Denis Jacquemin

List of Publications by Year
in descending order

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		8755	11052
624	28,347	75	137
papers	citations	h-index	g-index

640	640	640	18740
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The calculations of excited-state properties with Time-Dependent Density Functional Theory. Chemical Society Reviews, 2013, 42, 845-856.	38.1	1,424
2	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. Journal of Chemical Theory and Computation, 2009, 5, 2420-2435.	5.3	942
3	TD-DFT benchmarks: A review. International Journal of Quantum Chemistry, 2013, 113, 2019-2039.	2.0	938
4	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes:â€‰Conventional versus Long-Range Hybrids. Journal of Chemical Theory and Computation, 2008, 4, 123-135.	5.3	766
5	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Pushâ^'Pull Ï€-Conjugated Systemsâ€. Journal of Physical Chemistry A, 2000, 104, 4755-4763.	2.5	501
6	Accurate Simulation of Optical Properties in Dyes. Accounts of Chemical Research, 2009, 42, 326-334.	15.6	435
7	TD-DFT Assessment of Functionals for Optical 0â€“0 Transitions in Solvated Dyes. Journal of Chemical Theory and Computation, 2012, 8, 2359-2372.	5.3	403
8	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 2071-2085.	5.3	383
9	Enhanced Efficiency of Organic Dye-Sensitized Solar Cells: Triphenylamine Derivatives. Journal of Physical Chemistry C, 2009, 113, 16821-16833.	3.1	328
10	Multiphotochromic molecular systems. Chemical Society Reviews, 2015, 44, 3719-3759.	38.1	302
11	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. Physical Chemistry Chemical Physics, 2011, 13, 16987.	2.8	301
12	Dye chemistry with time-dependent density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 14334-14356.	2.8	294
13	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. Journal of Chemical Physics, 2007, 126, 144105.	3.0	290
14	What is the â€œbestâ€•atomic charge model to describe through-space charge-transfer excitations?. Physical Chemistry Chemical Physics, 2012, 14, 5383.	2.8	290
15	Taking Up the Cyanine Challenge with Quantum Tools. Accounts of Chemical Research, 2015, 48, 530-537.	15.6	254
16	Thioindigo Dyes:Â Highly Accurate Visible Spectra with TD-DFT. Journal of the American Chemical Society, 2006, 128, 2072-2083.	13.7	245
17	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. Journal of Chemical Theory and Computation, 2013, 9, 2749-2760.	5.3	243
18	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. Journal of Physical Chemistry C, 2012, 116, 11946-11955.	3.1	222

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19	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. Journal of Chemical Theory and Computation, 2018, 14, 4360-4379.	5.3	211
20	0â€“0 Energies Using Hybrid Schemes: Benchmarks of TD-DFT, CIS(D), ADC(2), CC2, and BSE/GW formalisms for 80 Real-Life Compounds. Journal of Chemical Theory and Computation, 2015, 11, 5340-5359.	5.3	208
21	Assessment of Functionals for TD-DFT Calculations of Singletâ^'Triplet Transitions. Journal of Chemical Theory and Computation, 2010, 6, 1532-1537.	5.3	194
22	Second-Order NLO Switches from Molecules to Polymer Films Based on Photochromic Cyclometalated Platinum(II) Complexes. Journal of the American Chemical Society, 2014, 136, 5367-5375.	13.7	184
23	Going beyond the vertical approximation with timeâ€dependent density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 460-486.	14.6	174
24	Benchmarking the Betheâ€“Salpeter Formalism on a Standard Organic Molecular Set. Journal of Chemical Theory and Computation, 2015, 11, 3290-3304.	5.3	172
25	Tuning ESIPT fluorophores into dual emitters. Chemical Science, 2016, 7, 3763-3774.	7.4	168
26	Single Molecule Multiphotochromism with Diarylethenes. Accounts of Chemical Research, 2012, 45, 1173-1182.	15.6	166
27	Solvent polarity scales: determination of new E_T(30) values for 84 organic solvents. Journal of Physical Organic Chemistry, 2014, 27, 512-518.	1.9	161
28	First hyperpolarizability of polymethineimine with long-range corrected functionals. Journal of Chemical Physics, 2007, 126, 191108.	3.0	158
29	The Betheâ€“Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. Chemical Society Reviews, 2018, 47, 1022-1043.	38.1	158
30	Towards new efficient dye-sensitised solar cells. Energy and Environmental Science, 2010, 3, 891.	30.8	156
31	Revisiting the optical signatures of BODIPY with ab initio tools. Chemical Science, 2013, 4, 1950.	7.4	140
32	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0â€“0 Electronic Excitation Energies. Journal of Chemical Theory and Computation, 2014, 10, 1677-1685.	5.3	135
33	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
34	Assessment of the Ï‰B97 family for excited-state calculations. Theoretical Chemistry Accounts, 2011, 128, 127-136.	1.4	132
35	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. Journal of Chemical Theory and Computation, 2011, 7, 369-376.	5.3	131
36	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. Physical Chemistry Chemical Physics, 2010, 12, 8016.	2.8	126

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37	Verdict: Time-Dependent Density Functional Theory â€œNot Guiltyâ€•of Large Errors for Cyanines. Journal of Chemical Theory and Computation, 2012, 8, 1255-1259.	5.3	122
38	Improvement of the efficiency of thiophene-bridged compounds for dye-sensitized solar cells. Chemical Physics, 2010, 376, 56-68.	1.9	120
39	Assessment of long-range corrected functionals performance for nâ†'Ï€* transitions in organic dyes. Journal of Chemical Physics, 2007, 127, 094102.	3.0	119
40	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Medium Sized Molecules. Journal of Chemical Theory and Computation, 2020, 16, 1711-1741.	5.3	119
41	Ruthenium polypyridine complexes as sensitizers in NiO based p-type dye-sensitized solar cells: Effects of the anchoring groups. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 219, 235-242.	3.9	117
42	Reference Energies for Double Excitations. Journal of Chemical Theory and Computation, 2019, 15, 1939-1956.	5.3	116
43	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. Journal of Chemical Physics, 2006, 125, 164324.	3.0	115
44	Theoretical investigation of substituted anthraquinone dyes. Journal of Chemical Physics, 2004, 121, 1736-1743.	3.0	113
45	A TD-DFT study of the absorption spectra of fast dye salts. Chemical Physics Letters, 2005, 410, 254-259.	2.6	113
46	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. Journal of Chemical Theory and Computation, 2011, 7, 1882-1892.	5.3	113
47	Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. Journal of Chemical Theory and Computation, 2015, 11, 5782-5790.	5.3	112
48	Cyclometalated Ir(<scp>iii</scp>) complexes with styryl-BODIPY ligands showing near IR absorption/emission: preparation, study of photophysical properties and application as photodynamic/luminescence imaging materials. Journal of Materials Chemistry B, 2014, 2, 2838-2854.	5.8	111
49	Substitution and chemical environment effects on the absorption spectrum of indigo. Journal of Chemical Physics, 2006, 124, 074104.	3.0	110
50	Molecular Structureâ€“Intersystem Crossing Relationship of Heavy-Atom-Free BODIPY Triplet Photosensitizers. Journal of Organic Chemistry, 2015, 80, 5958-5963.	3.2	109
51	Ab initio calculations of the colour of closed-ring diarylethenes: TD-DFT estimates for molecular switches. Chemical Physics Letters, 2006, 429, 147-152.	2.6	106
52	On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes. Journal of Chemical Theory and Computation, 2012, 8, 3303-3313.	5.3	102
53	Aza-boron-dipyrromethene dyes: TD-DFT benchmarks, spectral analysis and design of original near-IR structures. Physical Chemistry Chemical Physics, 2012, 14, 157-164.	2.8	100
54	The Quest for Highly Accurate Excitation Energies: A Computational Perspective. Journal of Physical Chemistry Letters, 2020, 11, 2374-2383.	4.6	100

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55	N,Nâ€²-Disubstituted Indigos as Readily Available Red-Light Photoswitches with Tunable Thermal Half-Lives. Journal of the American Chemical Society, 2017, 139, 15205-15211.	13.7	99
56	Assessing the Importance of Proton Transfer Reactions in DNA. Accounts of Chemical Research, 2014, 47, 2467-2474.	15.6	98
57	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
58	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. Chemical Physics Letters, 2008, 465, 226-229.	2.6	96
59	The Betheâ€“Salpeter Equation Formalism: From Physics to Chemistry. Journal of Physical Chemistry Letters, 2020, 11, 7371-7382.	4.6	96
60	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
61	Toward a Theoretical Quantitative Estimation of the Î»max of Anthraquinones-Based Dyes. Journal of Chemical Theory and Computation, 2006, 2, 434-440.	5.3	94
62	Expanding the Polymethine Paradigm: Evidence for the Contribution of a Bis-Dipolar Electronic Structure. Journal of Physical Chemistry A, 2014, 118, 4038-4047.	2.5	91
63	Ab Initio Coupled Hartreeâ€“Fock Investigation of the Static First Hyperpolarizability of Model all-trans-Polymethineimine Oligomers of Increasing Size. Journal of Physical Chemistry A, 1997, 101, 3158-3165.	2.5	88
64	Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Betheâ€“Salpeter Approach. Journal of Chemical Theory and Computation, 2014, 10, 1212-1218.	5.3	88
65	Computational insights into the photodeactivation dynamics of phosphors for OLEDs: a perspective. Dalton Transactions, 2015, 44, 8346-8355.	3.3	88
66	Shedding Light on the Photoisomerization Pathway of Donorâ€“Acceptor Stenhouse Adducts. Journal of the American Chemical Society, 2017, 139, 15596-15599.	13.7	88
67	Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments. Journal of Chemical Theory and Computation, 2021, 17, 1117-1132.	5.3	88
68	<scp>QUESTDB</scp>: A database of highly accurate excitation energies for the electronic structure community. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1517.	14.6	84
69	Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. Journal of Physical Chemistry Letters, 2012, 3, 468-471.	4.6	82
70	Molecular Engineering of Excited-state Intramolecular Proton Transfer (ESIPT) Dual and Triple Emitters. Chemistry Letters, 2018, 47, 1083-1089.	1.3	82
71	Charge transfer from the carotenoid can quench chlorophyll excitation in antenna complexes of plants. Nature Communications, 2020, 11, 662.	12.8	81
72	General Principles for the Design of Visibleâ€Lightâ€Responsive Photoswitches: Tetraâ€orthoâ€Chloroâ€Azobenzenes. Angewandte Chemie - International Edition, 2020, 59, 21663-21670.	13.8	80

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73	TD-DFT Investigation of the UV Spectra of Pyranone Derivatives. Journal of Physical Chemistry A, 2006, 110, 8144-8150.	2.5	78
74	Is the Betheâ€“Salpeter Formalism Accurate for Excitation Energies? Comparisons with TD-DFT, CASPT2, and EOM-CCSD. Journal of Physical Chemistry Letters, 2017, 8, 1524-1529.	4.6	78
75	Assessment of Several Hybrid DFT Functionals for the Evaluation of Bond Length Alternation of Increasingly Long Oligomers. Journal of Physical Chemistry A, 2006, 110, 5952-5959.	2.5	77
76	Intermolecular Proton Transfer in Microhydrated Guanineâ^'Cytosine Base Pairs: a New Mechanism for Spontaneous Mutation in DNA. Journal of Physical Chemistry A, 2009, 113, 10549-10556.	2.5	77
77	Boron Difluoride Curcuminoid Fluorophores with Enhanced Twoâ€Photon Excited Fluorescence Emission and Versatile Livingâ€Cell Imaging Properties. Chemistry - A European Journal, 2016, 22, 5219-5232.	3.3	77
78	Second Generation of Diketopyrrolopyrrole Dyes for NiO-Based Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2016, 120, 7923-7940.	3.1	77
79	An ab Initio Study of the Absorption Spectra of Indirubin, Isoindigo, and Related Derivatives. Journal of Physical Chemistry A, 2006, 110, 5629-5635.	2.5	76
80	On the TD-DFT Accuracy in Determining Single and Double Bonds in Excited-State Structures of Organic Molecules. Journal of Physical Chemistry A, 2010, 114, 13402-13410.	2.5	76
81	Copper-catalyzed free-radical Câ€“H arylation of pyrroles. Chemical Communications, 2014, 50, 5236-5238.	4.1	76
82	The short device lifetimes of blue PhOLEDs: insights into the photostability of blue Ir(<scp>iii</scp>) complexes. Chemical Science, 2017, 8, 7844-7850.	7.4	76
83	Proton-Stabilized Photochemically Reversible E/Z Isomerization of Spiropyrans. Journal of Physical Chemistry B, 2018, 122, 6423-6430.	2.6	76
84	Correlated frequency-dependent electronic first hyperpolarizability of small pushâ€“pull conjugated chains. Chemical Physics Letters, 2000, 319, 327-334.	2.6	75
85	Boranil and Related NBO Dyes: Insights From Theory. Journal of Chemical Theory and Computation, 2013, 9, 3127-3135.	5.3	74
86	Accuracy of TD-DFT Geometries: A Fresh Look. Journal of Chemical Theory and Computation, 2018, 14, 3715-3727.	5.3	74
87	Long-Lived Charge Separated State in NiO-Based p-Type Dye-Sensitized Solar Cells with Simple Cyclometalated Iridium Complexes. Journal of Physical Chemistry Letters, 2014, 5, 2254-2258.	4.6	73
88	Diketopyrrolopyrrole derivatives for efficient NiO-based dye-sensitized solar cells. Chemical Communications, 2013, 49, 8018.	4.1	72
89	Effects of Hydration on the Proton Transfer Mechanism in the Adenineâ^'Thymine Base Pair. Journal of Physical Chemistry A, 2009, 113, 7892-7898.	2.5	71
90	Absorption and emission spectra in gas-phase and solution using TD-DFT: Formaldehyde and benzene as case studies. Chemical Physics Letters, 2006, 421, 272-276.	2.6	70

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91	A water soluble probe with near infrared two-photon absorption and polarity-induced fluorescence for cerebral vascular imaging. Chemical Science, 2013, 4, 2833.	7.4	70
92	General Approach To Compute Phosphorescent OLED Efficiency. Journal of Physical Chemistry C, 2018, 122, 6340-6347.	3.1	70
93	A Blue Diketopyrrolopyrrole Sensitizer with High Efficiency in Nickelâ€Oxideâ€based Dyeâ€Sensitized Solar Cells. ChemSusChem, 2017, 10, 2618-2625.	6.8	69
94	Triplet state CPL active heliceneâ€“dithiolene platinum bipyridine complexes. Chemical Communications, 2017, 53, 9210-9213.	4.1	69
95	Geometry, dipole moment, polarizability and first hyperpolarizability of polymethineimine: An assessment of electron correlation contributions. Journal of Chemical Physics, 2004, 121, 4389-4396.	3.0	68
96	A Database of Dispersion-Induction DI, Electrostatic ES, and Hydrogen Bonding Î±₁ and Î²₁ Solvent Parameters and Some Applications to the Multiparameter Correlation Analysis of Solvent Effects. Journal of Physical Chemistry B, 2015, 119, 3174-3184.	2.6	68
97	Zwitterionic [4]helicene: a water-soluble and reversible pH-triggered ECD/CPL chiroptical switch in the UV and red spectral regions. Organic and Biomolecular Chemistry, 2016, 14, 4590-4594.	2.8	67
98	A compact diketopyrrolopyrrole dye as efficient sensitizer in titanium dioxide dye-sensitized solar cells. Journal of Photochemistry and Photobiology A: Chemistry, 2011, 226, 9-15.	3.9	66
99	On the Fineâ€Tuning of the Excitedâ€State Intramolecular Proton Transfer (ESIPT) Process in 2â€(2â€²â€Hydroxybenzofuran)benzazole (HBBX) Dyes. Chemistry - A European Journal, 2017, 23, 7324-7336.	3.3	66
100	Ab initiostatic polarizability and first hyperpolarizability of model polymethineimine chains. II. Effects of conformation and of substitution by donor/acceptor end groups. Journal of Chemical Physics, 1997, 107, 5076-5087.	3.0	65
101	Design of New Triphenylamine-Sensitized Solar Cells: A Theoretical Approach. Environmental Science & Technology, 2010, 44, 5666-5671.	10.0	65
102	Benchmark of Bethe-Salpeter for Triplet Excited-States. Journal of Chemical Theory and Computation, 2017, 13, 767-783.	5.3	65
103	Determination of a Solvent Hydrogen-Bond Acidity Scale by Means of the Solvatochromism of Pyridinium-N-phenolate Betaine Dye 30 and PCM-TD-DFT Calculations. Journal of Physical Chemistry B, 2014, 118, 4605-4614.	2.6	64
104	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. Chemical Physics Letters, 2007, 438, 208-212.	2.6	63
105	Excited-states of BODIPYâ€“cyanines: ultimate TD-DFT challenges?. RSC Advances, 2014, 4, 49449-49456.	3.6	63
106	Red Thermally Activated Delayed Fluorescence and the Intersystem Crossing Mechanisms in Compact Naphthalimideâ€“Phenothiazine Electron Donor/Acceptor Dyads. Journal of Physical Chemistry C, 2019, 123, 30171-30186.	3.1	63
107	A qualitative failure of B3LYP for textbook organic reactions. Physical Chemistry Chemical Physics, 2012, 14, 7170.	2.8	62
108	Ab Initio Investigation of the n â†' Ï€* Transitions in Thiocarbonyl Dyes. Journal of Physical Chemistry A, 2006, 110, 9145-9152.	2.5	61

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109	Boron difluorides with formazanate ligands: redox-switchable fluorescent dyes with large stokes shifts. Dalton Transactions, 2016, 45, 9477-9484.	3.3	61
110	A generalized Romberg differentiation procedure for calculation of hyperpolarizabilities. Computational and Theoretical Chemistry, 2007, 847, 39-46.	1.5	59
111	On the geometries and UV/Vis spectra of substituted trans-azobenzenes. Chemical Physics Letters, 2007, 435, 257-262.	2.6	58
112	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. Chemical Physics, 2010, 372, 61-66.	1.9	58
113	Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. Journal of Chemical Theory and Computation, 2019, 15, 4581-4590.	5.3	58
114	Use of Pyrimidine and Pyrazine Bridges as a Design Strategy To Improve the Performance of Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes. ACS Applied Materials & Interfaces, 2019, 11, 45171-45179.	8.0	58
115	Spectral properties of self-assembled squaraineâ€“tetralactam: a theoretical assessment. Physical Chemistry Chemical Physics, 2009, 11, 1258.	2.8	57
116	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. Journal of Chemical Theory and Computation, 2013, 9, 2368-2379.	5.3	57
117	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. Theoretical Chemistry Accounts, 2008, 120, 405-410.	1.4	56
118	Sequential double second-order nonlinear optical switch by an acido-triggered photochromic cyclometallated platinum(<scp>ii</scp>) complex. Chemical Communications, 2015, 51, 7805-7808.	4.1	56
119	Low-Lying Ï€Ï€* States of Heteroaromatic Molecules: A Challenge for Excited State Methods. Journal of Chemical Theory and Computation, 2016, 12, 2652-2660.	5.3	56
120	Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Exotic Molecules and Radicals. Journal of Chemical Theory and Computation, 2020, 16, 3720-3736.	5.3	56
121	Electron correlation effects upon the static (hyper)polarizabilities of push-pull conjugated polyenes and polyynes. , 1997, 65, 679-688.		55
122	Substitution effects on the visible spectra of 1,4-diNHPh-9,10-anthraquinones. Chemical Physics Letters, 2005, 405, 429-433.	2.6	55
123	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
124	Efficient Intersystem Crossing in Heavy-Atom-Free Perylenebisimide Derivatives. Journal of Physical Chemistry C, 2016, 120, 10162-10175.	3.1	55
125	The Betheâ€“Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. Chemical Science, 2018, 9, 4430-4443.	7.4	55
126	Electronic Communication between two [10]cycloparaphenylenes and Bis(azafullerene) (C₅₉N)₂ Induced by Cooperative Complexation. Angewandte Chemie - International Edition, 2018, 57, 6930-6934.	13.8	55

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127	Is solvated trans-azobenzene twisted or planar?. Chemical Physics Letters, 2006, 417, 190-195.	2.6	54
128	Modeling optical signatures and excited-state reactivities of substituted hydroxyphenylbenzoxazole (HBO) ESIPT dyes. Physical Chemistry Chemical Physics, 2014, 16, 1319-1321.	2.8	53
129	Electron nuclear dynamics of proton collisions with methane at 30 eV. Journal of Chemical Physics, 1997, 107, 6146-6155.	3.0	52
130	Photochromic properties of dithienylazoles and other conjugated diarylethenes. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 192, 211-219.	3.9	52
131	Combined effect of stacking and solvation on the spontaneous mutation in DNA. Physical Chemistry Chemical Physics, 2011, 13, 14584.	2.8	52
132	Photoswitching of the second-order nonlinearity of a tetrahedral octupolar multi DTE-based copper(i) complex. Chemical Communications, 2012, 48, 10395.	4.1	52
133	Diketopyrrolopyrroleâ€“Porphyrin Conjugates as Broadly Absorbing Sensitizers for Dyeâ€Sensitized Solar Cells. ChemSusChem, 2012, 5, 1568-1577.	6.8	52
134	Optical Signatures of OBO Fluorophores: A Theoretical Analysis. Journal of Chemical Theory and Computation, 2014, 10, 805-815.	5.3	52
135	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
136	Accurate Excited-State Geometries: A CASPT2 and Coupled-Cluster Reference Database for Small Molecules. Journal of Chemical Theory and Computation, 2017, 13, 6237-6252.	5.3	52
137	Assessment of recently developed density functional approaches for the evaluation of the bond length alternation in polyacetylene. Chemical Physics Letters, 2005, 405, 376-381.	2.6	51
138	Theoretical investigations of the UV spectra of coumarin derivatives. Chemical Physics Letters, 2005, 415, 20-24.	2.6	51
139	Reference Energies for Intramolecular Charge-Transfer Excitations. Journal of Chemical Theory and Computation, 2021, 17, 3666-3686.	5.3	51
140	MÃ¸llerâ€“Plesset evaluation of the static first hyperpolarizability of polymethineimine. Chemical Physics Letters, 1998, 284, 24-30.	2.6	50
141	Second-Order ab Initio MÃ¸llerâ^'Plesset Study of Optimum Chain Length for Total (Electronic Plus) Tj ETQq1 1 0.784314 rgBT /Overlo 9748-9755.	2.5	50
142	Interplay Between Electronic and Steric Effects in Multiphotochromic Diarylethenes. Journal of Physical Chemistry C, 2011, 115, 9193-9203.	3.1	50
143	Using Timeâ€Dependent Density Functional Theory to Probe the Nature of Donorâ€“Acceptor Stenhouse Adduct Photochromes. ChemPhysChem, 2016, 17, 1846-1851.	2.1	50
144	Arylazoindazole Photoswitches: Facile Synthesis and Functionalization via S_NAr Substitution. Journal of the American Chemical Society, 2017, 139, 3328-3331.	13.7	50

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145	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. Journal of Chemical Physics, 2018, 149, 034108.	3.0	50
146	Doubly Closing or Not? Theoretical Analysis for Coupled Photochromes. Journal of Physical Chemistry C, 2010, 114, 9489-9497.	3.1	49
147	Perylene-Derived Triplet Acceptors with Optimized Excited State Energy Levels for Tripletâ€"Triplet Annihilation Assisted Upconversion. Journal of Organic Chemistry, 2014, 79, 2038-2048.	3.2	48
148	Isoindigo derivatives for application in p-type dye sensitized solar cells. RSC Advances, 2015, 5, 85530-85539.	3.6	48
149	Symmetry Breaking in Pyrrolo[3,2â€b]pyrroles: Synthesis, Solvatofluorochromism and Twoâ€photon Absorption. Chemistry - an Asian Journal, 2017, 12, 1736-1748.	3.3	48
150	First-principles investigation of the double ESIPT process in a thiophene-based dye. Physical Chemistry Chemical Physics, 2019, 21, 2307-2317.	2.8	48
151	Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications. Molecules, 2022, 27, 2443.	3.8	48
152	Excitation spectra of nitro-diphenylaniline: Accurate time-dependent density functional theory predictions for charge-transfer dyes. Journal of Chemical Physics, 2006, 124, 204321.	3.0	47
153	Synthesis, photovoltaic performances and TD-DFT modeling of pushâ€"pull diacetylide platinum complexes in TiO₂ based dye-sensitized solar cells. Dalton Transactions, 2014, 43, 11233-11242.	3.3	47
154	Electric field induced DNA damage: an open door for selective mutations. Chemical Communications, 2013, 49, 7578.	4.1	46
155	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. Journal of Chemical Physics, 2016, 144, 164106.	3.0	46
156	Electric-field induced mutation of DNA: a theoretical investigation of the GC base pair. Physical Chemistry Chemical Physics, 2013, 15, 4548.	2.8	45
157	Diketopyrrolopyrrole-zinc porphyrin, a tuned panchromatic association for dye-sensitized solar cells. Journal of Materials Chemistry A, 2013, 1, 7572.	10.3	45
158	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
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