.	3.3	11
57	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
58	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
59	Light-inducedin situchemical activation of a fluorescent probe for monitoring intracellular G-quadruplex structures. Nanoscale, 2021, 13, 13795-13808.	5.6	11
60	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
61	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	2.8	10
62	Interstrand cross-linking implies contrasting structural consequences for DNA: insights from molecular dynamics. Nucleic Acids Research, 2017, 45, gkw1253.	14.5	10
63	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
64	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
65	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
66	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
67	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
68	The dark side of disulfide-based dynamic combinatorial chemistry. Chemical Science, 2020, 11, 8151-8156.	7.4	9
69	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
70	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
71	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
72	Wetting the lock and key enthalpically favours polyelectrolyte binding. Chemical Science, 2019, 10, 277-283.	7.4	8

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73	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
74	Editorial: Radiation-induced and oxidative DNA damages. Frontiers in Chemistry, 2015, 3, 54.	3.6	7
75	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
76	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
77	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
78	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
79	Dynamic Molecular Metamorphism Involving Palladiumâ€Assisted Dimerization of Ïâ€Cation Radicals. Chemistry - A European Journal, 2019, 25, 1573-1580.	3.3	6
80	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
81	Electron-Triggered Metamorphism in Palladium-Driven Self-Assembled Architectures. Inorganic Chemistry, 2021, 60, 3543-3555.	4.0	6
82	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
83	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
84	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
85	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
86	Diastereoselective Synthesis of a Dyn[3]arene with Distinct Binding Behaviors toward Linear Biogenic Polyamines. Organic Letters, 2018, 20, 2420-2423.	4.6	5
87	Organoâ€Polyoxometalateâ€Based Hydrogenâ€Bond Catalysis. Chemistry - A European Journal, 2021, 27, 17761-17764.	3.3	5
88	Reactivity of Singlet Oxygen with DNA, an Update^{â€}. Photochemistry and Photobiology, 2022, 98, 564-571.	2.5	5
89	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
90	Grafting of Secondary Diolamides onto [P₂W₁₅V₃O₆₂]^{9â^'} Generates Hybrid Heteropoly Acids. Angewandte Chemie, 2016, 128, 6065-6069.	2.0	4

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91	Molecular Mechanisms Associated with Clustered Lesion-Induced Impairment of 8-oxoG Recognition by the Human Glycosylase OGG1. Molecules, 2021, 26, 6465.	3.8	4
92	Synthesis and Electrochemistry of Freeâ€Base Porphyrins Bearing Trifluoromethyl mesoâ€Substituents. ChemElectroChem, 2022, 9, .	3.4	4
93	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
94	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
95	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
96	Influence of Divalent Cations in the Protein Crystallization Process Assisted by Lanthanide-Based Additives. Inorganic Chemistry, 2021, 60, 15208-15214.	4.0	3
97	Unraveling Gold(I)â€Specific Action Towards Peptidic Disulfide Cleavage: A DFT Investigation. ChemPhysChem, 2011, 12, 2596-2603.	2.1	2
98	Synthesis and Properties of Higher Nuclearity Polyazanes. Chemistry - A European Journal, 2021, 27, 3670-3674.	3.3	2
99	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
100	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
101	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
102	Towards an accurate treatment of Ïƒâˆ—â†Ïƒ transitions: Moving onto. Chemical Physics Letters, 2013, 580, 14-20.	2.6	0
103	A Halogenâ€Bond Donor Catalyst for Templated Macrocyclization. Angewandte Chemie, 2019, 131, 15082-15085.	2.0	0
104	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Supramolecular Polymers. ECS Meeting Abstracts, 2021, MA2021-01, 778-778.	0.0	0
105	Electron-Triggered Metamorphism in Porphyrin-Based Self-Assembled Supramolecular Polymers. ECS Meeting Abstracts, 2020, MA2020-01, 932-932.	0.0	0