Denis Jacquemin

List of Publications by Citations

604 papers	22,926 citations	69 h-index	124 g-index
640 ext. papers	25,727 ext. citations	4.9 avg, IF	7.56 L-index

#	Paper	IF	Citations
604	The calculations of excited-state properties with Time-Dependent Density Functional Theory. *Chemical Society Reviews*, **2013**, 42, 845-56	58.5	1048
603	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 2420-35	6.4	799
602	TD-DFT benchmarks: A review. *International Journal of Quantum Chemistry*, **2013**, 113, 2019-2039	2.1	715
601	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. *Journal of Chemical Theory and Computation*, **2008**, 4, 123-35	6.4	681
600	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of Push□Pull □Conjugated Systems□ *Journal of Physical Chemistry A*, **2000**, 104, 4755-4763	2.8	473
599	Accurate simulation of optical properties in dyes. *Accounts of Chemical Research*, **2009**, 42, 326-34	24.3	404
598	TD-DFT Assessment of Functionals for Optical 0-0 Transitions in Solvated Dyes. *Journal of Chemical Theory and Computation*, **2012**, 8, 2359-72	6.4	342
597	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2010**, 6, 2071-85	6.4	335
596	Enhanced Efficiency of Organic Dye-Sensitized Solar Cells: Triphenylamine Derivatives. *Journal of Physical Chemistry C*, **2009**, 113, 16821-16833	3.8	287
595	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. *Journal of Chemical Physics*, **2007**, 126, 144105	3.9	264
594	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. *Physical Chemistry Chemical Physics*, **2011**, 13, 16987-98	3.6	258
593	Multiphotochromic molecular systems. *Chemical Society Reviews*, **2015**, 44, 3719-59	58.5	248
592	What is the "best" atomic charge model to describe through-space charge-transfer excitations?. *Physical Chemistry Chemical Physics*, **2012**, 14, 5383-8	3.6	242
591	Dye chemistry with time-dependent density functional theory. *Physical Chemistry Chemical Physics*, **2014**, 16, 14334-56	3.6	225
590	Thioindigo dyes: highly accurate visible spectra with TD-DFT. *Journal of the American Chemical Society*, **2006**, 128, 2072-83	16.4	220
589	Taking up the cyanine challenge with quantum tools. *Accounts of Chemical Research*, **2015**, 48, 530-7	24.3	207
588	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. *Journal of Chemical Theory and Computation*, **2013**, 9, 2749-60	6.4	196

587	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. *Journal of Physical Chemistry C*, **2012**, 116, 11946-11955	3.8	193
586	Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions. *Journal of Chemical Theory and Computation*, **2010**, 6, 1532-7	6.4	173
585	0-0 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, 5340-59	6.4	166
584	Second-order NLO switches from molecules to polymer films based on photochromic cyclometalated platinum(II) complexes. *Journal of the American Chemical Society*, **2014**, 136, 5367-75	16.4	159
583	First hyperpolarizability of polymethineimine with long-range corrected functionals. *Journal of Chemical Physics*, **2007**, 126, 191108	3.9	151
582	Single molecule multiphotochromism with diarylethenes. *Accounts of Chemical Research*, **2012**, 45, 1173-82	24.3	147
581	Benchmarking the Bethe-Salpeter Formalism on a Standard Organic Molecular Set. *Journal of Chemical Theory and Computation*, **2015**, 11, 3290-304	6.4	145
580	Towards new efficient dye-sensitised solar cells. *Energy and Environmental Science*, **2010**, 3, 891	35.4	145
579	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. *Journal of Chemical Theory and Computation*, **2018**, 14, 4360-4379	6.4	145
578	Going beyond the vertical approximation with time-dependent density functional theory. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 460-486	7.9	137
577	Revisiting the optical signatures of BODIPY with ab initio tools. *Chemical Science*, **2013**, 4, 1950	9.4	124
576	Tuning ESIPT fluorophores into dual emitters. *Chemical Science*, **2016**, 7, 3763-3774	9.4	122
575	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. *Journal of Chemical Theory and Computation*, **2011**, 7, 369-76	6.4	119
574	Assessment of the B97 family for excited-state calculations. *Theoretical Chemistry Accounts*, **2011**, 128, 127-136	1.9	115
573	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0-0 Electronic Excitation Energies. *Journal of Chemical Theory and Computation*, **2014**, 10, 1677-85	6.4	113
572	White emitters by tuning the excited-state intramolecular proton-transfer fluorescence emission in 2-(2'-hydroxybenzofuran)benzoxazole dyes. *Chemistry - A European Journal*, **2014**, 20, 12843-57	4.8	113
571	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. *Physical Chemistry Chemical Physics*, **2010**, 12, 8016-23	3.6	113
570	Assessment of long-range corrected functionals performance for n-->pi* transitions in organic dyes. *Journal of Chemical Physics*, **2007**, 127, 094102	3.9	112

569	The Bethe-Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. *Chemical Society Reviews*, **2018**, 47, 1022-1043	58.5	110
568	Verdict: Time-Dependent Density Functional Theory "Not Guilty" of Large Errors for Cyanines. *Journal of Chemical Theory and Computation*, **2012**, 8, 1255-9	6.4	110
567	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	4.7	107
566	Solvent polarity scales: determination of new ET(30) values for 84 organic solvents. *Journal of Physical Organic Chemistry*, **2014**, 27, 512-518	2.1	105
565	A TD-DFT study of the absorption spectra of fast dye salts. *Chemical Physics Letters*, **2005**, 410, 254-259	2.5	105
564	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. *Journal of Chemical Physics*, **2006**, 125, 164324	3.9	104
563	Theoretical investigation of substituted anthraquinone dyes. *Journal of Chemical Physics*, **2004**, 121, 1736-43	3.9	102
562	Improvement of the efficiency of thiophene-bridged compounds for dye-sensitized solar cells. *Chemical Physics*, **2010**, 376, 56-68	2.3	100
561	Substitution and chemical environment effects on the absorption spectrum of indigo. *Journal of Chemical Physics*, **2006**, 124, 74104	3.9	100
560	Cyclometalated Ir(iii) 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	7.3	99
559	Ab initio calculations of the colour of closed-ring diarylethenes: TD-DFT estimates for molecular switches. *Chemical Physics Letters*, **2006**, 429, 147-152	2.5	99
558	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, 1882-92	6.4	96
557	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, 5782-90	6.4	95
556	Aza-boron-dipyrromethene dyes: TD-DFT benchmarks, spectral analysis and design of original near-IR structures. *Physical Chemistry Chemical Physics*, **2012**, 14, 157-64	3.6	92
555	On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes. *Journal of Chemical Theory and Computation*, **2012**, 8, 3303-13	6.4	91
554	Molecular Structure-Intersystem Crossing Relationship of Heavy-Atom-Free BODIPY Triplet Photosensitizers. *Journal of Organic Chemistry*, **2015**, 80, 5958-63	4.2	90
553	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. *Chemical Physics Letters*, **2008**, 465, 226-229	2.5	88
552	Toward a Theoretical Quantitative Estimation of the λ_{max} of Anthraquinones-Based Dyes. *Journal of Chemical Theory and Computation*, **2006**, 2, 434-40	6.4	86

551	Computational insights into the photodeactivation dynamics of phosphors for OLEDs: a perspective. *Dalton Transactions*, **2015**, 44, 8346-55	4.3	81
550	Ab Initio Coupled Hartree–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	2.8	81
549	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, 4574-82	6.4	80
548	Reference Energies for Double Excitations. *Journal of Chemical Theory and Computation*, **2019**, 15, 1939-1956	6.4	78
547	A theoretical investigation of microhydration of amino acids. *Journal of Cheminformatics*, **2010**, 2,	8.6	78
546	Is the Tamm-Dancoff Approximation Reliable for the Calculation of Absorption and Fluorescence Band Shapes?. *Journal of Chemical Theory and Computation*, **2013**, 9, 4517-25	6.4	75
545	Assessing the importance of proton transfer reactions in DNA. *Accounts of Chemical Research*, **2014**, 47, 2467-74	24.3	74
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542	An ab initio study of the absorption spectra of indirubin, isoindigo, and related derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 5629-35	2.8	72
541	Copper-catalyzed free-radical C-H arylation of pyrroles. *Chemical Communications*, **2014**, 50, 5236-8	5.8	71
540	Assessment of several hybrid DFT functionals for the evaluation of bond length alternation of increasingly long oligomers. *Journal of Physical Chemistry A*, **2006**, 110, 5952-9	2.8	71
539	Second Generation of Diketopyrrolopyrrole Dyes for NiO-Based Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2016**, 120, 7923-7940	3.8	69
538	Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. *Journal of Physical Chemistry Letters*, **2012**, 3, 468-71	6.4	69
537	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, 13402-10	2.8	69
536	TD-DFT investigation of the UV spectra of pyranone derivatives. *Journal of Physical Chemistry A*, **2006**, 110, 8144-50	2.8	69
535	Geometry, dipole moment, polarizability and first hyperpolarizability of polymethineimine: an assessment of electron correlation contributions. *Journal of Chemical Physics*, **2004**, 121, 4389-96	3.9	68
534	Expanding the polymethine paradigm: evidence for the contribution of a bis-dipolar electronic structure. *Journal of Physical Chemistry A*, **2014**, 118, 4038-47	2.8	67

533	Boranil and Related NBO Dyes: Insights From Theory. *Journal of Chemical Theory and Computation*, **2013**, 9, 3127-35	6.4	67
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531	Diketopyrrolopyrrole derivatives for efficient NiO-based dye-sensitized solar cells. *Chemical Communications*, **2013**, 49, 8018-20	5.8	66
530	Intermolecular proton transfer in microhydrated guanine-cytosine base pairs: a new mechanism for spontaneous mutation in DNA. *Journal of Physical Chemistry A*, **2009**, 113, 10549-56	2.8	66
529	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	2.5	66
528	Shedding Light on the Photoisomerization Pathway of Donor-Acceptor Stenhouse Adducts. *Journal of the American Chemical Society*, **2017**, 139, 15596-15599	16.4	63
527	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	6.4	63
526	Effects of hydration on the proton transfer mechanism in the adenine-thymine base pair. *Journal of Physical Chemistry A*, **2009**, 113, 7892-8	2.8	63
525	Ab initio static 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	3.9	63
524	Boron Difluoride Curcuminoid Fluorophores with Enhanced Two-Photon Excited Fluorescence Emission and Versatile Living-Cell Imaging Properties. *Chemistry - A European Journal*, **2016**, 22, 5219-32	4.8	62
523	Is the Bethe-Salpeter Formalism Accurate for Excitation Energies? Comparisons with TD-DFT, CASPT2, and EOM-CCSD. *Journal of Physical Chemistry Letters*, **2017**, 8, 1524-1529	6.4	61
522	A water soluble probe with near infrared two-photon absorption and polarity-induced fluorescence for cerebral vascular imaging. *Chemical Science*, **2013**, 4, 2833	9.4	61
521	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. *Chemical Physics Letters*, **2007**, 438, 208-212	2.5	60
520	N,N'-Disubstituted Indigos as Readily Available Red-Light Photoswitches with Tunable Thermal Half-Lives. *Journal of the American Chemical Society*, **2017**, 139, 15205-15211	16.4	59
519	Ab initio investigation of the n --> pi* transitions in thiocarbonyl dyes. *Journal of Physical Chemistry A*, **2006**, 110, 9145-52	2.8	59
518	The short device lifetimes of blue PhOLEDs: insights into the photostability of blue Ir(iii) complexes. *Chemical Science*, **2017**, 8, 7844-7850	9.4	58
517	The Quest for Highly Accurate Excitation Energies: A Computational Perspective. *Journal of Physical Chemistry Letters*, **2020**, 11, 2374-2383	6.4	58
516	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	4.7	58

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514	General Approach To Compute Phosphorescent OLED Efficiency. *Journal of Physical Chemistry C*, **2018**, 122, 6340-6347	3.8	57
513	Spectral properties of self-assembled squaraine-tetralactam: a theoretical assessment. *Physical Chemistry Chemical Physics*, **2009**, 11, 1258-62	3.6	57
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511	On the geometries and UV/Vis spectra of substituted trans-azobenzenes. *Chemical Physics Letters*, **2007**, 435, 257-262	2.5	55
510	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. *Journal of Chemical Theory and Computation*, **2013**, 9, 2368-79	6.4	54
509	A generalized Romberg differentiation procedure for calculation of hyperpolarizabilities. *Computational and Theoretical Chemistry*, **2007**, 847, 39-46		54
508	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. *Chemical Physics*, **2010**, 372, 61-66	2.3	53
507	Excited-states of BODIPY□yanines: ultimate TD-DFT challenges?. *RSC Advances*, **2014**, 4, 49449-49456	3.7	52
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503	Benchmark of Bethe-Salpeter for Triplet Excited-States. *Journal of Chemical Theory and Computation*, **2017**, 13, 767-783	6.4	51
502	Sequential double second-order nonlinear optical switch by an acido-triggered photochromic cyclometallated platinum(II) complex. *Chemical Communications*, **2015**, 51, 7805-8	5.8	51
501	Photoswitching of the second-order nonlinearity of a tetrahedral octupolar multi DTE-based copper(I) complex. *Chemical Communications*, **2012**, 48, 10395-7	5.8	51
500	Electron nuclear dynamics of proton collisions with methane at 30 eV. *Journal of Chemical Physics*, **1997**, 107, 6146-6155	3.9	51
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498	Substitution effects on the visible spectra of 1,4-diNHPh-9,10-anthraquinones. *Chemical Physics Letters*, **2005**, 405, 429-433	2.5	51

497	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. *Theoretical Chemistry Accounts*, **2008**, 120, 405-410	1.9	50
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494	A database of dispersion-induction DI, electrostatic ES, and hydrogen bonding □ and □ solvent parameters and some applications to the multiparameter correlation analysis of solvent effects. *Journal of Physical Chemistry B*, **2015**, 119, 3174-84	3.4	49
493	Combined effect of stacking and solvation on the spontaneous mutation in DNA. *Physical Chemistry Chemical Physics*, **2011**, 13, 14584-9	3.6	49
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490	Doubly Closing or Not? Theoretical Analysis for Coupled Photochromes. *Journal of Physical Chemistry C*, **2010**, 114, 9489-9497	3.8	48
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486	Excitation spectra of nitro-diphenylaniline: accurate time-dependent density functional theory predictions for charge-transfer dyes. *Journal of Chemical Physics*, **2006**, 124, 204321	3.9	47
485	Assessment of recently developed density functional approaches for the evaluation of the bond length alternation in polyacetylene. *Chemical Physics Letters*, **2005**, 405, 376-381	2.5	47
484	Low-Lying □ States of Heteroaromatic Molecules: A Challenge for Excited State Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 2652-60	6.4	47
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481	Optical Signatures of OBO Fluorophores: A Theoretical Analysis. *Journal of Chemical Theory and Computation*, **2014**, 10, 805-15	6.4	46
480	Molecular Engineering of Excited-state Intramolecular Proton Transfer (ESIPT) Dual and Triple Emitters. *Chemistry Letters*, **2018**, 47, 1083-1089	1.7	45

479	Diketopyrrolopyrrole-porphyrin conjugates as broadly absorbing sensitizers for dye-sensitized solar cells. *ChemSusChem*, **2012**, 5, 1568-77	8.3	45
478	Physicochemical and Electronic Properties of Cationic [6]Helicenes: from Chemical and Electrochemical Stabilities to Far-Red (Polarized) Luminescence. *Chemistry - A European Journal*, **2016**, 22, 18394-18403	4.8	44
477	Isoindigo derivatives for application in p-type dye sensitized solar cells. *RSC Advances*, **2015**, 5, 85530-85539	3.7	43
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471	Diketopyrrolopyrrole-zinc porphyrin, a tuned panchromatic association for dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2013**, 1, 7572	13	41
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469	Arylazoindazole Photoswitches: Facile Synthesis and Functionalization via SAr Substitution. *Journal of the American Chemical Society*, **2017**, 139, 3328-3331	16.4	40
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459	Perylene-derived triplet acceptors with optimized excited state energy levels for triplet-triplet annihilation assisted upconversion. *Journal of Organic Chemistry*, **2014**, 79, 2038-48	4.2	39
458	Electric-field induced mutation of DNA: a theoretical investigation of the GC base pair. *Physical Chemistry Chemical Physics*, **2013**, 15, 4548-53	3.6	39
457	Triplet state CPL active helicene-dithiolene platinum bipyridine complexes. *Chemical Communications*, **2017**, 53, 9210-9213	5.8	39
456	Electronic Communication between two [10]cycloparaphenylenes and Bis(azafullerene) (C N) Induced by Cooperative Complexation. *Angewandte Chemie - International Edition*, **2018**, 57, 6930-6934	16.4	38
455	The Influence of the Conjugated Spacer on Photophysical Properties of Difluoroboranyls Derived from Amides Carrying a Donor Group. *Journal of Organic Chemistry*, **2016**, 81, 2280-92	4.2	38
454	The Bethe-Salpeter Equation Formalism: From Physics to Chemistry. *Journal of Physical Chemistry Letters*, **2020**, 11, 7371-7382	6.4	38
453	Controlling Triplet Triplet Annihilation Upconversion by Tuning the PET in Aminomethyleneanthracene Derivatives. *Journal of Physical Chemistry C*, **2015**, 119, 23801-23812	3.8	37
452	The Bethe-Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. *Chemical Science*, **2018**, 9, 4430-4443	9.4	37
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450	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 4599-608	6.4	36
449	Synthesis and properties of push ull porphyrins as sensitizers for NiO based dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2015**, 3, 3908-3917	13	36
448	General Principles for the Design of Visible-Light-Responsive Photoswitches: Tetra-ortho-Chloro-Azobenzenes. *Angewandte Chemie - International Edition*, **2020**, 59, 21663-21670	16.4	36
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446	Homochiral Emissive and [Ir Pd] Supramolecular Cages. *Chemistry - A European Journal*, **2017**, 23, 14358-14366	4.8	35
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