AdÃ¨le D Laurent

List of Publications by Year
in descending order

92 papers	6,164 citations	186265 28 h-index	69250 77 g-index
93 all docs	93 docs citations	93 times ranked	8003 citing authors

#	Article	IF	Citations
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
2	TD-DFT benchmarks: A review. International Journal of Quantum Chemistry, 2013, 113, 2019-2039.	2.0	938
3	Dye chemistry with time-dependent density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 14334-14356.	2.8	294
4	Tuning ESIPT fluorophores into dual emitters. Chemical Science, 2016, 7, 3763-3774.	7.4	168
5	Revisiting the optical signatures of BODIPY with ab initio tools. Chemical Science, 2013, 4, 1950.	7.4	140
6	White Emitters by Tuning the Excitedâ€State Intramolecular Protonâ€Transfer Fluorescence Emission in 2â€(2â€²â€Hydroxybenzofuran)benzoxazole Dyes. Chemistry - A European Journal, 2014, 20, 12843-12857.	3.3	135
7	Improving the Accuracy of Excited-State Simulations of BODIPY and Aza-BODIPY Dyes with a Joint SOS-CIS(D) and TD-DFT Approach. Journal of Chemical Theory and Computation, 2014, 10, 4574-4582.	5.3	98
8	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. Journal of Chemical Theory and Computation, 2013, 9, 4517-4525.	5.3	95
9	Shedding Light on the Photoisomerization Pathway of Donorâ€“Acceptor Stenhouse Adducts. Journal of the American Chemical Society, 2017, 139, 15596-15599.	13.7	88
10	Solvent Effects on the Actinic Step of Donorâ€“Acceptor Stenhouse Adduct Photoswitching. Angewandte Chemie - International Edition, 2018, 57, 8063-8068.	13.8	70
11	Iminothioindoxyl as a molecular photoswitch with 100â€‰nm band separation in the visible range. Nature Communications, 2019, 10, 2390.	12.8	63
12	Spectral properties of self-assembled squaraineâ€“tetralactam: a theoretical assessment. Physical Chemistry Chemical Physics, 2009, 11, 1258.	2.8	57
13	TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in Hydroxyphenylbenzimidazole (HBI) Dyes. Journal of Physical Chemistry B, 2015, 119, 2180-2192.	2.6	55
14	Tailoring Photoisomerization Pathways in Donorâ€“Acceptor Stenhouse Adducts: The Role of the Hydroxy Group. Journal of Physical Chemistry A, 2018, 122, 955-964.	2.5	54
15	Modeling optical signatures and excited-state reactivities of substituted hydroxyphenylbenzoxazole (HBO) ESIPT dyes. Physical Chemistry Chemical Physics, 2014, 16, 1319-1321.	2.8	53
16	Photochromic properties of dithienylazoles and other conjugated diarylethenes. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 192, 211-219.	3.9	52
17	Physicochemical and Electronic Properties of Cationic [6]Helicenes: from Chemical and Electrochemical Stabilities to Farâ€Red (Polarized) Luminescence. Chemistry - A European Journal, 2016, 22, 18394-18403.	3.3	52
18	Using Timeâ€Dependent Density Functional Theory to Probe the Nature of Donorâ€“Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1846-1851.	2.1	50

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19	Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications. Molecules, 2022, 27, 2443.	3.8	48
20	The Influence of the Ï€-Conjugated Spacer on Photophysical Properties of Difluoroboranyls Derived from Amides Carrying a Donor Group. Journal of Organic Chemistry, 2016, 81, 2280-2292.	3.2	45
21	Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes. Journal of Physical Chemistry C, 2014, 118, 28831-28841.	3.1	41
22	Photophysical Properties of Phenacylphenantridine Difluoroboranyls: Effect of Substituent and Double Benzannulation. Journal of Organic Chemistry, 2017, 82, 1529-1537.	3.2	37
23	Dual Solution-/Solid-State Emissive Excited-State Intramolecular Proton Transfer (ESIPT) Dyes: A Combined Experimental and Theoretical Approach. Journal of Organic Chemistry, 2021, 86, 17606-17619.	3.2	36
24	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. Chemical Physics Letters, 2009, 475, 120-123.	2.6	35
25	Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches. Journal of Physical Chemistry C, 2014, 118, 4334-4345.	3.1	34
26	Impact of tautomers on the absorption spectra of neutral and anionic alizarin and quinizarin dyes. Computational and Theoretical Chemistry, 2009, 901, 24-30.	1.5	33
27	Exploring Structural and Optical Properties of Fluorescent Proteins by Squeezing: Modeling High-Pressure Effects on the mStrawberry and mCherry Red Fluorescent Proteins. Journal of Physical Chemistry B, 2012, 116, 12426-12440.	2.6	32
28	ESIPT or not ESIPT? Revisiting recent results on 2,1,3-benzothiadiazole under the TD-DFT light. RSC Advances, 2014, 4, 14189-14192.	3.6	30
29	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. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	30
30	How To Make Nitroaromatic Compounds Glow: Nextâ€Generation Large Xâ€Shaped, Centrosymmetric Diketopyrrolopyrroles. Angewandte Chemie - International Edition, 2020, 59, 16104-16113.	13.8	30
31	Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2014, 10, 1848-1851.	5.3	29
32	Effect of the Enhanced Cyan Fluorescent Protein framework on the UV/visible absorption spectra of some chromophores. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 38-47.	3.6	27
33	Electroactive polymerâ€“peptide conjugates for adhesive biointerfaces. Biomaterials Science, 2015, 3, 1395-1405.	5.4	26
34	Investigation of ESIPT in a panel of chromophores presenting Nâ€“Hâ‹¯N intramolecular hydrogen bonds. Physical Chemistry Chemical Physics, 2014, 16, 25288-25295.	2.8	24
35	Theoretical Investigation of the Geometries and UVâ^'vis Spectra of Poly(<scp>l</scp>-glutamic acid) Featuring a Photochromic Azobenzene Side Chain. Journal of Chemical Theory and Computation, 2008, 4, 637-645.	5.3	23
36	Molecular features and toxicological properties of four common pesticides, acetamiprid, deltamethrin, chlorpyriphos and fipronil. Bioorganic and Medicinal Chemistry, 2015, 23, 1540-1550.	3.0	23

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37	Solvatochromic Shifts in UVâ€“Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide. Journal of Chemical Theory and Computation, 2016, 12, 1919-1929.	5.3	23
38	Methodological keys for accurate simulations. Physical Chemistry Chemical Physics, 2013, 15, 11875.	2.8	22
39	Influence of the Nature of the Amino Group in Highly Fluorescent Difluoroborates Exhibiting Intramolecular Charge Transfer. Journal of Organic Chemistry, 2018, 83, 7779-7788.	3.2	22
40	Solvent Effects on the Actinic Step of Donorâ€“Acceptor Stenhouse Adduct Photoswitching. Angewandte Chemie, 2018, 130, 8195-8200.	2.0	21
41	Determining the most promising anchors for CuSCN: ab initio insights towards p-type DSSCs. Journal of Materials Chemistry A, 2016, 4, 2217-2227.	10.3	20
42	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. Chemical Physics Letters, 2011, 501, 245-251.	2.6	19
43	TD-DFT study of the for coumarins. Chemical Physics Letters, 2013, 583, 218-221.	2.6	19
44	Investigating the optical properties of BOIMPY dyes using ab initio tools. Physical Chemistry Chemical Physics, 2017, 19, 10554-10561.	2.8	19
45	Similar Comparative Low and High Doses of Deltamethrin and Acetamiprid Differently Impair the Retrieval of the Proboscis Extension Reflex in the Forager Honey Bee (Apis mellifera). Insects, 2015, 6, 805-814.	2.2	18
46	Exploring the Solvatochromism of Betaineâ€…30 with Ab Initio Tools: From Accurate Gasâ€Phase Calculations to Implicit and Explicit Solvation Models. Chemistry - A European Journal, 2017, 23, 4108-4119.	3.3	18
47	Modelling solvent effects on the absorption and emission spectra of constrained cyanines with both implicit and explicit QM/EFP models. Computational and Theoretical Chemistry, 2014, 1040-1041, 321-327.	2.5	15
48	Interplay between TiO₂ Surfaces and Organic Photochromes: A DFT Study of Adsorbed Azobenzenes and Diarylethenes. Journal of Physical Chemistry C, 2015, 119, 3684-3696.	3.1	15
49	Exploring the excited-states of squaraine dyes with TD-DFT, SOS-CIS(D) and ADC(2). Dyes and Pigments, 2017, 138, 169-175.	3.7	15
50	Photo-isomerization upshifts the pKa of the Photoactive Yellow Protein chromophore to contribute to photocycle propagation. Journal of Photochemistry and Photobiology A: Chemistry, 2013, 270, 43-52.	3.9	14
51	Exceptional Stability of Azacalixphyrin and Its Dianion. Journal of Physical Chemistry A, 2014, 118, 8883-8888.	2.5	14
52	Photostable orange-red fluorescent unsymmetrical diketopyrrolopyrroleâ€“BF₂ hybrids. Journal of Materials Chemistry C, 2020, 8, 7708-7717.	5.5	14
53	Hemi-indigo photochroms: A theoretical investigation. Chemical Physics Letters, 2007, 436, 84-88.	2.6	13
54	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

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55	Spectral Signatures of Perylene Diimide Derivatives: Insights From Theory. Journal of Physical Chemistry C, 2013, 117, 21682-21691.	3.1	13
56	Excited States of Ladder-Type Ï€-Conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach. Journal of Physical Chemistry A, 2015, 119, 5417-5425.	2.5	13
57	Imidacloprid and thiacloprid neonicotinoids bind more favourably to cockroach than to honeybee Î±6 nicotinic acetylcholine receptor: Insights from computational studies. Journal of Molecular Graphics and Modelling, 2015, 55, 1-12.	2.4	13
58	Tailoring the optical and dynamic properties of iminothioindoxyl photoswitches through acidochromism. Chemical Science, 2021, 12, 4588-4598.	7.4	13
59	Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes. Journal of Physical Chemistry A, 2015, 119, 3112-3124.	2.5	12
60	Time-Dependent Density Functional Theory: A Tool to Explore Excited States. , 2017, , 927-961.		12
61	An ab initio simulation of the UV/visible spectra of Nâ€benzylideneaniline dyes. International Journal of Quantum Chemistry, 2009, 109, 3506-3515.	2.0	11
62	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
63	Theoretical spectroscopy of BASHY dyes. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	10
64	The â€œhydrazinoturnâ€•hydrogen bonding network in hydrazinopeptides and aza-Î²3-peptides as probed by an AIM topological analysis of the electronic density. Computational and Theoretical Chemistry, 2008, 869, 41-46.	1.5	8
65	Molecular recognition of thiaclopride by Aplysia californica AChBP: new insights from a computational investigation. Journal of Computer-Aided Molecular Design, 2015, 29, 1151-1167.	2.9	8
66	Phosphonic Acid Fluorescent Organic Nanoparticles for High-Contrast and Selective Staining of Gram-Positive Bacteria. ACS Omega, 2018, 3, 17392-17402.	3.5	8
67	Binding of Sulfoxaflor to Aplysia californica-AChBP: Computational Insights from Multiscale Approaches. Journal of Chemical Information and Modeling, 2019, 59, 3755-3769.	5.4	8
68	Substitution effects on the optical spectra of diarylethene photochroms:ab initioinsights. Molecular Simulation, 2010, 36, 74-78.	2.0	7
69	Conformational Exploration of Two Peptides and Their Hybrid Polymer Conjugates: Potentialities As Self-Aggregating Materials. Journal of Physical Chemistry B, 2012, 116, 13941-13952.	2.6	7
70	Design of hybrid conjugates based on chemical similarity. RSC Advances, 2013, 3, 21069.	3.6	7
71	Formazanate boron difluoride dyes: discrepancies between TD-DFT and wavefunction descriptions. Journal of Molecular Modeling, 2016, 22, 263.	1.8	7
72	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

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73	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
74	Key Building Block of Photoresponsive Biomimetic Systems. Journal of Physical Chemistry B, 2011, 115, 1232-1242.	2.6	6
75	Analyzing excited-state processes and optical signatures of a ratiomeric fluorine anion sensor: a quantum look. Science China Chemistry, 2014, 57, 1363-1368.	8.2	6
76	IL-15RÎ± membrane-anchorage either in cis or in trans is required for stabilization of IL-15 and optimal signaling. Journal of Cell Science, 2019, 133, .	2.0	6
77	A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives. ChemPhysChem, 2016, 17, 2434-2445.	2.1	5
78	Investigating cyclic peptides inhibiting CD2â€“CD58 interactions through molecular dynamics and molecular docking methods. Journal of Computer-Aided Molecular Design, 2018, 32, 1295-1313.	2.9	5
79	Investigation of Phospholipase CÎ³1 Interaction with SLP76 Using Molecular Modeling Methods for Identifying Novel Inhibitors. International Journal of Molecular Sciences, 2019, 20, 4721.	4.1	5
80	How To Make Nitroaromatic Compounds Glow: Nextâ€Generation Large Xâ€Shaped, Centrosymmetric Diketopyrrolopyrroles. Angewandte Chemie, 2020, 132, 16238-16247.	2.0	5
81	Exploiting Light Interferences to Generate Micrometerâ€High Superstructures from Monomeric Azo Materials with Extensive Orientational Mobility. Advanced Optical Materials, 2021, 9, 2100525.	7.3	4
82	Structural insights into the catalytic mechanism of granzyme B upon substrate and inhibitor binding. Journal of Molecular Graphics and Modelling, 2022, 114, 108167.	2.4	4
83	Toward the understanding of the environmental effects on core ionizations. Journal of Computational Chemistry, 2014, 35, 1131-1139.	3.3	3
84	Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. Chemical Physics Letters, 2014, 599, 73-79.	2.6	3
85	Interactions of the Rad51 inhibitor DIDS with human and bovine serum albumins: Optical spectroscopy and isothermal calorimetry approaches. Biochimie, 2019, 167, 187-197.	2.6	3
86	First computational step towards the understanding of the antioxidant activity of the Phycocyanobilin:Ferredoxin Oxidoreductase in complex with biliverdin IXÎ±. Computational and Theoretical Chemistry, 2016, 1077, 58-64.	2.5	2
87	Computational simulations determining disulfonic stilbene derivative bioavailability within human serum albumin. Physical Chemistry Chemical Physics, 2018, 20, 18020-18030.	2.8	2
88	Mechanistic and Structural Insights on the IL-15 System through Molecular Dynamics Simulations. Molecules, 2019, 24, 3261.	3.8	2
89	Structure-based identification of inhibitors disrupting the CD2â€“CD58 interactions. Journal of Computer-Aided Molecular Design, 2021, 35, 337-353.	2.9	1
90	Time-Dependent Density Functional Theory: A Tool to Explore Excited States. , 2015, , 1-35.		1

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91	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1712-1712.	2.1	0
92	Exploring Structural Dynamics and Optical Properties of UnaG Fluorescent Protein upon N57 Mutations. Physical Chemistry Chemical Physics, 2022, , .	2.8	0