

Denis Jacquemin

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	2,2,4,6-Tetraaryl-2H-benzo[h]chromenes: The influence of electronic communication between aryl substituents on their photochromism. <i>Dyes and Pigments</i> , 2022 , 199, 110036	4.6	0
603	The Krönke synthesis of benzo[a]indolizines revisited: towards small, red light emitters. <i>Organic Chemistry Frontiers</i> , 2022 , 9, 1861-1874	5.2	0
602	Blue-Emitting 2-(2'-Hydroxyphenyl)benzazole Fluorophores by Modulation of Excited-State Intramolecular Proton Transfer: Spectroscopic Studies and Theoretical Calculations.. <i>Journal of Physical Chemistry B</i> , 2022 ,	3.4	3
601	Excited-State Intramolecular Proton Transfer Dyes with Dual-State Emission Properties: Concept, Examples and Applications.. <i>Molecules</i> , 2022 , 27,	4.8	4
600	Si-containing polycyclic aromatic hydrocarbons: synthesis and opto-electronic properties. <i>Chemical Communications</i> , 2021 ,	5.8	1
599	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 ,	4.2	7
598	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Bicyclic Systems. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 10174-10188	2.8	0
597	Going beyond the borders: pyrrolo[3,2-]pyrroles with deep red emission.. <i>Chemical Science</i> , 2021 , 12, 15935-15946	9.4	3
596	Boranils: Versatile Multifunctional Organic Fluorophores for Innovative Applications. <i>Organics</i> , 2021 , 2, 365-375	9	2
595	Chiral Near-Infrared Fluorophores by Self-Promoted Oxidative Coupling of Cationic Helicenes with Amines/Enamines. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8733-8738	16.4	3
594	Thermally Activated Delayed Fluorescence Emitters with Intramolecular Proton Transfer for High Luminescence Solution-Processed Organic Light-Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 15459-15474	9.5	9
593	Using Theory To Extend the Scope of Azobenzene Drugs in Chemotherapy: Novel Combinations for a Specific Delivery. <i>ChemMedChem</i> , 2021 , 16, 1764-1774	3.7	0
592	Chiral Near-Infrared Fluorophores by Self-Promoted Oxidative Coupling of Cationic Helicenes with Amines/Enamines. <i>Angewandte Chemie</i> , 2021 , 133, 8815-8820	3.6	1
591	Electrochemical Ring-Opening and -Closing of a Spiropyran. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 3355-3361	2.8	4
590	High-field and benchtop NMR spectroscopy for the characterization of new psychoactive substances. <i>Forensic Science International</i> , 2021 , 321, 110718	2.6	5
589	Coumarin-Pyronin Hybrid Dyes: Synthesis, Fluorescence Properties and Theoretical Calculations**. <i>ChemPhotoChem</i> , 2021 , 5, 822-838	3.3	0
588	Reference Energies for Intramolecular Charge-Transfer Excitations. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 3666-3686	6.4	14

587	How accurate are EOM-CC4 vertical excitation energies?. <i>Journal of Chemical Physics</i> , 2021 , 154, 221103	3.9	3
586	Modified Indulines: From Dyestuffs to Theranostic Agents. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 30337-30349	9.5	
585	Does Twisted π -Conjugation Framework Always Induce Efficient Intersystem Crossing? A Case Study with Benzo[<i>a</i>]- and [<i>b</i>]Phenanthrene-Fused BODIPY Derivatives and Identification of a Dark State. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 6280-6295	3.4	4
584	2,2-Dipicolylamino substituted 2-(2'-hydroxybenzofuranyl) benzoxazole (HBBO) derivative: Towards ratiometric sensing of divalent zinc cations. <i>Dyes and Pigments</i> , 2021 , 190, 109338	4.6	2
583	Excited States of Xanthophylls Revisited: Toward the Simulation of Biologically Relevant Systems. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 6604-6612	6.4	4
582	Mountaineering Strategy to Excited States: Highly Accurate Oscillator Strengths and Dipole Moments of Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 416-438	6.4	9
581	Stabilization of a 12- π -Electrons diamino-benzoquinonediimine tautomer. <i>Chemical Communications</i> , 2021 , 57, 548-551	5.8	1
580	Benzothiadiazole-Substituted Aza-BODIPY Dyes: Two-Photon Absorption Enhancement for Improved Optical Limiting Performances in the Short-Wave IR Range. <i>Chemistry - A European Journal</i> , 2021 , 27, 3517-3525	4.8	2
579	Impact of Heteroatom Substitution on Dual-State Emissive Rigidified 2-(2'-hydroxyphenyl)benzazole Dyes: Towards Ultra-Bright ESIPT Fluorophores*. <i>Chemistry - A European Journal</i> , 2021 , 27, 3483-3495	4.8	15
578	Switch-On Diketopyrrolopyrrole-Based Chemosensors for Cations Possessing Lewis Acid Character. <i>Chemistry - an Asian Journal</i> , 2021 , 16, 355-362	4.5	1
577	Quenching of the phosphorescence of thermally reversible photochromic naphthopyran Re(i) complexes initiated by either visible or ultraviolet radiation. <i>Dalton Transactions</i> , 2021 , 50, 830-834	4.3	0
576	Azacalixpyrins as an innovative alternative for the free-radical photopolymerization under visible and NIR irradiation without the need of co-initiators. <i>Chemical Communications</i> , 2021 , 57, 8973-8976	5.8	0
575	Investigation of second-order nonlinear optical responses in a series of V-shaped binuclear platinum(ii) complexes. <i>Dalton Transactions</i> , 2021 , 50, 4623-4633	4.3	1
574	Helical donor-acceptor platinum complexes displaying dual luminescence and near-infrared circularly polarized luminescence. <i>Dalton Transactions</i> , 2021 , 50, 13220-13226	4.3	3
573	QUESTDB: A database of highly accurate excitation energies for the electronic structure community. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021 , 11, e1517	7.9	24
572	Dual-State Emissive π -Extended Salicylaldehyde Fluorophores: Synthesis, Photophysical Properties and First-Principle Calculations. <i>European Journal of Organic Chemistry</i> , 2021 , 2021, 3726-3736	3.2	6
571	Simple Protocol for Capturing Both Linear-Response and State-Specific Effects in Excited-State Calculations with Continuum Solvation Models. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 5155-5164	6.4	9
570	The Synthesis and Photophysical Properties of Weakly Coupled Diketopyrrolopyrroles. <i>Molecules</i> , 2021 , 26,	4.8	1

569	Attochemistry: Is Controlling Electrons the Future of Photochemistry?. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 8404-8415	6.4	3
568	Dye-Sensitized Photoelectrosynthesis Cells for Benzyl Alcohol Oxidation Using a Zinc Porphyrin Sensitizer and TEMPO Catalyst. <i>ACS Catalysis</i> , 2021 , 11, 12075-12086	13.1	2
567	Photoluminescent properties of the carbon-dimer defect in hexagonal boron-nitride: A many-body finite-size cluster approach. <i>Physical Review Materials</i> , 2021 , 5,	3.2	2
566	Accurate full configuration interaction correlation energy estimates for five- and six-membered rings. <i>Journal of Chemical Physics</i> , 2021 , 155, 134104	3.9	4
565	-> photoisomerisation of azobenzene: a fresh theoretical look. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 19155-19165	3.6	6
564	Benchmarking TD-DFT and Wave Function Methods for Oscillator Strengths and Excited-State Dipole Moments. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 1117-1132	6.4	27
563	Structure illumination microscopy imaging of lipid vesicles in live bacteria with naphthalimide-appended organometallic complexes. <i>Analyst, The</i> , 2021 , 146, 3818-3822	5	2
562	Versatile naphthalimide tetrazines for fluorogenic bioorthogonal labelling. <i>RSC Chemical Biology</i> , 2021 , 2, 1491-1498	3	0
561	Synthesis of Nitro-Aryl Functionalised 4-Amino-1,8-Naphthalimides and Their Evaluation as Fluorescent Hypoxia Sensors. <i>Chemistry - A European Journal</i> , 2020 , 26, 10064-10071	4.8	4
560	Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Exotic Molecules and Radicals. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 3720-3736	6.4	29
559	Comparative studies of new pyranilidene-based sensitizers bearing single or double anchoring groups for dye-sensitized solar cells. <i>Solar Energy</i> , 2020 , 205, 310-319	6.8	12
558	How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 16104-16113	16.4	14
557	Observation of Collective Photoswitching in Free-Standing TATA-Based Azobenzenes on Au(111). <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 17192-17196	16.4	3
556	N-Arylation of Diketopyrrolopyrroles with Aryl Triflates. <i>Chemistry - an Asian Journal</i> , 2020 , 15, 1369-1375	4.5	7
555	Multi-Stage Redox Systems Based on Dicationic P-Containing Polycyclic Aromatic Hydrocarbons. <i>Chemistry - A European Journal</i> , 2020 , 26, 8226-8229	4.8	9
554	The Quest for Highly Accurate Excitation Energies: A Computational Perspective. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 2374-2383	6.4	58
553	Controlling Two-Photon Action Cross Section by Changing a Single Heteroatom Position in Fluorescent Dyes. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5920-5925	6.4	4
552	Ground- and Excited-State Symmetry Breaking and Solvatofluorochromism in Centrosymmetric Pyrrolo[3,2-b]pyrroles Possessing two Nitro Groups. <i>ChemPhotoChem</i> , 2020 , 4, 508-519	3.3	11

551	Charge transfer from the carotenoid can quench chlorophyll excitation in antenna complexes of plants. <i>Nature Communications</i> , 2020 , 11, 662	17.4	41
550	Is ADC(3) as Accurate as CC3 for Valence and Rydberg Transition Energies?. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 974-980	6.4	13
549	A Mountaineering Strategy to Excited States: Highly Accurate Energies and Benchmarks for Medium Sized Molecules. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 1711-1741	6.4	63
548	Tuning the Emission Color of Indolo[3,2-b]carbazole-Based Boron Complexes and their Application in Organic Field Effect Transistors and Bioimaging. <i>ChemPhotoChem</i> , 2020 , 4, 729	3.3	2
547	Pros and Cons of the Bethe-Salpeter Formalism for Ground-State Energies. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 3536-3545	6.4	15
546	Photostable orange-red fluorescent unsymmetrical diketopyrrolopyrroleBF ₂ hybrids. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 7708-7717	7.1	5
545	Small Panchromatic and NIR Absorbers from Quinoid Zwitterions. <i>Organic Letters</i> , 2020 , 22, 7997-8001	6.2	2
544	Dual fluorescence in strap ESIPT systems: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 854-863	3.6	13
543	Fused bis-azacalixpyrin that reaches NIR-II absorptions. <i>Chemical Communications</i> , 2020 , 56, 896-899	5.8	7
542	A Pd ₃ L ₆ supramolecular cage incorporating photoactive [2.2]paracyclophane units. <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 232-238	6.8	7
541	Mixed N-aryl/alkyl substitution favours an unusual tautomer of near-infrared absorbing azacalixpyrins. <i>New Journal of Chemistry</i> , 2020 , 44, 18130-18137	3.6	2
540	Synthesis of heterocyclic enamine-zinc complexes as precursors of stereocontrolled substitution of nitrogen position. <i>Tetrahedron Letters</i> , 2020 , 61, 152405	2	1
539	Daphnanes diterpenes from the latex of <i>Hura crepitans</i> L. And activity against human colorectal cancer cells Caco-2. <i>Bioorganic Chemistry</i> , 2020 , 103, 104132	5.1	1
538	Persistent Organic Room-Temperature Phosphorescence in Cyclohexane-1,2-Bisphthalimide Derivatives: The Dramatic Impact of Heterochiral vs Homochiral interactions. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 6426-6434	6.4	11
537	How To Make Nitroaromatic Compounds Glow: Next-Generation Large X-Shaped, Centrosymmetric Diketopyrrolopyrroles. <i>Angewandte Chemie</i> , 2020 , 132, 16238-16247	3.6	3
536	Hochkooperatives Photoschalten in Dihydropyren-Dimeren. <i>Angewandte Chemie</i> , 2020 , 132, 19517-19523	3.6	0
535	The Bethe-Salpeter Equation Formalism: From Physics to Chemistry. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 7371-7382	6.4	38
534	Unconventional access to a solvatochromic nickel (II) dye featuring a coordination-induced spin crossover behavior. <i>Dyes and Pigments</i> , 2020 , 183, 108645	4.6	0

533	Noncommutative Switching of Double Spiropyrans. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 6458-6467. 2.8	0
532	Highly Cooperative Photoswitching in Dihdropyrene Dimers. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 19352-19358	16.4 9
531	High-Performance Optical Power Limiting Filters at Telecommunication Wavelengths: When Aza-BODIPY Dyes Bond to Solid Materials. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 24344-24350	3.8 6
530	Luminescent molecular switches based on dicationic P-doped polycyclic aromatic hydrocarbons. <i>Materials Advances</i> , 2020 , 1, 3369-3377	3.3 4
529	TD-DFT and CC2 insights into the dual-emissive behaviour of 2-(2'-hydroxyphenyl)oxazoles core and their derivatives. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 25066-25074	3.6 8
528	Access to Chiral Rigid Hemicyanine Fluorophores from Tröger Bases and Amino Carbenes. <i>Organic Letters</i> , 2020 , 22, 7599-7603	6.2 4
527	General Principles for the Design of Visible-Light-Responsive Photoswitches: Tetra-ortho-Chloro-Azobenzenes. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 21663-21670	16.4 36
526	General Principles for the Design of Visible-Light-Responsive Photoswitches: Tetra-ortho-Chloro-Azobenzenes. <i>Angewandte Chemie</i> , 2020 , 132, 21847-21854	3.6 13
525	Unraveling the Two-Photon and Excited-State Absorptions of Aza-BODIPY Dyes for Optical Power Limiting in the SWIR Band. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 23661-23673	3.8 19
524	Reference Energies for Double Excitations. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 1939-1956	6.2 78
523	Electronic Communication in Pyrrolo[3,2-b]pyrroles Possessing Sterically Hindered Aromatic Substituents. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 5247-5253	3.2 5
522	First-principles investigation of the double ESIPT process in a thiophene-based dye. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 2307-2317	3.6 29
521	Structure of Electronically Reduced N-Donor Bidentate Ligands and Their Heteroleptic Four-Coordinate Zinc Complexes: A Survey of Density Functional Theory Results. <i>Inorganic Chemistry</i> , 2019 , 58, 7169-7179	5.1 5
520	3,4-Dideoxy-3,3,4,4-tetrafluoro- and 4-OH epimeric 3-deoxy-3,3-difluoro-β-GalCer analogues: Synthesis and biological evaluation on human iNKT cells stimulation. <i>European Journal of Medicinal Chemistry</i> , 2019 , 178, 195-213	6.8 9
519	Evaluating 00 Energies with Theoretical Tools: A Short Review. <i>ChemPhotoChem</i> , 2019 , 3, 684-696	3.3 21
518	A de novo strategy for predictive crystal engineering to tune excitonic coupling. <i>Nature Communications</i> , 2019 , 10, 2048	17.4 27
517	Design of Two-Photon-Excited Fluorescent Dyes Containing Fluoroborylene Groups. <i>ChemPhotoChem</i> , 2019 , 3, 719-726	3.3 4
516	The impact of the heteroatom in a five-membered ring on the photophysical properties of difluoroborates. <i>Dyes and Pigments</i> , 2019 , 170, 107481	4.6 6

515	Chemically Accurate 0-0 Energies with Not-so-Accurate Excited State Geometries. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 2481-2491	6.4	25
514	Divergent synthesis of 5',7'-difluorinated dihydroxanthene-hemicyanine fused near-infrared fluorophores. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 4291-4300	3.9	3
513	Fabrication of Robust Spatially Resolved Photochromic Patterns on Cellulose Papers by Covalent Printing for Anticounterfeiting Applications. <i>ACS Applied Polymer Materials</i> , 2019 , 1, 1240-1250	4.3	16
512	i-Motif DNA structures upon electric field exposure: completing the map of induced genetic errors. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	2
511	Natural Born Laser Dyes: Excited-State Intramolecular Proton Transfer (ESIPT) Emitters and Their Use in Random Lasing Studies. <i>Nanomaterials</i> , 2019 , 9,	5.4	21
510	Influence of pseudopotentials on excitation energies from selected configuration interaction and diffusion Monte Carlo. <i>Results in Chemistry</i> , 2019 , 1, 100002	2.1	11
509	Iridium effect in cyclometalated iridium complexes for p-type dye sensitized solar cells. <i>Dyes and Pigments</i> , 2019 , 171, 107693	4.6	10
508	Synthesis and properties of novel pyranilidene-based organic sensitizers for dye-sensitized solar cells. <i>Dyes and Pigments</i> , 2019 , 171, 107747	4.6	12
507	A theoretical elucidation of the mechanism of tuneable fluorescence in a full-colour emissive ESIPT dye. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 17400-17409	3.6	15
506	Fe(III)-Catalyzed synthesis of pyrrolo[3,2-b]pyrroles: formation of new dyes and photophysical studies. <i>Organic Chemistry Frontiers</i> , 2019 , 6, 2939-2948	5.2	11
505	Cross-Comparisons between Experiment, TD-DFT, CC, and ADC for Transition Energies. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4581-4590	6.4	34
504	Use of Pyrimidine and Pyrazine Bridges as a Design Strategy To Improve the Performance of Thermally Activated Delayed Fluorescence Organic Light Emitting Diodes. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 45171-45179	9.5	39
503	Performances of Density Functional Tight-Binding Methods for Describing Ground and Excited State Geometries of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 6267-6276	6.4	9
502	Merging polyacenes and cationic helicenes: from weak to intense chiroptical properties in the far red region. <i>Chemical Science</i> , 2019 , 11, 1165-1169	9.4	13
501	Reactivity of 4-phenylthiazoles in ruthenium catalyzed direct arylations. <i>Applied Organometallic Chemistry</i> , 2019 , 33, e4794	3.1	2
500	First principles investigation of the spectral properties of neutral, zwitterionic, and bis-cationic azaacenes. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 22910-22918	3.6	4
499	Red Thermally Activated Delayed Fluorescence and the Intersystem Crossing Mechanisms in Compact Naphthalimide-Phenothiazine Electron Donor/Acceptor Dyads. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 30171-30186	3.8	28
498	Solution and solid-state Excited-State Intramolecular Proton Transfer (ESIPT) emitters incorporating Bis-triethyl-or triphenylsilylethynyl units. <i>Dyes and Pigments</i> , 2019 , 160, 915-922	4.6	21

497	Thiodiketopiperazines with two spirocyclic centers extracted from <i>Botryosphaeria mamane</i> , an endophytic fungus isolated from <i>Bixa orellana</i> L. <i>Phytochemistry</i> , 2019 , 158, 142-148	4	12
496	Catalyst-Controlled Regiodivergent C-H Arylation Site of Fluorinated 2-Arylpyridine Derivatives: Application to Luminescent Iridium(III) Complexes. <i>ACS Catalysis</i> , 2019 , 9, 1320-1328	13.1	20
495	Turning ESIPT-Based triazine fluorophores into dual emitters: From theory to experiment. <i>Dyes and Pigments</i> , 2019 , 163, 475-482	4.6	13
494	Azacalixquinarenes: From Canonical to (Poly-)Zwitterionic Macrocycles. <i>Journal of Organic Chemistry</i> , 2019 , 84, 1387-1397	4.2	8
493	Analyzing the Relation between Structure and Aggregation Induced Emission (AIE) Properties of Iridium(III) Complexes through Modification of Non-Chromophoric Ancillary Ligands. <i>European Journal of Inorganic Chemistry</i> , 2019 , 2019, 135-135	2.3	
492	Analyzing the Relation between Structure and Aggregation Induced Emission (AIE) Properties of Iridium(III) Complexes through Modification of Non-Chromophoric Ancillary Ligands. <i>European Journal of Inorganic Chemistry</i> , 2019 , 2019, 152-163	2.3	15
491	Ethynyl-Tolyl Extended 2-(2'-Hydroxyphenyl)benzoxazole Dyes: Solution and Solid-state Excited-State Intramolecular Proton Transfer (ESIPT) Emitters. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 1134-1144	3.2	15
490	Synthesis of Bis(arylethynyl)pyrrolo[3,2-b]pyrroles and Effect of Intramolecular Charge Transfer on Their Photophysical Behavior. <i>Chemistry - A European Journal</i> , 2019 , 25, 598-608	4.8	16
489	Effiziente lichtinduzierte pKa-Modulation, gekoppelt mit basenkatalysierter Photochromie. <i>Angewandte Chemie</i> , 2018 , 130, 4888-4893	3.6	12
488	Efficient Light-Induced pK _a Modulation Coupled to Base-Catalyzed Photochromism. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 4797-4801	16.4	23
487	Phosphorescent cationic iridium(iii) complexes bearing a nonconjugated six-membered chelating ancillary ligand: a strategy for tuning the emission towards the blue. <i>Dalton Transactions</i> , 2018 , 47, 10564-10577	4.3	8
486	Phosphonate-Mediated Immobilization of Rhodium/Bipyridine Hydrogenation Catalysts. <i>Chemistry - A European Journal</i> , 2018 , 24, 2457-2465	4.8	4
485	General Approach To Compute Phosphorescent OLED Efficiency. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 6340-6347	3.8	57
484	A physico-chemical investigation of fluorine-enriched quinolines. <i>New Journal of Chemistry</i> , 2018 , 42, 10036-10047	3.6	3
483	Thermal equilibration between excited states or solvent effects: unveiling the origins of anomalous emissions in heteroleptic Ru(ii) complexes. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 11559-11563	3.6	9
482	The Bethe-Salpeter formalism with polarisable continuum embedding: reconciling linear-response and state-specific features. <i>Chemical Science</i> , 2018 , 9, 4430-4443	9.4	37
481	Electronic Communication between two [10]cycloparaphenylenes and Bis(azafullerene) (C ₆₀ N ₂) Induced by Cooperative Complexation. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 6930-6934	16.4	38
480	Rationalisation of the optical signatures of nor-dihydroxanthene-hemicyanine fused near-infrared fluorophores by first-principle tools. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 12120-12128	3.6	3

479	Synthesis and spectral properties of non-symmetrical red and near IR emitter dibenzoBODIPYs. <i>Tetrahedron Letters</i> , 2018 , 59, 878-881	2	5
478	Synthesis, Characterization, and Optoelectronic Properties of Iridium Complexes Bearing Nonconjugated Six-Membered Chelating Ligands. <i>Inorganic Chemistry</i> , 2018 , 57, 2023-2034	5.1	8
477	Excited State Dipole Moments in Solution: Comparison between State-Specific and Linear-Response TD-DFT Values. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1544-1553	6.4	31
476	Expanding the Breadth of 4-Amino-1,8-naphthalimide Photophysical Properties through Substitution of the Naphthalimide Core. <i>Chemistry - A European Journal</i> , 2018 , 24, 5569-5573	4.8	27
475	Synthesis and Photophysical Properties of N-Arylated Diketopyrrolopyrroles. <i>European Journal of Organic Chemistry</i> , 2018 , 2018, 6643-6648	3.2	7
474	What is the Key for Accurate Absorption and Emission Calculations, Energy or Geometry?. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 1534-1543	6.4	32
473	The Bethe-Salpeter equation in chemistry: relations with TD-DFT, applications and challenges. <i>Chemical Society Reviews</i> , 2018 , 47, 1022-1043	58.5	110
472	Bidirectional Solvatofluorochromism of a Pyrrolo[3,2-b]pyrroleDiketopyrrolopyrrole Hybrid. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 13424-13434	3.8	17
471	Iron(III) coordination properties of ladanein, a flavone lead with a broad-spectrum antiviral activity. <i>New Journal of Chemistry</i> , 2018 , 42, 8074-8087	3.6	4
470	Theoretical spectroscopy of a NIR-absorbing benzophthalocyanine dye. <i>Theoretical Chemistry Accounts</i> , 2018 , 137, 1	1.9	5
469	Searching for new borondifluoride β -diketonate complexes with enhanced absorption/emission properties using ab initio tools. <i>Dyes and Pigments</i> , 2018 , 155, 59-67	4.6	12
468	Synthesis and properties of new benzothiadiazole-based push-pull dyes for p-type dye sensitized solar cells. <i>Dyes and Pigments</i> , 2018 , 148, 154-166	4.6	21
467	Molecular Engineering of Excited-state Intramolecular Proton Transfer (ESIPT) Dual and Triple Emitters. <i>Chemistry Letters</i> , 2018 , 47, 1083-1089	1.7	45
466	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	4.2	12
465	Theoretical 0-0 Energies with Chemical Accuracy. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 4646-4654	4.4	33
464	Excitation energies from diffusion Monte Carlo using selected configuration interaction nodes. <i>Journal of Chemical Physics</i> , 2018 , 149, 034108	3.9	41
463	Mono- and Diplatinum Polyynediyl Complexes as Potential PushPull Chromophores: Synthesis, Characterization, TD-DFT Modeling, and Photophysical and NLO Properties. <i>Organometallics</i> , 2018 , 37, 2232-2244	3.8	12
462	An extended excited-state intramolecular proton transfer (ESIPT) emitter for random lasing applications. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 19958-19963	3.6	17

461	Central substitution of azacalixpyrins: a strategy towards acidochromic NIR dyes. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 20056-20069	3.6	4
460	Photoinduced Energy and Electron Transfer Between a Photoactive Cage Based on a Thermally Activate Delayed Fluorescence Ligand and Encapsulated Fluorescent Dyes. <i>ACS Applied Energy Materials</i> , 2018 , 1, 2971-2978	6.1	23
459	Versatile synthesis of Fused BODIPY displaying intense absorption in the NIR region and high electron affinity. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 9925-9931	7.1	17
458	Photochromic DTE-Substituted-1,3-di(2-pyridyl)benzene Platinum(II) Complexes: Photomodulation of Luminescence and Second-Order Nonlinear Optical Properties. <i>Inorganic Chemistry</i> , 2018 , 57, 7051-7063	5.1	32
457	Accuracy of TD-DFT Geometries: A Fresh Look. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3715-3727	6.4	40
456	Intriguing C-HCu interactions in bis-(phenanthroline)Cu(i) redox mediators for dye-sensitized solar cells. <i>Dalton Transactions</i> , 2018 , 47, 1018-1022	4.3	10
455	Modelling excitation energy transfer in covalently linked molecular dyads containing a BODIPY unit and a macrocycle. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 1993-2008	3.6	11
454	Unexpected Nucleophilic Substitution Reaction of BODIPY: Preparation of the BODIPY-TEMPO Triad Showing Radical-Enhanced Intersystem Crossing. <i>European Journal of Organic Chemistry</i> , 2018 , 2018, 885-895	3.2	16
453	A panchromatic, near infrared Ir(III) emitter bearing a tripodal C ^N C ligand as a dye for dye-sensitized solar cells. <i>Polyhedron</i> , 2018 , 140, 109-115	2.7	9
452	Azacalixpyrins as NIR photoacoustic contrast agents. <i>Chemical Communications</i> , 2018 , 54, 12365-12368	5.8	11
451	Hetero-Bimetallic Effect as a Route to Access Multinuclear Complexes. <i>Inorganic Chemistry</i> , 2018 , 57, 12536-12542	5.1	1
450	Investigating cyclic peptides inhibiting CD2-CD58 interactions through molecular dynamics and molecular docking methods. <i>Journal of Computer-Aided Molecular Design</i> , 2018 , 32, 1295-1313	4.2	4
449	Excited state intramolecular proton transfer in julolidine derivatives: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25031-25038	3.6	9
448	An investigation on the second-order nonlinear optical response of cationic bipyridine or phenanthroline iridium(iii) complexes bearing cyclometallated 2-phenylpyridines with a triphenylamine substituent. <i>Dalton Transactions</i> , 2018 , 47, 8292-8300	4.3	14
447	Controlling the canonical/zwitterionic balance through intramolecular proton transfer: a strategy for vapochromism. <i>Materials Chemistry Frontiers</i> , 2018 , 2, 1618-1625	7.8	11
446	Proton-Stabilized Photochemically Reversible E/Z Isomerization of Spiropyrans. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 6423-6430	3.4	40
445	A luminescent [PdRu] supramolecular cage. <i>Chemical Communications</i> , 2018 , 54, 6016-6019	5.8	15
444	A Mountaineering Strategy to Excited States: Highly Accurate Reference Energies and Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 4360-4379	6.4	145

443	The voltage-sensitive dye RH421 detects a Na,K-ATPase conformational change at the membrane surface. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017 , 1859, 813-823	3.8	10
442	Bethe-Salpeter study of cationic dyes: Comparisons with ADC(2) and TD-DFT. <i>Journal of Chemical Physics</i> , 2017 , 146, 034301	3.9	18
441	Benchmark of Bethe-Salpeter for Triplet Excited-States. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 767-783	6.4	51
440	Tuning the Spectroscopic Properties of Ratiometric Fluorescent Metal Indicators: Experimental and Computational Studies on Mag-fura-2 and Analogues. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 696-703	3.4	7
439	Photophysical Properties of Phenacylphenanthridine Difluoroboranyls: Effect of Substituent and Double Benzannulation. <i>Journal of Organic Chemistry</i> , 2017 , 82, 1529-1537	4.2	28
438	An ab initio investigation of photoswitches adsorbed onto metal oxide surfaces: the case of donor-acceptor Stenhouse adduct photochromes on TiO ₂ anatase. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 1624-1631	7.1	15
437	Time-Dependent Density Functional Theory: A Tool to Explore Excited States		5
436	Modeling excitation energy transfer in multi-BODIPY architectures. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 6443-6453	3.6	13
435	Photoinduced electron transfer in supramolecular ruthenium-porphyrin assemblies. <i>Dalton Transactions</i> , 2017 , 46, 2255-2262	4.3	8
434	Arylazoindazole Photoswitches: Facile Synthesis and Functionalization via SAr Substitution. <i>Journal of the American Chemical Society</i> , 2017 , 139, 3328-3331	16.4	40
433	Influence of the electron donor groups on the optical and electrochemical properties of borondifluoride complexes of curcuminoid derivatives: a joint theoretical and experimental study. <i>RSC Advances</i> , 2017 , 7, 10132-10142	3.7	22
432	Modeling the Photochrome-TiO Interface with Bethe-Salpeter and Time-Dependent Density Functional Theory Methods. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 936-940	6.4	14
431	2,5-Bis(azulenyl)pyrrolo[3,2-b]pyrroles: The key influence of the linkage position on the linear and nonlinear optical properties. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 2620-2628	7.1	25
430	Ethynylene-analogues of hemicurcuminoids: Synthesis and ground- and excited properties of their boron difluoride complexes. <i>Dyes and Pigments</i> , 2017 , 141, 38-47	4.6	6
429	Symmetry Breaking in Pyrrolo[3,2-b]pyrroles: Synthesis, Solvatochromism and Two-photon Absorption. <i>Chemistry - an Asian Journal</i> , 2017 , 12, 1736-1748	4.5	35
428	An Unprecedented Family of Luminescent Iridium(III) Complexes Bearing a Six-Membered Chelated Tridentate C ^N C Ligand. <i>Inorganic Chemistry</i> , 2017 , 56, 5182-5188	5.1	16
427	A Blue Diketopyrrolopyrrole Sensitizer with High Efficiency in Nickel-Oxide-based Dye-Sensitized Solar Cells. <i>ChemSusChem</i> , 2017 , 10, 2618-2625	8.3	56
426	Phosphorescent platinum(II) complexes bearing pentafluorosulfanyl substituted cyclometalating ligands. <i>RSC Advances</i> , 2017 , 7, 25566-25574	3.7	13

425	Theoretical investigation of the photochromic properties of [2.2]paracyclophane-bridged imidazole dimers and bis(imidazole) dimers. <i>Tetrahedron</i> , 2017 , 73, 4936-4949	2.4	8
424	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	4.6	12
423	Structural and Optical Properties of Subporphyrinoids: A TD-DFT Study. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 4306-4317	2.8	15
422	On the structures, spin states, and optical properties of titanium, platinum, and iron azacalixpyrins: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 15903-15913	3.6	4
421	Straightforward metal-free synthesis of an azacalix[6]arene forming a host-guest complex with fullerene C60. <i>New Journal of Chemistry</i> , 2017 , 41, 5284-5290	3.6	3
420	Excited state gradients for a state-specific continuum solvation approach: The vertical excitation model within a Lagrangian TDDFT formulation. <i>Journal of Chemical Physics</i> , 2017 , 146, 204106	3.9	17
419	Modeling Diarylethene Excited States with Ab Initio Tools: From Model Systems to Large Multimers 2017 , 321-341		1
418	On the Fine-Tuning of the Excited-State Intramolecular Proton Transfer (ESIPT) Process in 2-(2'-Hydroxybenzofuran)benzazole (HBBX) Dyes. <i>Chemistry - A European Journal</i> , 2017 , 23, 7324-7336	4.8	49
417	Investigating the optical properties of BOIMPY dyes using ab initio tools. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 10554-10561	3.6	18
416	Exposing the G-quadruplex to electric fields: the role played by telomeres in the propagation of DNA errors. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 9358-9365	3.6	4
415	Is the Bethe-Salpeter Formalism Accurate for Excitation Energies? Comparisons with TD-DFT, CASPT2, and EOM-CCSD. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1524-1529	6.4	61
414	Synthesis and Characterization of Ruffled Phosphorus meso-Ester Corroles. <i>European Journal of Inorganic Chemistry</i> , 2017 , 2017, 780-788	2.3	16
413	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	4.8	12
412	Is energy transfer limiting multiphotochromism? answers from ab initio quantifications. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 2044-2052	3.6	10
411	N,N'-Disubstituted Indigos as Readily Available Red-Light Photoswitches with Tunable Thermal Half-Lives. <i>Journal of the American Chemical Society</i> , 2017 , 139, 15205-15211	16.4	59
410	The short device lifetimes of blue PhOLEDs: insights into the photostability of blue Ir(III) complexes. <i>Chemical Science</i> , 2017 , 8, 7844-7850	9.4	58
409	Shedding Light on the Photoisomerization Pathway of Donor-Acceptor Stenhouse Adducts. <i>Journal of the American Chemical Society</i> , 2017 , 139, 15596-15599	16.4	63
408	Ultrafast Excited-State Dynamics in Cyclometalated Ir(III) Complexes Coordinated with Perylenebisimide and Its Radical Anion Ligands. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 21184-21198	3.8	10

407	Tuning the Optical Properties of Phenanthriplatin: Towards New Photoactivatable Analogues. <i>ChemPhotoChem</i> , 2017 , 1, 504-512	3.3	2
406	Calculations of $n \rightarrow \pi^*$ Transition Energies: Comparisons Between TD-DFT, ADC, CC, CASPT2, and BSE/GW Descriptions. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 6122-6134	2.8	17
405	Di- vs. tetra-substituted quinonediimines: a drastic effect on coordination chemistry. <i>Dalton Transactions</i> , 2017 , 46, 12794-12803	4.3	5
404	Triplet state CPL active helicene-dithiolen platinum bipyridine complexes. <i>Chemical Communications</i> , 2017 , 53, 9210-9213	5.8	39
403	Quantifying the Performances of DFT for Predicting Vibrationally Resolved Optical Spectra: Asymmetric Fluoroborate Dyes as Working Examples. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 4347-4356	6.4	14
402	Homochiral Emissive π and π [Ir Pd] Supramolecular Cages. <i>Chemistry - A European Journal</i> , 2017 , 23, 14358-14366	4.8	35
401	Accurate Excited-State Geometries: A CASPT2 and Coupled-Cluster Reference Database for Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6237-6252	6.4	40
400	Combined TD-DFT-SOS-CIS(D) Study of BOPHY Derivatives with Potential Application in Biosensing. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 10850-10858	3.4	17
399	Keto-polymethines: a versatile class of dyes with outstanding spectroscopic properties for and two-photon microscopy imaging. <i>Chemical Science</i> , 2017 , 8, 381-394	9.4	27
398	Synthesis, structure and photophysical properties of NIR aza-BODIPYs with F/N3/NH2 groups at 1,7-positions. <i>Dyes and Pigments</i> , 2017 , 136, 619-626	4.6	15
397	Correlated electron-hole mechanism for molecular doping in organic semiconductors. <i>Physical Review Materials</i> , 2017 , 1,	3.2	31
396	Controlling the emission in flexibly-linked (N ⁺ C ⁺ N)platinum dyads. <i>Dalton Transactions</i> , 2017 , 47, 224-232	4.3	5
395	Grafting Spiropyran Molecular Switches on TiO ₂ : A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 18281-18288	3.8	5
394	Theoretical Quantification of the Modified Photoactivity of Photochromes Grafted on Metallic Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 21827-21836	3.8	5
393	Computational investigation on the switching efficiency of diarylethene: Comparison between the first hyperpolarizability and exchange interaction. <i>Chemical Physics Letters</i> , 2016 , 659, 258-262	2.5	1
392	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	4.8	44
391	Effects of chemical substitutions on the properties of azacalixpyrins: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 27308-27316	3.6	8
390	Assessment of the Accuracy of the Bethe-Salpeter (BSE/GW) Oscillator Strengths. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3969-81	6.4	34

389	Contrasted photochromic and luminescent properties in dinuclear Pt(II) complexes linked through a central dithienylethene unit. <i>Chemical Communications</i> , 2016 , 52, 9833-6	5.8	15
388	Accidental degeneracy in the spiropyran radical cation: charge transfer between two orthogonal rings inducing ultra-efficient reactivity. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 31244-31253	3.6	6
387	A Joint Theoretical and Experimental Study of the Behavior of the DIDS Inhibitor and its Derivatives. <i>ChemPhysChem</i> , 2016 , 17, 2434-45	3.2	4
386	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. <i>ChemPhysChem</i> , 2016 , 17, 1846-51	3.2	41
385	Mechanism of Fluorescence Switching in One ESIPT-Based Al(3+) Probe. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 6730-8	3.4	28
384	Highly fluorescent extended 2-(2'-hydroxyphenyl)benzazole dyes: synthesis, optical properties and first-principle calculations. <i>Chemical Communications</i> , 2016 , 52, 9216-9	5.8	28
383	Synthesis and Photophysical Properties of Novel Donor-Acceptor N-(Pyridin-2-yl)-Substituted Benzo(thio)amides and Their Difluoroboranyl Derivatives. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 4116-23	2.8	18
382	Going beyond the vertical approximation with time-dependent density functional theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016 , 6, 460-486	7.9	137
381	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	13	17
380	Assessment of the convergence of partially self-consistent BSE/GW calculations. <i>Molecular Physics</i> , 2016 , 114, 957-967	1.7	16
379	Borondifluoride complexes of hemicurcuminoids as bio-inspired push-pull dyes for bioimaging. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 1311-24	3.9	36
378	Second Generation of Diketopyrrolopyrrole Dyes for NiO-Based Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 7923-7940	3.8	69
377	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	2	1
376	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, 2280-92	4.2	38
375	Tuning ESIPT fluorophores into dual emitters. <i>Chemical Science</i> , 2016 , 7, 3763-3774	9.4	122
374	Understanding the tautomerism in azacalixpyrins. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 9608-15	5.6	10
373	Solvatochromic Shifts in UV-Vis Absorption Spectra: The Challenging Case of 4-Nitropyridine N-Oxide. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1919-29	6.4	18
372	Optical properties of V-shaped bis-coumarins: Ab initio insights. <i>Computational and Theoretical Chemistry</i> , 2016 , 1076, 57-64	2	5

371	Accessing the free energy profile of a ring closure in a proline-catalyzed reaction using a reactive force field. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	4
370	Investigating the properties of PODIPYs (phosphorus-dipyrromethene) with ab initio tools. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 9358-66	3.6	16
369	Computational Molecular Electronic Spectroscopy with TD-DFT. <i>Topics in Current Chemistry</i> , 2016 , 368, 347-75		25
368	Using Time-Dependent Density Functional Theory to Probe the Nature of Donor-Acceptor Stenhouse Adduct Photochromes. <i>ChemPhysChem</i> , 2016 , 17, 1712-1712	3.2	
367	Coumarin-Phosphine-Based Smart Probes for Tracking Biologically Relevant Metal Complexes: From Theoretical to Biological Investigations. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 545-553	2.3	12
366	Radical Cyclisation of Halo Aluminium Acetals: A Mechanistic Study. <i>Chemistry - A European Journal</i> , 2016 , 22, 4809-24	4.8	1
365	Theoretical spectroscopy of BASHY dyes. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	8
364	Excited-State Dipole and Quadrupole Moments: TD-DFT versus CC2. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3993-4003	6.4	29
363	Boron Difluoride Curcuminoid Fluorophores with Enhanced Two-Photon Excited Fluorescence Emission and Versatile Living-Cell Imaging Properties. <i>Chemistry - A European Journal</i> , 2016 , 22, 5219-32	4.8	62
362	Combining the GW formalism with the polarizable continuum model: A state-specific non-equilibrium approach. <i>Journal of Chemical Physics</i> , 2016 , 144, 164106	3.9	30
361	Writing and erasing hidden optical information on covalently modified cellulose paper. <i>Chemical Communications</i> , 2016 , 52, 7672-5	5.8	13
360	¹ H NMR and computational studies of the conformations in solution of one host/guest complex formed with an usnic acid tweezer and 2,4,7-trinitro-9-fluorenone (TNF). <i>Tetrahedron</i> , 2016 , 72, 2890-2894	3.4	1
359	Minor Pyranonaphthoquinones from the Apothecia of the Lichen <i>Ophioparma ventosa</i> . <i>Journal of Natural Products</i> , 2016 , 79, 1005-11	4.9	12
358	Elucidating the Nature of Carbazole-Porphyrinoids with First-Principle Approaches. <i>Journal of Physical Chemistry A</i> , 2016 , 120, 2824-31	2.8	6
357	How Metals Can Help Multiphotochromism: An Ab Initio Study. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 11140-11150	3.8	9
356	Low-Lying π States of Heteroaromatic Molecules: A Challenge for Excited State Methods. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 2652-60	6.4	47
355	Efficient Intersystem Crossing in Heavy-Atom-Free Perylenebisimide Derivatives. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 10162-10175	3.8	40
354	Zwitterionic [4]helicene: a water-soluble and reversible pH-triggered ECD/CPL chiroptical switch in the UV and red spectral regions. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 4590-4	3.9	49

353	Boron difluorides with formazanate ligands: redox-switchable fluorescent dyes with large stokes shifts. <i>Dalton Transactions</i> , 2016 , 45, 9477-84	4.3	50
352	Singlet oxygen generation properties of isometrically dibromated thienyl-containing aza-BODIPYs. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 32686-32690	3.6	17
351	Spectroscopic and electrochemical properties of ruthenium complexes with photochromic triarylaminedithienyletheneacetylide ligands. <i>Inorganic Chemistry Frontiers</i> , 2016 , 3, 1432-1443	6.8	7
350	Exploring the self-assembly and energy transfer of dynamic supramolecular iridium-porphyrin systems. <i>Dalton Transactions</i> , 2016 , 45, 17195-17205	4.3	21
349	N-Substituted Azacalixpyrins: Synthesis, Properties, and Self-Assembly. <i>Chemistry - A European Journal</i> , 2016 , 22, 17820-17832	4.8	15
348	Formazanate boron difluoride dyes: discrepancies between TD-DFT and wavefunction descriptions. <i>Journal of Molecular Modeling</i> , 2016 , 22, 263	2	7
347	Parameterization of the ReaxFF reactive force field for a proline-catalyzed aldol reaction. <i>Journal of Computational Chemistry</i> , 2016 , 37, 2564-72	3.5	6
346	Molecular-structure control of electron transfer dynamics of pushpull porphyrins as sensitizers for NiO based dye sensitized solar cells. <i>RSC Advances</i> , 2016 , 6, 77184-77194	3.7	25
345	Asymmetrical 1,3-Bis(heteroazolyl)benzene Platinum Complexes with Tunable Second-Order Non-Linear Optical Properties. <i>European Journal of Inorganic Chemistry</i> , 2016 , 2016, 4774-4782	2.3	8
344	Trans -disubstituted benzodiazaporphyrin: A promising hybrid dye between porphyrin and phthalocyanine for application in dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016 , 330, 186-194	4.7	5
343	Excited-State Vibrations of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 847-50	6.4	17
342	Taking up the cyanine challenge with quantum tools. <i>Accounts of Chemical Research</i> , 2015 , 48, 530-7	24.3	207
341	Direct and indirect effects of dispersion interactions on the electric properties of weakly bound complexes. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 3112-24	2.8	11
340	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	1.9	24
339	Synthesis of NIR naphthyl-containing aza-BODIPYs and measure of the singlet oxygen generation. <i>Tetrahedron</i> , 2015 , 71, 7676-7680	2.4	15
338	Benchmarking the Bethe-Salpeter Formalism on a Standard Organic Molecular Set. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 3290-304	6.4	145
337	How Adsorption Onto TiO ₂ Modifies the Properties of Multiswitchable DTE Systems: Theoretical Insights. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 16860-16869	3.8	6
336	Electroactive polymer-peptide conjugates for adhesive biointerfaces. <i>Biomaterials Science</i> , 2015 , 3, 1395-405	7.4	25

335	Toward an Enhancement of the Photoactivity of Multiphotochromic Dimers Using Plasmon Resonance: A Theoretical Study. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 3067-73	6.4	6
334	A curve-crossing model to rationalize and optimize diarylethene dyads. <i>Chemical Science</i> , 2015 , 6, 5695-5702	5.4	6
333	Multiphotochromic molecular systems. <i>Chemical Society Reviews</i> , 2015 , 44, 3719-59	58.5	248
332	Computational insights into the photodeactivation dynamics of phosphors for OLEDs: a perspective. <i>Dalton Transactions</i> , 2015 , 44, 8346-55	4.3	81
331	DNA spontaneous mutation and its role in the evolution of GC-content: assessing the impact of the genetic sequence. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 7754-60	3.6	28
330	Molecular Structure-Intersystem Crossing Relationship of Heavy-Atom-Free BODIPY Triplet Photosensitizers. <i>Journal of Organic Chemistry</i> , 2015 , 80, 5958-63	4.2	90
329	Sequential double second-order nonlinear optical switch by an acido-triggered photochromic cyclometallated platinum(II) complex. <i>Chemical Communications</i> , 2015 , 51, 7805-8	5.8	51
328	Controlling Triplet-Triplet Annihilation Upconversion by Tuning the PET in Aminomethyleneanthracene Derivatives. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 23801-23812	3.8	37
327	0-0 Energies Using Hybrid Schemes: Benchmarks of TD-DFT, CIS(D), ADC(2), CC2, and BSE/GW formalisms for 80 Real-Life Compounds. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5340-59	6.4	166
326	H-atom loss and migration in hydrogen-rich peptide cation radicals: The role of chemical environment. <i>International Journal of Mass Spectrometry</i> , 2015 , 390, 28-38	1.9	6
325	Electronic Excitations in Solution: The Interplay between State Specific Approaches and a Time-Dependent Density Functional Theory Description. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5782-90	6.4	95
324	Isoindigo derivatives for application in p-type dye sensitized solar cells. <i>RSC Advances</i> , 2015 , 5, 85530-85539	5.39	43
323	Photoactivatable platinum(II) compounds: in search of novel anticancer drugs. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	5
322	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, 5417-25	2.8	13
321	TD-DFT assessment of the excited state intramolecular proton transfer in hydroxyphenylbenzimidazole (HBI) dyes. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 2180-92	3.4	46
320	Effect of the cation model on the equilibrium structure of poly-L-glutamate in aqueous sodium chloride solution. <i>Journal of Chemical Physics</i> , 2015 , 143, 224505	3.9	6
319	Unexpected benzimidazole ring formation from a quinoneimide species in the presence of ammonium acetate as supporting electrolyte used in the coupling of electrochemistry with mass spectrometry. <i>Rapid Communications in Mass Spectrometry</i> , 2015 , 29, 456-60	2.2	3
318	P-Type Photochromism of New Helical Naphthopyrans: Synthesis and Photochemical, Photophysical and Theoretical Study. <i>ChemPhysChem</i> , 2015 , 16, 2447-58	3.2	23

317	Mutagenic effects induced by the attack of NO ₂ radical to the guanine-cytosine base pair. <i>Frontiers in Chemistry</i> , 2015 , 3, 13	5	5
316	Tuning the Direction of Intramolecular Charge Transfer and the Nature of the Fluorescent State in a T-Shaped Molecular Dyad. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 6283-95	2.8	26
315	Designing efficient photochromic dithienylethene dyads. <i>Chemical Science</i> , 2015 , 6, 3495-3504	9.4	22
314	N-confused porphyrin tautomers: lessons from density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 5290-7	3.6	12
313	A database of dispersion-induction DI, electrostatic ES, and hydrogen bonding H and H solvent parameters and some applications to the multiparameter correlation analysis of solvent effects. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 3174-84	3.4	49
312	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	3.8	13
311	Dissymmetric Molecular Tweezers in Host-Guest Complexes: Internal or External Complexation?. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 3771-3779	3.8	4
310	Synthesis and properties of push-pull porphyrins as sensitizers for NiO based dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 3908-3917	13	36
309	Time-Dependent Density Functional Theory: A Tool to Explore Excited States 2015 , 1-35		
308	Strategies for Designing Diarylethenes as Efficient Nonlinear Optical Switches. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 4334-4345	3.8	31
307	Heck-Matsuda Arylation of Olefins Through a Bimetallic Approach: Improved Procedures and Rationalization. <i>Advanced Synthesis and Catalysis</i> , 2014 , 356, 1065-1071	5.6	31
306	Optical signatures of boronic dyes: a TD-DFT analysis. <i>Theoretical Chemistry Accounts</i> , 2014 , 133, 1	1.9	10
305	Optical Properties of Diarylethenes with TD-DFT: 0-0 Energies, Fluorescence, Stokes Shifts, and Vibronic Shapes. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3944-57	6.4	22
304	Assessing the importance of proton transfer reactions in DNA. <i>Accounts of Chemical Research</i> , 2014 , 47, 2467-74	24.3	74
303	NIR Emission in Boron Difluoride Complexes of 2'-Hydroxychalcone Derivatives Containing an Acetonaphthone Ring. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 11906-11918	3.8	22
302	Solvent polarity scales: determination of new ET(30) values for 84 organic solvents. <i>Journal of Physical Organic Chemistry</i> , 2014 , 27, 512-518	2.1	105
301	Excited-State Geometries of Solvated Molecules: Going Beyond the Linear-Response Polarizable Continuum Model. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1848-51	6.4	26
300	Performance of an Optimally Tuned Range-Separated Hybrid Functional for 0-0 Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1677-85	6.4	113

299	How DNA is damaged by external electric fields: selective mutation vs. random degradation. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 8243-6	3.6	30
298	Modeling optical signatures and excited-state reactivities of substituted hydroxyphenylbenzoxazole (HBO) ESIPT dyes. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 1319-21	3.6	46
297	Dye chemistry with time-dependent density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 14334-56	3.6	225
296	Optical Signatures of OBO Fluorophores: A Theoretical Analysis. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 805-15	6.4	46
295	Full cLR-PCM calculations of the solvatochromic effects on emission energies. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 26024-9	3.6	11
294	The photochemistry of inverse dithienylethene switches understood. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 26762-8	3.6	10
293	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	3.7	27
292	Electronic Band Shapes Calculated with Optimally Tuned Range-Separated Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4599-608	6.4	36
291	The first structural and spectroscopic characterisation of a ring-opened form of a 2H-naphtho[1,2-b]pyran: a novel photomerocyanine. <i>Chemical Communications</i> , 2014 , 50, 7900-3	5.8	18
290	Designing Efficient Azobenzene and Azothiophene Nonlinear Optical Photochromes. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 28831-28841	3.8	34
289	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. <i>Journal of Materials Chemistry B</i> , 2014 , 2, 2838-2854	7.3	99
288	Competitive direct vs. indirect photochromism dynamics of constrained inverse dithienylethene molecules. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 22262-72	3.6	7
287	New insights into the by-product fatigue mechanism of the photo-induced ring-opening in diarylethenes. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 18463-71	3.6	29
286	Unveiling solvents effect on excited-state polarizabilities with the corrected linear-response model. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5652-6	2.8	11
285	Aggregation effect on the luminescence properties of phenylbipyridine Pt(II) acetylide complexes. A theoretical prediction with experimental evidence. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 6278-86	2.8	23
284	Exceptional stability of azacalixpyrin and its dianion. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 8883-8	2.8	13
283	Vibronic spectra of organic electronic chromophores. <i>RSC Advances</i> , 2014 , 4, 55466-55472	3.7	13
282	Solvent effects on cyanine derivatives: a PCM investigation. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5343-8	2.8	26

281	Benzothiophene or benzofuran bridges in diaryl ethenes: two-step access by pd-catalyzed C-H activation and theoretical/experimental studies on their photoreactivity. <i>Chemistry - A European Journal</i> , 2014 , 20, 10073-83	4.8	10
280	Benchmarking DFT and TD-DFT Functionals for the Ground and Excited States of Hydrogen-Rich Peptide Radicals. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3308-18	6.4	28
279	Fluorescence in rhoda- and iridacyclopentadienes neglecting the spin-orbit coupling of the heavy atom: the ligand dominates. <i>Inorganic Chemistry</i> , 2014 , 53, 7055-69	5.1	29
278	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, 4574-82	6.4	80
277	Solution- and Solid-State Luminescent Borate Complexes Based on a Substituted π -Conjugated 2-(6'-Hydroxy-5'-benzofuryl) Scaffold. <i>European Journal of Organic Chemistry</i> , 2014 , 2014, 7156-7164	3.2	19
276	Excited-states of BODIPY dyes: ultimate TD-DFT challenges?. <i>RSC Advances</i> , 2014 , 4, 49449-49456	3.7	52
275	Expanding the polymethine paradigm: evidence for the contribution of a bis-dipolar electronic structure. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 4038-47	2.8	67
274	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	2	11
273	Synthesis, photovoltaic performances and TD-DFT modeling of push-pull diacetylide platinum complexes in TiO ₂ based dye-sensitized solar cells. <i>Dalton Transactions</i> , 2014 , 43, 11233-42	4.3	40
272	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. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 4605-14	3.4	41
271	Solvatomagnetic Comparison Method: A Proper Quantification of Solvent Hydrogen-Bond Basicity. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 7594-7608	3.4	16
270	Combining the Bethe-Salpeter Formalism with Time-Dependent DFT Excited-State Forces to Describe Optical Signatures: NBO Fluoroborates as Working Examples. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4548-56	6.4	30
269	Long-Lived Charge Separated State in NiO-Based p-Type Dye-Sensitized Solar Cells with Simple Cyclometalated Iridium Complexes. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 2254-8	6.4	66
268	Benchmark Study on the Triplet Excited-State Geometries and Phosphorescence Energies of Heterocyclic Compounds: Comparison Between TD-PBE0 and SAC-CI. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3969-79	6.4	32
267	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, 12843-57	4.8	113
266	Theoretical insights on the antioxidant activity of edaravone free radical scavengers derivatives. <i>Chemical Physics Letters</i> , 2014 , 599, 73-79	2.5	3
265	Acetylacetone anchoring group for NiO-based dye-sensitized solar cell. <i>Dyes and Pigments</i> , 2014 , 105, 174-179	4.6	25
264	Quantum mechanical investigations on the role of neutral and negatively charged enamine intermediates in organocatalyzed reactions. <i>Chemical Physics</i> , 2014 , 434, 30-36	2.3	9

263	Second-order NLO switches from molecules to polymer films based on photochromic cyclometalated platinum(II) complexes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 5367-75	16.4	159
262	Fast and Accurate Electronic Excitations in Cyanines with the Many-Body Bethe-Salpeter Approach. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 1212-8	6.4	73
261	Perylene-derived triplet acceptors with optimized excited state energy levels for triplet-triplet annihilation assisted upconversion. <i>Journal of Organic Chemistry</i> , 2014 , 79, 2038-48	4.2	39
260	Absorption and fluorescence signatures of 1,2,3-triazole based regioisomers: challenging compounds for TD-DFT. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 9064-73	3.6	22
259	Fluorescent 2-(2'-hydroxybenzofuran)benzoxazole (HBBO) borate complexes: synthesis, optical properties, and theoretical calculations. <i>Tetrahedron Letters</i> , 2014 , 55, 4136-4140	2	6
258	A methodological evaluation of volumetric measurement techniques including three-dimensional imaging in breast surgery. <i>BioMed Research International</i> , 2014 , 2014, 573249	3	22
257	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	7.9	6
256	Extendable nickel complex tapes that reach NIR absorptions. <i>Chemical Communications</i> , 2014 , 50, 15140-38	5.8	19
255	Investigation of ESIPT in a panel of chromophores presenting N-H... intramolecular hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 25288-95	3.6	22
254	Molecular Engineering of Efficient Dyes for p-Type Semiconductor Sensitization. <i>Springer Series in Materials Science</i> , 2014 , 215-246	0.9	4
253	Copper-catalyzed free-radical C-H arylation of pyrroles. <i>Chemical Communications</i> , 2014 , 50, 5236-8	5.8	71
252	Methodological keys for accurate pKa* simulations. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 11875-82	3.6	19
251	Charge-transfer in quasilinear push-pull polyene chains. <i>Chemical Physics Letters</i> , 2013 , 581, 52-56	2.5	15
250	Fluorescent carboxylic and phosphonic acids: comparative photophysics from solution to organic nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 12748-56	3.6	13
249	Perfluorocyclohexene bridges in inverse DiArylEthenes: synthesis through Pd-catalysed C-H bond activation, experimental and theoretical studies on their photoreactivity. <i>Chemical Communications</i> , 2013 , 49, 7896-8	5.8	9
248	Diketopyrrolopyrrole derivatives for efficient NiO-based dye-sensitized solar cells. <i>Chemical Communications</i> , 2013 , 49, 8018-20	5.8	66
247	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, 4517-25	6.4	75
246	Voltammetry coupled to mass spectrometry in the presence of isotope ¹⁸ O labeled water for the prediction of oxidative transformation pathways of activated aromatic ethers: acebutolol. <i>Analytica Chimica Acta</i> , 2013 , 762, 39-46	6.6	16

245	The Remarkable Hyperchromicity of Ketohydrazone Dyes and Pigment Lakes Derived from 4-Morpholino-2-naphthol. <i>European Journal of Organic Chemistry</i> , 2013 , 2013, 8097-8107	3.2	9
244	Spectral Signatures of Perylene Diimide Derivatives: Insights From Theory. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 21682-21691	3.8	10
243	Palladium-catalyzed direct arylation of luminescent bis-cyclometalated iridium(III) complexes incorporating C ^N - or O [^] O-coordinating thiophene-based ligands: an efficient method for color tuning. <i>Inorganic Chemistry</i> , 2013 , 52, 12416-28	5.1	26
242	Pretreatment of the cockroach cercal afferent/giant interneuron synapses with nicotinoids and neonicotinoids differently affects acetylcholine and nicotine-induced ganglionic depolarizations. <i>Invertebrate Neuroscience</i> , 2013 , 13, 91-7	1.2	
241	TD-DFT study of the for coumarins. <i>Chemical Physics Letters</i> , 2013 , 583, 218-221	2.5	17
240	Spectral signatures of thieno[3,4-b]pyrazines: Theoretical interpretations and design of improved structures. <i>Dyes and Pigments</i> , 2013 , 99, 972-978	4.6	19
239	Design of hybrid conjugates based on chemical similarity. <i>RSC Advances</i> , 2013 , 3, 21069	3.7	7
238	Tuning the NLO properties of polymethineimine chains by chemical substitution. <i>Chemical Physics</i> , 2013 , 415, 196-206	2.3	8
237	Do inverse dithienylethenes behave as normal ones? A joint spectroscopic and theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 6226-34	3.6	28
236	Excited-State Geometries of Heteroaromatic Compounds: A Comparative TD-DFT and SAC-CI Study. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2368-79	6.4	54
235	Revisiting the optical signatures of BODIPY with ab initio tools. <i>Chemical Science</i> , 2013 , 4, 1950	9.4	124
234	The calculations of excited-state properties with Time-Dependent Density Functional Theory. <i>Chemical Society Reviews</i> , 2013 , 42, 845-56	58.5	1048
233	Electric-field induced mutation of DNA: a theoretical investigation of the GC base pair. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 4548-53	3.6	39
232	Interplay between solvent models and predicted optical spectra: A TD-DFT study of 7-OH-coumarin. <i>Chemical Physics Letters</i> , 2013 , 556, 122-126	2.5	15
231	The first hexadithienylethene-substituted tris(bipyridine)metal complexes as quadratic NLO photoswitches: combined experimental and DFT studies. <i>Chemistry - A European Journal</i> , 2013 , 19, 5845-9	4.8	35
230	Choosing a Functional for Computing Absorption and Fluorescence Band Shapes with TD-DFT. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 2749-60	6.4	196
229	A water soluble probe with near infrared two-photon absorption and polarity-induced fluorescence for cerebral vascular imaging. <i>Chemical Science</i> , 2013 , 4, 2833	9.4	61
228	The NBO pattern in luminescent chromophores: unravelling excited-state features using TD-DFT. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 7534-40	3.6	28

227	Full ring closing in a diarylethene hexamer: insights from theory. <i>Chemical Communications</i> , 2013 , 49, 4247-9	5.8	10
226	Optical signatures of Boron adducts of Oxasmaragdyrin: insights from theory. <i>Molecular Physics</i> , 2013 , 111, 1303-1307	1.7	
225	Azacalixphyrin: the hidden porphyrin cousin brought to light. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 6250-4	16.4	25
224	Inverse versus Normal Dithienylethenes: Computational Investigation of the Photocyclization Reaction. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 2190-2196	6.4	35
223	Electric field induced DNA damage: an open door for selective mutations. <i>Chemical Communications</i> , 2013 , 49, 7578-80	5.8	40
222	Boranil and Related NBO Dyes: Insights From Theory. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 3127-35	6.4	67
221	Acebutolol and alprenolol metabolism predictions: comparative study of electrochemical and cytochrome P450-catalyzed reactions using liquid chromatography coupled to high-resolution mass spectrometry. <i>Analytical and Bioanalytical Chemistry</i> , 2013 , 405, 6077-85	4.4	24
220	Ruthenium Sensitizer Functionalized by Acetylacetone Anchoring Groups for Dye-Sensitized Solar Cells. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 8652-8660	3.8	30
219	TD-DFT benchmarks: A review. <i>International Journal of Quantum Chemistry</i> , 2013 , 113, 2019-2039	2.1	715
218	Diketopyrrolopyrrole-zinc porphyrin, a tuned panchromatic association for dye-sensitized solar cells. <i>Journal of Materials Chemistry A</i> , 2013 , 1, 7572	13	41
217	New insights on the molecular recognition of imidacloprid with Aplysia californica AChBP: a computational study. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 3944-53	3.4	18
216	Stereoselective Synthesis of a Bicyclic Norsesquiterpene Backbone [A Possible Route to Nardosinane Derivatives. <i>European Journal of Organic Chemistry</i> , 2013 , 2013, 7083-7094	3.2	3
215	Impact of DNA environment on the intrastrand cross-link lesions: hydrogen atom release as the last step of formation of G[8-5m]T. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 16397-404	3.4	5
214	Probing the performances of HISS functionals for the description of excited states of molecular systems. <i>Theoretical Chemistry Accounts</i> , 2013 , 132, 1	1.9	1
213	Azacalixphyrin: The Hidden Porphyrin Cousin Brought to Light. <i>Angewandte Chemie</i> , 2013 , 125, 6370-6374	346	7
212	Impact of DFT functionals on the predicted magnesium-DNA interaction: an ONIOM study. <i>Highlights in Theoretical Chemistry</i> , 2013 , 271-279		
211	A theoretical spectroscopy investigation of oxosumanenes. <i>Chemical Physics Letters</i> , 2012 , 519-520, 49-52	535	13
210	A DFT-D evaluation of the complexation of a molecular tweezer with small aromatic molecules. <i>Chemical Physics Letters</i> , 2012 , 522, 11-16	2.5	16

209	Excited-state nature in benzodifuranone dyes: Insights from ab initio simulations. <i>Dyes and Pigments</i> , 2012 , 92, 1144-1152	4.6	12
208	TD-DFT Assessment of Functionals for Optical 0-0 Transitions in Solvated Dyes. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2359-72	6.4	342
207	3-fluoro- and 3,3-difluoro-3,4-dideoxy-KRN7000 analogues as new potent immunostimulator agents: total synthesis and biological evaluation in human invariant natural killer T cells and mice. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 1227-41	8.3	20
206	Verdict: Time-Dependent Density Functional Theory "Not Guilty" of Large Errors for Cyanines. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1255-9	6.4	110
205	Intermolecular interactions in electron transfer through stretched helical peptides. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 10332-44	3.6	22
204	Aza-boron-dipyrromethene dyes: TD-DFT benchmarks, spectral analysis and design of original near-IR structures. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 157-64	3.6	92
203	Molecular Tweezers in Host-Guest Complexes: A Computational Study through a DFT-D Approach. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 23067-23074	3.8	7
202	Superior performance of range-separated hybrid functionals for describing $\pi \leftarrow \pi^*$ UV-vis signatures of three-electron two-center anions. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 3237-46	2.8	9
201	Impact of Vibronic Couplings on Perceived Colors: Two Anthraquinones as a Working Example. <i>Journal of Physical Chemistry Letters</i> , 2012 , 3, 468-71	6.4	69
200	Through-Space Charge Transfer in Rod-Like Molecules: Lessons from Theory. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 11946-11955	3.8	193
199	Long-range electron transfer in zinc-phthalocyanine-oligo(phenylene-ethynylene)-based donor-bridge-acceptor dyads. <i>Inorganic Chemistry</i> , 2012 , 51, 11500-12	5.1	35
198	On the photochromic properties of dithienylethenes grafted on gold clusters. <i>Computational and Theoretical Chemistry</i> , 2012 , 990, 167-176	2	10
197	A DFT study of magnetic interactions in photoswitchable systems. <i>Chemical Physics Letters</i> , 2012 , 542, 13-18	2.5	11
196	Ab initio quantum chemical and ReaxFF-based study of the intramolecular iminium-enamine conversion in a proline-catalyzed reaction. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	7
195	A qualitative failure of B3LYP for textbook organic reactions. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 7170-5	3.6	52
194	Photoswitching of the second-order nonlinearity of a tetrahedral octupolar multi DTE-based copper(I) complex. <i>Chemical Communications</i> , 2012 , 48, 10395-7	5.8	51
193	Interplay between hydroxyl radical attack and H-bond stability in guanine-cytosine. <i>RSC Advances</i> , 2012 , 2, 11867	3.7	15
192	Cisplatin cytotoxicity: a theoretical study of induced mutations. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 12457-64	3.6	33

191	On the Computation of Adiabatic Energies in Aza-Boron-Dipyrromethene Dyes. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 3303-13	6.4	91
190	Ab initio modeling of optical spectra in pH-sensitive diarylethenes. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 1122-1133	2.1	2
189	Spectroscopic properties of mono- and bis-azopyrroles. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 2043-2050	2.1	1
188	Basis set and functional effects on excited-state properties: Three bicyclic chromogens as working examples. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 2135-2141	2.1	35
187	Computing redox potentials for dyes used in p-type dye-sensitized solar cells. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 3763-3768	2.1	4
186	Single molecule multiphotochromism with diarylethenes. <i>Accounts of Chemical Research</i> , 2012 , 45, 1173-1183	2.3	147
185	What is the "best" atomic charge model to describe through-space charge-transfer excitations?. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 5383-8	3.6	242
184	Diketopyrrolopyrrole-porphyrin conjugates as broadly absorbing sensitizers for dye-sensitized solar cells. <i>ChemSusChem</i> , 2012 , 5, 1568-77	8.3	45
183	Impact of DFT functionals on the predicted magnesium-DNA interaction: an ONIOM study. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	23
182	TD-DFT Vibronic Couplings in Anthraquinones: From Basis Set and Functional Benchmarks to Applications for Industrial Dyes. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 1882-92	6.4	96
181	New cyanine dyes or not? Theoretical insights for model chains. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 2442-5	2.8	8
180	Multiswitchable Acidichromic and Photochromic Bisdiarylethene. An Experimental and Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 23096-23106	3.8	23
179	Diarylethene-dihydroazulene multimode photochrome: a theoretical spectroscopic investigation. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 13791-9	3.6	17
178	Comparison of microhydration methods: protonated glycine as a working example. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 3604-13	3.4	16
177	Combined effect of stacking and solvation on the spontaneous mutation in DNA. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 14584-9	3.6	49
176	A compact diketopyrrolopyrrole dye as efficient sensitizer in titanium dioxide dye-sensitized solar cells. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011 , 226, 9-15	4.7	58
175	New insights on the molecular features and electrophysiological properties of dinotefuran, imidacloprid and acetamiprid neonicotinoid insecticides. <i>Bioorganic and Medicinal Chemistry</i> , 2011 , 19, 7623-34	3.4	27
174	Key building block of photoresponsive biomimetic systems. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 1232-42	3.4	6

173	Excited-state calculations with TD-DFT: from benchmarks to simulations in complex environments. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 16987-98	3.6	258
172	Assessment of the B97 family for excited-state calculations. <i>Theoretical Chemistry Accounts</i> , 2011 , 128, 127-136	1.9	115
171	Performances of recently-proposed functionals for describing disulfide radical anions and similar systems. <i>Chemical Physics Letters</i> , 2011 , 501, 245-251	2.5	18
170	Structural study of piracetam polymorphs and cocrystals: crystallography redetermination and quantum mechanics calculations. <i>Acta Crystallographica Section B: Structural Science</i> , 2011 , 67, 499-507		5
169	Absorption spectra of azobenzenes simulated with time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 4224-4240	2.1	32
168	Influence of Mg(2+) on the guanine-cytosine tautomeric equilibrium: simulations of the induced intermolecular proton transfer. <i>ChemPhysChem</i> , 2011 , 12, 2615-23	3.2	18
167	Bond Length Alternation of Conjugated Oligomers: Wave Function and DFT Benchmarks. <i>Journal of Chemical Theory and Computation</i> , 2011 , 7, 369-76	6.4	119
166	Ground Electronic State of Peptide Cation Radicals: A Delocalized Unpaired Electron?. <i>Journal of Physical Chemistry Letters</i> , 2011 , 2, 1426-1431	6.4	16
165	Interplay Between Electronic and Steric Effects in Multiphotochromic Diarylethenes. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 9193-9203	3.8	48
164	Photochromic properties of a dithienylethene-indolinooxazolidine switch: A theoretical investigation. <i>Computational and Theoretical Chemistry</i> , 2011 , 963, 63-70	2	7
163	A theoretical spectroscopy investigation of bifunctional platinum-bridged diarylethenes. <i>Chemical Physics Letters</i> , 2011 , 502, 77-81	2.5	25
162	Nature of the excited states in large photochromic dimers: A TD-DFT examination. <i>Chemical Physics Letters</i> , 2011 , 509, 129-133	2.5	10
161	An ab initio simulation of a dithienylethene/phenoxy naphthacenequinone photochromic hybrid. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011 , 218, 33-40	4.7	8
160	Ruthenium polypyridine complexes as sensitizers in NiO based p-type dye-sensitized solar cells: Effects of the anchoring groups. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2011 , 219, 235-242	4.7	107
159	Shoulder function after latissimus dorsi transfer in breast reconstruction. <i>Clinical Physiology and Functional Imaging</i> , 2010 , 30, 406-12	2.4	34
158	Communication: Bond length alternation of conjugated oligomers: Another step on the fifth rung of Perdew's ladder of functional. <i>Journal of Chemical Physics</i> , 2010 , 133, 151104	3.9	19
157	Doubly Closing or Not? Theoretical Analysis for Coupled Photochromes. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 9489-9497	3.8	48
156	On the TD-DFT accuracy in determining single and double bonds in excited-state structures of organic molecules. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 13402-10	2.8	69

155	Assessment of Functionals for TD-DFT Calculations of Singlet-Triplet Transitions. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1532-7	6.4	173
154	Theoretical study of the tautomerism in the one-electron oxidized guanine-cytosine base pair. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 13439-45	3.4	27
153	On the Performances of the M06 Family of Density Functionals for Electronic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2071-85	6.4	335
152	On the absorption spectra of recently synthesized carbonyl dyes: TD-DFT insights. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 9579-82	2.8	17
151	Ab Initio Investigation of the Electronic Properties of Coupled Dithienylethenes. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 434-438	6.4	27
150	Simulation of the Properties of a Photochromic Triad. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 2104-2108	2.5	25
149	Planar vs. twisted intramolecular charge transfer mechanism in Nile Red: new hints from theory. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 8016-23	3.6	113
148	Hybrid dithienylethene-naphthopyran multi-addressable photochromes: an ab initio analysis. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 13144-52	3.6	23
147	TD-DFT simulations of the electronic properties of star-shaped photochromes. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 7994-8000	3.6	24
146	Substitution effects on the optical spectra of diarylethene photochroms: ab initio insights. <i>Molecular Simulation</i> , 2010 , 36, 74-78	2	7
145	Design of new triphenylamine-sensitized solar cells: a theoretical approach. <i>Environmental Science & Technology</i> , 2010 , 44, 5666-71	10.3	58
144	Towards new efficient dye-sensitized solar cells. <i>Energy and Environmental Science</i> , 2010 , 3, 891	35.4	145
143	Improvement of the efficiency of thiophene-bridged compounds for dye-sensitized solar cells. <i>Chemical Physics</i> , 2010 , 376, 56-68	2.3	100
142	Electrochemical synthesis and characterisation of alternating tripyridyl-dipyrrole molecular strands with multiple nitrogen-based donor-acceptor binding sites. <i>Chemistry - A European Journal</i> , 2010 , 16, 11876-89	4.8	10
141	Excited-state properties from ground-state DFT descriptors: A QSPR approach for dyes. <i>Journal of Molecular Graphics and Modelling</i> , 2010 , 28, 465-71	2.8	22
140	Absorption and emission spectra of 1,8-naphthalimide fluorophores: A PCM-TD-DFT investigation. <i>Chemical Physics</i> , 2010 , 372, 61-66	2.3	53
139	Photochromic molecular wires: Insights from theory. <i>Chemical Physics Letters</i> , 2010 , 488, 193-197	2.5	31
138	Visible spectrum of naphthazarin investigated through Time-Dependent Density Functional Theory. <i>Chemical Physics Letters</i> , 2010 , 493, 67-71	2.5	19

137	A theoretical investigation of microhydration of amino acids. <i>Journal of Cheminformatics</i> , 2010 , 2,	8.6	78
136	Absorption spectra of recently synthesised organic dyes: A TD-DFT study. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, 2121-2129	2.1	23
135	A UV/VIS spectra investigation of pH-sensitive dyes using time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, 2147-2154	2.1	13
134	An ab initio simulation of the UV/visible spectra of N-benzylideneaniline dyes. <i>International Journal of Quantum Chemistry</i> , 2009 , 109, 3506-3515	2.1	10
133	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		29
132	Enhancement of the second-order NLO responses of boron–nitrogen oligomers by copolymerization with polyyne. <i>Computational and Theoretical Chemistry</i> , 2009 , 901, 194-201		4
131	TD-DFT benchmark for indigo–dyes. <i>Computational and Theoretical Chemistry</i> , 2009 , 914, 100-105		32
130	Ab initio investigation of the hydration of deprotonated amino acids. <i>Journal of the American Society for Mass Spectrometry</i> , 2009 , 20, 632-8	3.5	19
129	Electronic transitions of neutral and anionic quinolinone HIV-1 integrase inhibitor: Joint theory/experiment investigation. <i>Chemical Physics Letters</i> , 2009 , 478, 243-248	2.5	2
128	Double proton transfer mechanism in the adenine–uracil base pair and spontaneous mutation in RNA duplex. <i>Chemical Physics Letters</i> , 2009 , 484, 64-68	2.5	30
127	Quantitative evaluation of solvation and packing effects on the visible absorption of anthraquinone derivatives. <i>Dyes and Pigments</i> , 2009 , 81, 97-102	4.6	2
126	Extensive TD-DFT Benchmark: Singlet-Excited States of Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 2420-35	6.4	799
125	Accurate simulation of optical properties in dyes. <i>Accounts of Chemical Research</i> , 2009 , 42, 326-34	24.3	404
124	Enhanced Efficiency of Organic Dye-Sensitized Solar Cells: Triphenylamine Derivatives. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 16821-16833	3.8	287
123	Intermolecular proton transfer in microhydrated guanine-cytosine base pairs: a new mechanism for spontaneous mutation in DNA. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 10549-56	2.8	66
122	Effects of hydration on the proton transfer mechanism in the adenine-thymine base pair. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 7892-8	2.8	63
121	Spectral properties of spirooxazine photochromes: TD-DFT insights. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 13004-12	2.8	28
120	Spectral properties of self-assembled squaraine-tetralactam: a theoretical assessment. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 1258-62	3.6	57

119	Fast and reliable theoretical determination of pKa* for photoacids. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 794-6	2.8	32
118	Modeling the microhydration of protonated alanine. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 9896-9023	3.4	21
117	Microhydration of protonated glycine: an ab initio family tree. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 2430-8	3.4	40
116	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, 637-45	6.4	22
115	Stepwise hydration of protonated proline. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 7702-5	3.4	14
114	Assessment of the Accuracy of TD-DFT Absorption Spectra: Substituted Benzenes. <i>Collection of Czechoslovak Chemical Communications</i> , 2008 , 73, 898-908		4
113	A quantitative prediction of the electronic spectra of thiocarbonyl chromophores: TD-DFT versus SAC-CI. <i>Theoretical Chemistry Accounts</i> , 2008 , 119, 463-468	1.9	11
112	On the TD-DFT UV/vis spectra accuracy: the azoalkanes. <i>Theoretical Chemistry Accounts</i> , 2008 , 120, 405-419	4.0	50
111	Revisiting the relationship between the bond length alternation and the first hyperpolarizability with range-separated hybrid functionals. <i>Journal of Computational Chemistry</i> , 2008 , 29, 921-5	3.5	27
110	A theoretical study of the perfluoro-diarylethenes electronic spectra. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2008 , 199, 211-223	4.7	31
109	Delocalisation in conjugated triazene chromophores: Insights from theory. <i>Chemical Physics Letters</i> , 2008 , 451, 37-42	2.5	29
108	Revisiting the nonlinear optical properties of polybutatriene and polydiacetylene with density functional theory. <i>Chemical Physics Letters</i> , 2008 , 456, 101-104	2.5	22
107	Modelling the acidochromism of pyridylazulenes. <i>Chemical Physics Letters</i> , 2008 , 457, 91-95	2.5	6
106	Extensive TD-DFT investigation of the first electronic transition in substituted azobenzenes. <i>Chemical Physics Letters</i> , 2008 , 465, 226-229	2.5	88
105	Modelling the UV/visible spectrum of tetrakis(phenylethynyl)benzene. <i>Computational and Theoretical Chemistry</i> , 2008 , 863, 123-127		7
104	Fluorescein isothiocyanate: Molecular characterization by theoretical calculations. <i>Chemical Physics</i> , 2008 , 354, 155-161	2.3	17
103	TD-DFT Performance for the Visible Absorption Spectra of Organic Dyes: Conventional versus Long-Range Hybrids. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 123-35	6.4	681
102	Comparison of theoretical approaches for predicting the UV/Vis spectra of anthraquinones. <i>Molecular Physics</i> , 2007 , 105, 325-331	1.7	35

101	TD-DFT investigation of diarylethene dyes with cyclopentene, dihydrothiophene, and dihydropyrrole bridges. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 5528-35	2.8	32
100	On the basis set convergence of TD-DFT oscillator strengths: Dinitrophenylhydrazones as a case study. <i>Computational and Theoretical Chemistry</i> , 2007 , 804, 31-34		17
99	A TD-DFT investigation of UV spectra of pyranodic dyes: A NCM vs PCM comparison. <i>Computational and Theoretical Chemistry</i> , 2007 , 808, 85-91		11
98	NLO responses of small polymethineimine oligomers: A CCSD(T) study. <i>Computational and Theoretical Chemistry</i> , 2007 , 821, 160-165		6
97	A generalized Romberg differentiation procedure for calculation of hyperpolarizabilities. <i>Computational and Theoretical Chemistry</i> , 2007 , 847, 39-46		54
96	On the geometries and UV/Vis spectra of substituted trans-azobenzenes. <i>Chemical Physics Letters</i> , 2007 , 435, 257-262	2.5	55
95	Hemi-indigo photochroms: A theoretical investigation. <i>Chemical Physics Letters</i> , 2007 , 436, 84-88	2.5	9
94	The geometries, absorption and fluorescence wavelengths of solvated fluorescent coumarins: A CIS and TD-DFT comparative study. <i>Chemical Physics Letters</i> , 2007 , 438, 208-212	2.5	60
93	A theoretical investigation of the hydrated glycine cation energetics and structures. <i>Chemical Physics Letters</i> , 2007 , 445, 57-61	2.5	27
92	Fluorescence of 1,8-naphthalimide: A PCM-TD-DFT investigation. <i>Chemical Physics Letters</i> , 2007 , 448, 3-6	2.5	40
91	Towards the understanding of the absorption spectra of NAD(P)H/NAD(P) ⁺ as a common indicator of dehydrogenase enzymatic activity. <i>Chemical Physics Letters</i> , 2007 , 450, 119-122	2.5	34
90	Évaluation ab initio de la couleur de diaryléthènes présentant un pont malimide. <i>Comptes Rendus Chimie</i> , 2007 , 10, 1227-1233	2.7	3
89	A TD-DFT investigation of the visible spectra of fluoro-anthraquinones. <i>Dyes and Pigments</i> , 2007 , 72, 185-191	4.6	9
88	Towards the understanding of the chromatic behaviour of triphenylmethane derivatives. <i>Chemical Physics</i> , 2007 , 335, 177-186	2.3	24
87	An ab initio scheme for quantitative predictions of the visible spectra of diarylethenes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007 , 187, 40-44	4.7	26
86	Ab initio tools for the accurate prediction of the visible spectra of anthraquinones. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007 , 67, 334-41	4.4	42
85	Ab initio studies of the lambda(max) of naphthoquinones dyes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007 , 68, 1326-33	4.4	26
84	DFT and TD-DFT investigation of IR and UV spectra of solvated molecules: Comparison of two SCRF continuum models. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 574-585	2.1	33

83	Ab initio investigation of the solvent and electron correlation effects on the geometries and first hyperpolarizabilities of pushpull oligomers. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 2066-2074	2.1	7
82	Tayloring standard TDDFT approaches for computing UV/Vis transitions in thiocarbonyl chromophores. <i>International Journal of Quantum Chemistry</i> , 2007 , 108, 762-773	2.1	2
81	Comparison of theoretical approaches for computing the bond length alternation of polymethineimine. <i>Chemical Physics</i> , 2007 , 332, 79-85	2.3	19
80	First hyperpolarizability of polymethineimine with long-range corrected functionals. <i>Journal of Chemical Physics</i> , 2007 , 126, 191108	3.9	151
79	Photochromic properties of dithienylazoles and other conjugated diarylethenes. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007 , 192, 211-219	4.7	51
78	Assessment of long-range corrected functionals performance for n->pi* transitions in organic dyes. <i>Journal of Chemical Physics</i> , 2007 , 127, 094102	3.9	112
77	Assessment of the efficiency of long-range corrected functionals for some properties of large compounds. <i>Journal of Chemical Physics</i> , 2007 , 126, 144105	3.9	264
76	Time-dependent density functional theory determination of the absorption spectra of naphthoquinones. <i>Chemical Physics</i> , 2006 , 328, 324-332	2.3	29
75	Excitation spectra of nitro-diphenylaniline: accurate time-dependent density functional theory predictions for charge-transfer dyes. <i>Journal of Chemical Physics</i> , 2006 , 124, 204321	3.9	47
74	TD-DFT investigation of the UV spectra of pyranone derivatives. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 8144-50	2.8	69
73	Substitution and chemical environment effects on the absorption spectrum of indigo. <i>Journal of Chemical Physics</i> , 2006 , 124, 74104	3.9	100
72	Time-dependent density functional theory investigation of the absorption, fluorescence, and phosphorescence spectra of solvated coumarins. <i>Journal of Chemical Physics</i> , 2006 , 125, 164324	3.9	104
71	Toward a Theoretical Quantitative Estimation of the λ_{max} of Anthraquinones-Based Dyes. <i>Journal of Chemical Theory and Computation</i> , 2006 , 2, 434-40	6.4	86
70	Assessment of several hybrid DFT functionals for the evaluation of bond length alternation of increasingly long oligomers. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 5952-9	2.8	71
69	Ab initio investigation of the n->pi* transitions in thiocarbonyl dyes. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 9145-52	2.8	59
68	An ab initio study of the absorption spectra of indirubin, isoindigo, and related derivatives. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 5629-35	2.8	72
67	Calculation of Hartree-Fock Energy Derivatives in Polymers. <i>Computer Aided Chemical Engineering</i> , 2006 , 3-30	0.6	
66	2,6-Dihydroxyanthraquinone: an isomer of the well known alizarin dye. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2006 , 62, o4503-o4505		1

65	Assessment of PBE0 for evaluating the absorption spectra of carbonyl molecules. <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 1853-1859	2.1	18
64	Is solvated trans-azobenzene twisted or planar?. <i>Chemical Physics Letters</i> , 2006 , 417, 190-195	2.5	52
63	The n- π^* transition in nitroso compounds: A TD-DFT study. <i>Chemical Physics Letters</i> , 2006 , 420, 529-533	2.5	31
62	Absorption and emission spectra in gas-phase and solution using TD-DFT: Formaldehyde and benzene as case studies. <i>Chemical Physics Letters</i> , 2006 , 421, 272-276	2.5	66
61	Ab initio calculations of the colour of closed-ring diarylethenes: TD-DFT estimates for molecular switches. <i>Chemical Physics Letters</i> , 2006 , 429, 147-152	2.5	99
60	Thioindigo dyes: highly accurate visible spectra with TD-DFT. <i>Journal of the American Chemical Society</i> , 2006 , 128, 2072-83	16.4	220
59	Linear and Nonlinear Optics Properties of Polyphosphazene/Polynitrile Alternating Copolymers. <i>Journal of Chemical Theory and Computation</i> , 2005 , 1, 307-14	6.4	11
58	Second-order Møller-Plesset evaluation of the bond length alternation of several series of linear oligomers. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 5734-41	2.8	28
57	Ab initio assessment of the first hyperpolarizability of saturated and unsaturated polyaminoborane/polyphosphinoborane copolymers. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 6380-6	2.8	12
56	Theoretical investigation of the absorption spectrum of thioindigo dyes. <i>Computational and Theoretical Chemistry</i> , 2005 , 731, 67-72		41
55	Assessment of recently developed density functional approaches for the evaluation of the bond length alternation in polyacetylene. <i>Chemical Physics Letters</i> , 2005 , 405, 376-381	2.5	47
54	Substitution effects on the visible spectra of 1,4-diNHP-9,10-anthraquinones. <i>Chemical Physics Letters</i> , 2005 , 405, 429-433	2.5	51
53	Ab initio studies of the static electronic first hyperpolarizability of polysilanenitrile. <i>Chemical Physics Letters</i> , 2005 , 408, 226-231	2.5	6
52	A TD-DFT study of the absorption spectra of fast dye salts. <i>Chemical Physics Letters</i> , 2005 , 410, 254-259	2.5	105
51	Theoretical investigations of the UV spectra of coumarin derivatives. <i>Chemical Physics Letters</i> , 2005 , 415, 20-24	2.5	48
50	Ab initio prediction of extremely large first hyperpolarizability of polyphosphaacetylene and polyphosphasilyne. <i>Chemical Physics Letters</i> , 2005 , 416, 277-281	2.5	12
49	Longitudinal NLO properties of C ₂ H ₂ , HCCF, and C ₂ F ₂ : Electron correlation and vibration effects. <i>International Journal of Quantum Chemistry</i> , 2005 , 102, 209-223	2.1	7
48	Linear phosphorusBoron chains: model system with huge electronic first hyperpolarizability. <i>International Journal of Quantum Chemistry</i> , 2005 , 103, 226-234	2.1	14

47	NLO response of polymethineimine and polymethineimine/polyacetylene conformers: Assessment of electron correlation effects. <i>International Journal of Quantum Chemistry</i> , 2005 , 105, 553-563	2.1	11
46	Second-order nonlinear optical coefficient of polyphosphazene-based materials: a theoretical study. <i>Journal of Chemical Physics</i> , 2004 , 120, 9401-9	3.9	34
45	Theoretical study of the longitudinal first hyperpolarizability of polysilaacetylene. <i>Journal of Chemical Physics</i> , 2004 , 120, 10317-27	3.9	30
44	Theoretical investigation of substituted anthraquinone dyes. <i>Journal of Chemical Physics</i> , 2004 , 121, 1736-43	3.9	102
43	Solvent effects on the geometry and first hyperpolarizability of polymethineimine. <i>Computational and Theoretical Chemistry</i> , 2004 , 710, 13-17		7
42	Structures and Properties of Polyphosphinoborane: an Oligomeric Theoretical Study. <i>Macromolecules</i> , 2004 , 37, 1009-1015	5.5	28
41	Effects of Chain Substitution on the Structures and Properties of Polyphosphinoborane. <i>Macromolecules</i> , 2004 , 37, 5040-5046	5.5	3
40	Geometry, dipole moment, polarizability and first hyperpolarizability of polymethineimine: an assessment of electron correlation contributions. <i>Journal of Chemical Physics</i> , 2004 , 121, 4389-96	3.9	68
39	First Hyperpolarizability of Polyaminoborane and Polyiminoborane Oligomers. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 9260-9266	2.8	27
38	Theoretical Study of Dehydrogenation Effects upon the First Hyperpolarizability of Polyphosphinoborane. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 500-506	2.8	18
37	Ab Initio Investigation of the Structures and Properties of Polyaminoborane. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 9616-9624	2.8	19
36	Pseudo linear-dependence and long-range interaction effects on the polarizability and hyperpolarizabilities of stereoregular polymers. <i>Chemical Physics Letters</i> , 2003 , 373, 539-549	2.5	10
35	Copolymerization Effects upon the Second-Order NLO Responses of Polyacetylene/Polymethineimine. <i>Macromolecules</i> , 2003 , 36, 3980-3985	5.5	16
34	Analytic ab initio determination of the elastic modulus in stereoregular polymers: Analytical integral derivatives, long-range effects, implementation, and examples. <i>Journal of Chemical Physics</i> , 2003 , 118, 373-388	3.9	12
33	Analytic ab initio determination of the IR intensities in stereoregular polymers. <i>Journal of Chemical Physics</i> , 2003 , 118, 3956-3965	3.9	14
32	Integral algorithm and density matrix integration scheme for ab initio band structure calculations on polymeric systems. <i>Journal of Computational Chemistry</i> , 2002 , 23, 1430-44	3.5	10
31	Convergence of exchange lattice summations in direct-space polymer calculations. <i>International Journal of Quantum Chemistry</i> , 2002 , 89, 452-463	2.1	9
30	First hyperpolarizability of H(BN)NH oligomers: analysis of geometry, asymmetry and delocalization effects. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 432-440	3.6	30

29	Intramolecular charge transfer and first-order hyperpolarizability of planar and twisted sesquifulvalenes. <i>Physical Chemistry Chemical Physics</i> , 2002 , 4, 5566-5571	3.6	26
28	Long-range effects in optimizing the geometry of stereoregular polymersIV: Explicit determination of the helical angle. <i>International Journal of Quantum Chemistry</i> , 2001 , 85, 539-545	2.1	6
27	Analysis of the sign reversal of the second-order molecular polarizability in polymethineimine chains. <i>Journal of Chemical Physics</i> , 2001 , 115, 6766-6774	3.9	21
26	MP2 correlation effects upon the electronic and vibrational properties of polyyne. <i>Journal of Chemical Physics</i> , 2001 , 114, 5917-5922	3.9	25
25	Second-Order ab Initio MøllerPlesset Study of Optimum Chain Length for Total (Electronic Plus Vibrational) $\beta(0,0)$ of a Prototype Push-Pull Polyene. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 9748-9755	2.8	48
24	Comment on "Calculation of ab initio dynamic hyperpolarizabilities of polymers"[J. Chem. Phys. 110, 2717 (1999)]. <i>Journal of Chemical Physics</i> , 2000 , 112, 1616-1617	3.9	12
23	Optimizing the geometry of stereoregular polymers. III. Polyyne and the basis set quasi-linear dependence. <i>International Journal of Quantum Chemistry</i> , 2000 , 80, 863-870	2.1	26
22	Correlated frequency-dependent electronic first hyperpolarizability of small pushPull conjugated chains. <i>Chemical Physics Letters</i> , 2000 , 319, 327-334	2.5	74
21	Electronic and vibrational first hyperpolarizabilities of polymethineimine oligomers. <i>Computational and Theoretical Chemistry</i> , 2000 , 529, 65-71		14
20	Structure and nonlinear electrical properties of squaric acid derivatives: a theoretical study of the conformation and deprotonation effects. <i>Computational and Theoretical Chemistry</i> , 2000 , 528, 151-159		23
19	Assessment of Conventional Density Functional Schemes for Computing the Dipole Moment and (Hyper)polarizabilities of PushPull π -Conjugated Systems <i>Journal of Physical Chemistry A</i> , 2000 , 104, 4755-4763	2.8	473
18	Long-range effects in optimizing the geometry of stereoregular polymers. II. Hydrogen fluoride chains as a working example. <i>Journal of Chemical Physics</i> , 1999 , 111, 5324-5330	3.9	20
17	Long-range effects in optimizing the geometry of stereoregular polymers. I. Formalism. <i>Journal of Chemical Physics</i> , 1999 , 111, 5306-5323	3.9	31
16	Asymmetric unit cell polymers with large first hyperpolarizabilities. <i>Synthetic Metals</i> , 1999 , 101, 490-4913.6		2
15	MøllerPlesset evaluation of the static first hyperpolarizability of polymethineimine. <i>Chemical Physics Letters</i> , 1998 , 284, 24-30	2.5	49
14	Static first hyperpolarizability of small all-trans polymethineimine oligomers. Basis set and electron correlation effects. <i>Computational and Theoretical Chemistry</i> , 1998 , 425, 69-79		20
13	Ab initio determination of the vibrational and electronic first hyperpolarizabilities of reference compounds for non-linear optical (NLO) applications 3-Methyl 4-nitropyridine 1-oxide (POM) and N-(4-nitrophenyl)-(L)-prolinol (NPP). <i>Journal of the Chemical Society, Faraday Transactions</i> , 1998 , 94, 1547-1553		25
12	Ab initio band structure of polymethineimine isomers. <i>Journal of Chemical Physics</i> , 1998 , 108, 1023-10303.9		17

11	Ab initio static polarizability and first hyperpolarizability of model polymethineimine chains. II. Effects of conformation and of substitution by donor/acceptor end groups. <i>Journal of Chemical Physics</i> , 1997 , 107, 5076-5087	3.9	63
10	Electron nuclear dynamics of proton collisions with methane at 30 eV. <i>Journal of Chemical Physics</i> , 1997 , 107, 6146-6155	3.9	51
9	Ab Initio Coupled Hartree-Fock Investigation of the Static First Hyperpolarizability of Model all-trans-Polymethineimine Oligomers of Increasing Size. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 3158-3165	2.8	81
8	Electron correlation effects upon the static (hyper)polarizabilities of push-pull conjugated polyenes and polyynes 1997 , 65, 679-688		52
7	Electronic first hyperpolarizability of polymethineimine chains with donor and acceptor groups. <i>Synthetic Metals</i> , 1996 , 80, 205-210	3.6	20
6	Exploratory Pariser-Parr-Pople investigation of the static first hyperpolarizability of polymethineimine chains. <i>Chemical Physics</i> , 1996 , 213, 217-228	2.3	12
5	Molecular orbital expressions for approximate uncoupled Hartree-Fock second hyperpolarizabilities. A Pariser-Parr-Pople assessment for model polyacetylene chains. <i>Chemical Physics</i> , 1995 , 197, 107-127	2.3	10
4	Model calculations of the first hyperpolarisability per unit cell of finite and infinite polymethineimine chains 1995 ,		19
3	Coordination-enhanced photochromism in dysprosium dinuclear complexes with photomodulated single-molecule magnet behavior	4, 2	
2	BN-Substituted coronene diimide donor-acceptor-donor triads: photophysical, (spectro)-electrochemical studies and Lewis behavior. <i>Journal of Materials Chemistry C</i> ,	7.1	3
1	Less is more: on the effect of benzannulation on the solid-state emission of difluoroborates. <i>Journal of Materials Chemistry C</i> ,	7.1	1