AdÃ¨le D Laurent

List of Publications by Year
in descending order

92 papers	6,164 citations	185998 28 h-index	69108 77 g-index
93 all docs	93 docs citations	93 times ranked	8003 citing authors

#	Article	IF	Citations
1	Exploring Structural Dynamics and Optical Properties of UnaG Fluorescent Protein upon N57 Mutations. Physical Chemistry Chemical Physics, 2022, , .	1.3	0
2	Structural insights into the catalytic mechanism of granzyme B upon substrate and inhibitor binding. Journal of Molecular Graphics and Modelling, 2022, 114, 108167.	1.3	4
3	Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications. Molecules, 2022, 27, 2443.	1.7	48
4	Tailoring the optical and dynamic properties of iminothioindoxyl photoswitches through acidochromism. Chemical Science, 2021, 12, 4588-4598.	3.7	13
5	Structure-based identification of inhibitors disrupting the CD2â€“CD58 interactions. Journal of Computer-Aided Molecular Design, 2021, 35, 337-353.	1.3	1
6	Exploiting Light Interferences to Generate Micrometerâ€High Superstructures from Monomeric Azo Materials with Extensive Orientational Mobility. Advanced Optical Materials, 2021, 9, 2100525.	3.6	4
7	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.	1.7	36
8	How To Make Nitroaromatic Compounds Glow: Nextâ€Generation Large Xâ€Shaped, Centrosymmetric Diketopyrrolopyrroles. Angewandte Chemie, 2020, 132, 16238-16247.	1.6	5
9	How To Make Nitroaromatic Compounds Glow: Nextâ€Generation Large Xâ€Shaped, Centrosymmetric Diketopyrrolopyrroles. Angewandte Chemie - International Edition, 2020, 59, 16104-16113.	7.2	30
10	Photostable orange-red fluorescent unsymmetrical diketopyrrolopyrroleâ€“BF₂ hybrids. Journal of Materials Chemistry C, 2020, 8, 7708-7717.	2.7	14
11	Binding of Sulfoxaflor to Aplysia californica-AChBP: Computational Insights from Multiscale Approaches. Journal of Chemical Information and Modeling, 2019, 59, 3755-3769.	2.5	8
12	Interactions of the Rad51 inhibitor DIDS with human and bovine serum albumins: Optical spectroscopy and isothermal calorimetry approaches. Biochimie, 2019, 167, 187-197.	1.3	3
13	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, .	1.2	6
14	Mechanistic and Structural Insights on the IL-15 System through Molecular Dynamics Simulations. Molecules, 2019, 24, 3261.	1.7	2
15	Investigation of Phospholipase CÎ³1 Interaction with SLP76 Using Molecular Modeling Methods for Identifying Novel Inhibitors. International Journal of Molecular Sciences, 2019, 20, 4721.	1.8	5
16	Iminothioindoxyl as a molecular photoswitch with 100â€‰nm band separation in the visible range. Nature Communications, 2019, 10, 2390.	5.8	63
17	Tailoring Photoisomerization Pathways in Donorâ€“Acceptor Stenhouse Adducts: The Role of the Hydroxy Group. Journal of Physical Chemistry A, 2018, 122, 955-964.	1.1	54
18	Phosphonic Acid Fluorescent Organic Nanoparticles for High-Contrast and Selective Staining of Gram-Positive Bacteria. ACS Omega, 2018, 3, 17392-17402.	1.6	8

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19	Investigating cyclic peptides inhibiting CD2â€“CD58 interactions through molecular dynamics and molecular docking methods. Journal of Computer-Aided Molecular Design, 2018, 32, 1295-1313.	1.3	5
20	Solvent Effects on the Actinic Step of Donorâ€“Acceptor Stenhouse Adduct Photoswitching. Angewandte Chemie - International Edition, 2018, 57, 8063-8068.	7.2	70
21	Solvent Effects on the Actinic Step of Donorâ€“Acceptor Stenhouse Adduct Photoswitching. Angewandte Chemie, 2018, 130, 8195-8200.	1.6	21
22	Influence of the Nature of the Amino Group in Highly Fluorescent Difluoroborates Exhibiting Intramolecular Charge Transfer. Journal of Organic Chemistry, 2018, 83, 7779-7788.	1.7	22
23	Computational simulations determining disulfonic stilbene derivative bioavailability within human serum albumin. Physical Chemistry Chemical Physics, 2018, 20, 18020-18030.	1.3	2
24	Photophysical Properties of Phenacylphenantridine Difluoroboranyls: Effect of Substituent and Double Benzannulation. Journal of Organic Chemistry, 2017, 82, 1529-1537.	1.7	37
25	Time-Dependent Density Functional Theory: A Tool to Explore Excited States. , 2017, , 927-961.		12
26	Exploring the excited-states of squaraine dyes with TD-DFT, SOS-CIS(D) and ADC(2). Dyes and Pigments, 2017, 138, 169-175.	2.0	15
27	Investigating the optical properties of BOIMPY dyes using ab initio tools. Physical Chemistry Chemical Physics, 2017, 19, 10554-10561.	1.3	19
28	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.	1.7	18
29	Shedding Light on the Photoisomerization Pathway of Donorâ€“Acceptor Stenhouse Adducts. Journal of the American Chemical Society, 2017, 139, 15596-15599.	6.6	88
30	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1712-1712.	1.0	0
31	Theoretical spectroscopy of BASHY dyes. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	10
32	Formazanate boron difluoride dyes: discrepancies between TD-DFT and wavefunction descriptions. Journal of Molecular Modeling, 2016, 22, 263.	0.8	7
33	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.	1.7	52
34	A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives. ChemPhysChem, 2016, 17, 2434-2445.	1.0	5
35	Using Timeâ€Dependent Density Functional Theory to Probe the Nature of Donorâ€“Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1846-1851.	1.0	50
36	Determining the most promising anchors for CuSCN: ab initio insights towards p-type DSSCs. Journal of Materials Chemistry A, 2016, 4, 2217-2227.	5.2	20

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37	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.	1.1	2
38	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.	1.7	45
39	Tuning ESIPT fluorophores into dual emitters. Chemical Science, 2016, 7, 3763-3774.	3.7	168
40	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.	2.3	23
41	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.	1.0	18
42	Molecular recognition of thiaclopride by Aplysia californica AChBP: new insights from a computational investigation. Journal of Computer-Aided Molecular Design, 2015, 29, 1151-1167.	1.3	8
43	Molecular features and toxicological properties of four common pesticides, acetamiprid, deltamethrin, chlorpyriphos and fipronil. Bioorganic and Medicinal Chemistry, 2015, 23, 1540-1550.	1.4	23
44	Interplay between TiO₂ Surfaces and Organic Photochromes: A DFT Study of Adsorbed Azobenzenes and Diarylethenes. Journal of Physical Chemistry C, 2015, 119, 3684-3696.	1.5	15
45	Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes. Journal of Physical Chemistry A, 2015, 119, 3112-3124.	1.1	12
46	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.	0.5	30
47	Electroactive polymerâ€“peptide conjugates for adhesive biointerfaces. Biomaterials Science, 2015, 3, 1395-1405.	2.6	26
48	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.	1.1	13
49	TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in Hydroxyphenylbenzimidazole (HBI) Dyes. Journal of Physical Chemistry B, 2015, 119, 2180-2192.	1.2	55
50	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.	1.3	13
51	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
52	Time-Dependent Density Functional Theory: A Tool to Explore Excited States. , 2015, , 1-35.		1
53	Analyzing excited-state processes and optical signatures of a ratiomeric fluorine anion sensor: a quantum look. Science China Chemistry, 2014, 57, 1363-1368.	4.2	6
54	Investigation of ESIPT in a panel of chromophores presenting Nâ€“Hâ‹¯N intramolecular hydrogen bonds. Physical Chemistry Chemical Physics, 2014, 16, 25288-25295.	1.3	24

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55	Toward the understanding of the environmental effects on core ionizations. Journal of Computational Chemistry, 2014, 35, 1131-1139.	1.5	3
56	Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches. Journal of Physical Chemistry C, 2014, 118, 4334-4345.	1.5	34
57	Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. Journal of Chemical Theory and Computation, 2014, 10, 1848-1851.	2.3	29
58	Modeling optical signatures and excited-state reactivities of substituted hydroxyphenylbenzoxazole (HBO) ESIPT dyes. Physical Chemistry Chemical Physics, 2014, 16, 1319-1321.	1.3	53
59	Dye chemistry with time-dependent density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 14334-14356.	1.3	294
60	ESIPT or not ESIPT? Revisiting recent results on 2,1,3-benzothiadiazole under the TD-DFT light. RSC Advances, 2014, 4, 14189-14192.	1.7	30
61	Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes. Journal of Physical Chemistry C, 2014, 118, 28831-28841.	1.5	41
62	Exceptional Stability of Azacalixphyrin and Its Dianion. Journal of Physical Chemistry A, 2014, 118, 8883-8888.	1.1	14
63	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.	2.3	98
64	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.	1.1	15
65	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.	1.7	135
66	Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. Chemical Physics Letters, 2014, 599, 73-79.	1.2	3
67	Methodological keys for accurate simulations. Physical Chemistry Chemical Physics, 2013, 15, 11875.	1.3	22
68	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.	2.3	95
69	Spectral Signatures of Perylene Diimide Derivatives: Insights From Theory. Journal of Physical Chemistry C, 2013, 117, 21682-21691.	1.5	13
70	TD-DFT study of the for coumarins. Chemical Physics Letters, 2013, 583, 218-221.	1.2	19
71	Design of hybrid conjugates based on chemical similarity. RSC Advances, 2013, 3, 21069.	1.7	7
72	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.	2.0	14

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73	Revisiting the optical signatures of BODIPY with ab initio tools. Chemical Science, 2013, 4, 1950.	3.7	140
74	TD-DFT benchmarks: A review. International Journal of Quantum Chemistry, 2013, 113, 2019-2039.	1.0	938
75	Conformational Exploration of Two Peptides and Their Hybrid Polymer Conjugates: Potentialities As Self-Aggregating Materials. Journal of Physical Chemistry B, 2012, 116, 13941-13952.	1.2	7
76	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.	1.2	32
77	Key Building Block of Photoresponsive Biomimetic Systems. Journal of Physical Chemistry B, 2011, 115, 1232-1242.	1.2	6
78	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. Chemical Physics Letters, 2011, 501, 245-251.	1.2	19
79	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.	2.2	27
80	Electronic effects and ring strain influences on the electron uptake by seleniumâ€containing bonds. International Journal of Quantum Chemistry, 2010, 110, 513-523.	1.0	6
81	Intersulfur Distance Is a Key Factor in Tuning Disulfide Radical Anion Vertical UVâ^Visible Absorption. Journal of Physical Chemistry Letters, 2010, 1, 581-586.	2.1	6
82	Substitution effects on the optical spectra of diarylethene photochroms:ab initioinsights. Molecular Simulation, 2010, 36, 74-78.	0.9	7
83	An ab initio simulation of the UV/visible spectra of Nâ€benzylideneaniline dyes. International Journal of Quantum Chemistry, 2009, 109, 3506-3515.	1.0	11
84	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
85	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. Chemical Physics Letters, 2009, 475, 120-123.	1.2	35
86	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.	2.3	11
87	Spectral properties of self-assembled squaraineâ€“tetralactam: a theoretical assessment. Physical Chemistry Chemical Physics, 2009, 11, 1258.	1.3	57
88	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
89	Huge Disulfide-Linkageâ€™S Electron Capture Variation Induced by Î±-Helix Orientation. Journal of Chemical Theory and Computation, 2008, 4, 1171-1173.	2.3	13
90	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.	2.3	23

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91	Photochromic properties of dithienylazoles and other conjugated diarylethenes. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 192, 211-219.	2.0	52
92	Hemi-indigo photochroms: A theoretical investigation. Chemical Physics Letters, 2007, 436, 84-88.	1.2	13