

Adèle D Laurent

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2181014/publications.pdf>

Version: 2024-02-01

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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
2	TD-DFT benchmarks: A review. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2019-2039.	1.0	938
3	Dye chemistry with time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14334-14356.	1.3	294
4	Tuning ESIPT fluorophores into dual emitters. <i>Chemical Science</i> , 2016, 7, 3763-3774.	3.7	168
5	Revisiting the optical signatures of BODIPY with ab initio tools. <i>Chemical Science</i> , 2013, 4, 1950.	3.7	140
6	White Emitters by Tuning the Excited-State Intramolecular Proton-Transfer Fluorescence Emission in 2-(2-Hydroxybenzofuran)benzoxazole Dyes. <i>Chemistry - A European Journal</i> , 2014, 20, 12843-12857.	1.7	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. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4574-4582.	2.3	98
8	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4517-4525.	2.3	95
9	Shedding Light on the Photoisomerization Pathway of Donor-Acceptor Stenhouse Adducts. <i>Journal of the American Chemical Society</i> , 2017, 139, 15596-15599.	6.6	88
10	Solvent Effects on the Actinic Step of Donor-Acceptor Stenhouse Adduct Photoswitching. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8063-8068.	7.2	70
11	Iminothioindoxyl as a molecular photoswitch with 100% nm band separation in the visible range. <i>Nature Communications</i> , 2019, 10, 2390.	5.8	63
12	Spectral properties of self-assembled squaraine-tetralactam: a theoretical assessment. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 1258.	1.3	57
13	TD-DFT Assessment of the Excited State Intramolecular Proton Transfer in Hydroxyphenylbenzimidazole (HBI) Dyes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2180-2192.	1.2	55
14	Tailoring Photoisomerization Pathways in Donor-Acceptor Stenhouse Adducts: The Role of the Hydroxy Group. <i>Journal of Physical Chemistry A</i> , 2018, 122, 955-964.	1.1	54
15	Modeling optical signatures and excited-state reactivities of substituted hydroxyphenylbenzoxazole (HBO) ESIPT dyes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 1319-1321.	1.3	53
16	Photochromic properties of dithienylazoles and other conjugated diarylethenes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 192, 211-219.	2.0	52
17	Physicochemical and Electronic Properties of Cationic [6]Helicenes: from Chemical and Electrochemical Stabilities to Far-Red (Polarized) Luminescence. <i>Chemistry - A European Journal</i> , 2016, 22, 18394-18403.	1.7	52
18	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. <i>ChemPhysChem</i> , 2016, 17, 1846-1851.	1.0	50

#	ARTICLE	IF	CITATIONS
19	Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications. <i>Molecules</i> , 2022, 27, 2443.	1.7	48
20	The Influence of the π -Conjugated Spacer on Photophysical Properties of Difluoroboranyls Derived from Amides Carrying a Donor Group. <i>Journal of Organic Chemistry</i> , 2016, 81, 2280-2292.	1.7	45
21	Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28831-28841.	1.5	41
22	Photophysical Properties of Phenacylphenantridine Difluoroboranyls: Effect of Substituent and Double Benzannulation. <i>Journal of Organic Chemistry</i> , 2017, 82, 1529-1537.	1.7	37
23	Dual Solution-/Solid-State Emissive Excited-State Intramolecular Proton Transfer (ESIPT) Dyes: A Combined Experimental and Theoretical Approach. <i>Journal of Organic Chemistry</i> , 2021, 86, 17606-17619.	1.7	36
24	Important effects of neighbouring nucleotides on electron induced DNA single-strand breaks. <i>Chemical Physics Letters</i> , 2009, 475, 120-123.	1.2	35
25	Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches. <i>Journal of Physical Chemistry C</i> , 2014, 118, 4334-4345.	1.5	34
26	Impact of tautomers on the absorption spectra of neutral and anionic alizarin and quinizarin dyes. <i>Computational and Theoretical Chemistry</i> , 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. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12426-12440.	1.2	32
28	ESIPT or not ESIPT? Revisiting recent results on 2,1,3-benzothiadiazole under the TD-DFT light. <i>RSC Advances</i> , 2014, 4, 14189-14192.	1.7	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. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	30
30	How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 16104-16113.	7.2	30
31	Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1848-1851.	2.3	29
32	Effect of the Enhanced Cyan Fluorescent Protein framework on the UV/visible absorption spectra of some chromophores. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010, 2, 38-47.	2.2	27
33	Electroactive polymer-peptide conjugates for adhesive biointerfaces. <i>Biomaterials Science</i> , 2015, 3, 1395-1405.	2.6	26
34	Investigation of ESIPT in a panel of chromophores presenting N-H \cdots N intramolecular hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25288-25295.	1.3	24
35	Theoretical Investigation of the Geometries and UV-vis Spectra of Poly(L-glutamic acid) Featuring a Photochromic Azobenzene Side Chain. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 637-645.	2.3	23
36	Molecular features and toxicological properties of four common pesticides, acetamiprid, deltamethrin, chlorpyrifos and fipronil. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 1540-1550.	1.4	23

#	ARTICLE	IF	CITATIONS
37	Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine <i>N</i> -Oxide. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1919-1929.	2.3	23
38	Methodological keys for accurate simulations. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 11875.	1.3	22
39	Influence of the Nature of the Amino Group in Highly Fluorescent Difluoroborates Exhibiting Intramolecular Charge Transfer. <i>Journal of Organic Chemistry</i> , 2018, 83, 7779-7788.	1.7	22
40	Solvent Effects on the Actinic Step of Donor-Acceptor Stenhouse Adduct Photoswitching. <i>Angewandte Chemie</i> , 2018, 130, 8195-8200.	1.6	21
41	Determining the most promising anchors for CuSCN: ab initio insights towards p-type DSSCs. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2217-2227.	5.2	20
42	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. <i>Chemical Physics Letters</i> , 2011, 501, 245-251.	1.2	19
43	TD-DFT study of the for coumarins. <i>Chemical Physics Letters</i> , 2013, 583, 218-221.	1.2	19
44	Investigating the optical properties of BOIMPY dyes using ab initio tools. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10554-10561.	1.3	19
45	Similar Comparative Low and High Doses of Deltamethrin and Acetamidid Differently Impair the Retrieval of the Proboscis Extension Reflex in the Forager Honey Bee (<i>Apis mellifera</i>). <i>Insects</i> , 2015, 6, 805-814.	1.0	18
46	Exploring the Solvatochromism of Betaine...30 with Ab Initio Tools: From Accurate Gas-Phase Calculations to Implicit and Explicit Solvation Models. <i>Chemistry - A European Journal</i> , 2017, 23, 4108-4119.	1.7	18
47	Modelling solvent effects on the absorption and emission spectra of constrained cyanines with both implicit and explicit QM/EFP models. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 321-327.	1.1	15
48	Interplay between TiO ₂ Surfaces and Organic Photochromes: A DFT Study of Adsorbed Azobenzenes and Diarylethenes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3684-3696.	1.5	15
49	Exploring the excited-states of squaraine dyes with TD-DFT, SOS-CIS(D) and ADC(2). <i>Dyes and Pigments</i> , 2017, 138, 169-175.	2.0	15
50	Photo-isomerization upshifts the pKa of the Photoactive Yellow Protein chromophore to contribute to photocycle propagation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013, 270, 43-52.	2.0	14
51	Exceptional Stability of Azacalixpyrin and Its Dianion. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8883-8888.	1.1	14
52	Photostable orange-red fluorescent unsymmetrical diketopyrrolopyrrole-BF ₂ hybrids. <i>Journal of Materials Chemistry C</i> , 2020, 8, 7708-7717.	2.7	14
53	Hemi-indigo photochroms: A theoretical investigation. <i>Chemical Physics Letters</i> , 2007, 436, 84-88.	1.2	13
54	Huge Disulfide-Linkage-TMS Electron Capture Variation Induced by Î±-Helix Orientation. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1171-1173.	2.3	13

#	ARTICLE	IF	CITATIONS
55	Spectral Signatures of Perylene Diimide Derivatives: Insights From Theory. <i>Journal of Physical Chemistry C</i> , 2013, 117, 21682-21691.	1.5	13
56	Excited States of Ladder-Type π -Conjugated Dyes with a Joint SOS-CIS(D) and PCM-TD-DFT Approach. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5417-5425.	1.1	13
57	Imidacloprid and thiacloprid neonicotinoids bind more favourably to cockroach than to honeybee α 6 nicotinic acetylcholine receptor: Insights from computational studies. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 55, 1-12.	1.3	13
58	Tailoring the optical and dynamic properties of iminothioindoxyl photoswitches through acidochromism. <i>Chemical Science</i> , 2021, 12, 4588-4598.	3.7	13
59	Direct and Indirect Effects of Dispersion Interactions on the Electric Properties of Weakly Bound Complexes. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3112-3124.	1.1	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 <i>N</i> -benzylideneaniline dyes. <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3506-3515.	1.0	11
62	Analyzing the Selectivity and Successiveness of a Two-Electron Capture on a Multiply Disulfide-Linked Protein. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1700-1708.	2.3	11
63	Theoretical spectroscopy of BASHY dyes. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	10
64	The α -hydrazinoturn-hydrogen bonding network in hydrazinopeptides and aza- β 3-peptides as probed by an AIM topological analysis of the electronic density. <i>Computational and Theoretical Chemistry</i> , 2008, 869, 41-46.	1.5	8
65	Molecular recognition of thiaclopride by <i>Aplysia californica</i> AChBP: new insights from a computational investigation. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 1151-1167.	1.3	8
66	Phosphonic Acid Fluorescent Organic Nanoparticles for High-Contrast and Selective Staining of Gram-Positive Bacteria. <i>ACS Omega</i> , 2018, 3, 17392-17402.	1.6	8
67	Binding of Sulfoxaflor to <i>Aplysia californica</i> -AChBP: Computational Insights from Multiscale Approaches. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3755-3769.	2.5	8
68	Substitution effects on the optical spectra of diarylethene photochroms: <i>ab initio</i> insights. <i>Molecular Simulation</i> , 2010, 36, 74-78.	0.9	7
69	Conformational Exploration of Two Peptides and Their Hybrid Polymer Conjugates: Potentialities As Self-Aggregating Materials. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13941-13952.	1.2	7
70	Design of hybrid conjugates based on chemical similarity. <i>RSC Advances</i> , 2013, 3, 21069.	1.7	7
71	Formazanate boron difluoride dyes: discrepancies between TD-DFT and wavefunction descriptions. <i>Journal of Molecular Modeling</i> , 2016, 22, 263.	0.8	7
72	Electronic effects and ring strain influences on the electron uptake by selenium-containing bonds. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 513-523.	1.0	6

#	ARTICLE	IF	CITATIONS
73	Intersulfur Distance Is a Key Factor in Tuning Disulfide Radical Anion Vertical UV-Visible Absorption. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 581-586.	2.1	6
74	Key Building Block of Photoresponsive Biomimetic Systems. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1232-1242.	1.2	6
75	Analyzing excited-state processes and optical signatures of a ratiometric fluorine anion sensor: a quantum look. <i>Science China Chemistry</i> , 2014, 57, 1363-1368.	4.2	6
76	IL-15 membrane-anchorage either in cis or in trans is required for stabilization of IL-15 and optimal signaling. <i>Journal of Cell Science</i> , 2019, 133, .	1.2	6
77	A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives. <i>ChemPhysChem</i> , 2016, 17, 2434-2445.	1.0	5
78	Investigating cyclic peptides inhibiting CD28-CD58 interactions through molecular dynamics and molecular docking methods. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1295-1313.	1.3	5
79	Investigation of Phospholipase C β 1 Interaction with SLP76 Using Molecular Modeling Methods for Identifying Novel Inhibitors. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4721.	1.8	5
80	How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. <i>Angewandte Chemie</i> , 2020, 132, 16238-16247.	1.6	5
81	Exploiting Light Interferences to Generate Micrometer-High Superstructures from Monomeric Azo Materials with Extensive Orientational Mobility. <i>Advanced Optical Materials</i> , 2021, 9, 2100525.	3.6	4
82	Structural insights into the catalytic mechanism of granzyme B upon substrate and inhibitor binding. <i>Journal of Molecular Graphics and Modelling</i> , 2022, 114, 108167.	1.3	4
83	Toward the understanding of the environmental effects on core ionizations. <i>Journal of Computational Chemistry</i> , 2014, 35, 1131-1139.	1.5	3
84	Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. <i>Chemical Physics Letters</i> , 2014, 599, 73-79.	1.2	3
85	Interactions of the Rad51 inhibitor DIDS with human and bovine serum albumins: Optical spectroscopy and isothermal calorimetry approaches. <i>Biochimie</i> , 2019, 167, 187-197.	1.3	3
86	First computational step towards the understanding of the antioxidant activity of the Phycocyanobilin:Ferredoxin Oxidoreductase in complex with biliverdin IX β . <i>Computational and Theoretical Chemistry</i> , 2016, 1077, 58-64.	1.1	2
87	Computational simulations determining disulfonic stilbene derivative bioavailability within human serum albumin. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18020-18030.	1.3	2
88	Mechanistic and Structural Insights on the IL-15 System through Molecular Dynamics Simulations. <i>Molecules</i> , 2019, 24, 3261.	1.7	2
89	Structure-based identification of inhibitors disrupting the CD28-CD58 interactions. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 337-353.	1.3	1
90	Time-Dependent Density Functional Theory: A Tool to Explore Excited States. , 2015, , 1-35.		1

#	ARTICLE	IF	CITATIONS
91	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. <i>ChemPhysChem</i> , 2016, 17, 1712-1712.	1.0	0
92	Exploring Structural Dynamics and Optical Properties of UnaG Fluorescent Protein upon N57 Mutations. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	1.3	0