

# A new hybrid exchangeâ€‘correlation functional using (CAM-B3LYP)

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Citation Report

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2810	Fullerene-Based Photoactive Layers for Heterojunction Solar Cells: Structure, Absorption Spectra and Charge Transfer Process. <i>Materials</i> , 2015, 8, 42-56.	1.3	41

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2849	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19306-19314.	1.3	160
2850	Accurate Diels-Alder Reaction Energies from Efficient Density Functional Calculations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2879-2888.	2.3	19
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2881	Reduced Density Matrix Functional Theory (RDMFT) and Linear Response Time-Dependent RDMFT (TD-RDMFT). <i>Topics in Current Chemistry</i> , 2015, 368, 125-183.	4.0	61
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3861	On the ultrafast charge migration dynamics in isolated ionized halogen, chalcogen, pnictogen, and tetrel bonded clusters. <i>Chemical Physics</i> , 2016, 472, 61-71.	0.9	12
3862	Platinum anti-cancer drugs: Free radical mechanism of Pt-DNA adduct formation and anti-neoplastic effect. <i>Free Radical Biology and Medicine</i> , 2016, 95, 216-229.	1.3	50
3863	Nonlinear optical properties of curcumin: solvatochromism-based approach and computational study. <i>Molecular Physics</i> , 2016, 114, 1867-1879.	0.8	51
3864	Exploring the limits of recent exchange-correlation functionals in modeling lithium/benzene interaction. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	26
3865	Four-Component Damped Density Functional Response Theory Study of UV/Vis Absorption Spectra and Phosphorescence Parameters of Group 12 Metal-Substituted Porphyrins. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2324-2334.	2.3	9
3866	Introducing QMC/MMpol: Quantum Monte Carlo in Polarizable Force Fields for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1674-1683.	2.3	28
3867	Gaussian-based range-separation approach on Hartree-Fock exchange interaction and second-order perturbation theory. <i>Chemical Physics Letters</i> , 2016, 647, 132-138.	1.2	3
3868	Predicting $^{17}\text{O}$ NMR chemical shifts of polyoxometalates using density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8235-8241.	1.3	4
3869	Interaction of $\alpha$ -proline with group IIB ( $\text{Zn}^{2+}$ , $\text{Cd}^{2+}$ ) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tt 50 Canadian Journal of Chemistry, 2016, 94, 501-508.	0.6	6
3870	Second- and third-order nonlinear optical properties of unsubstituted and mono-substituted chalcones. <i>Chemical Physics Letters</i> , 2016, 648, 91-96.	1.2	57
3871	Theoretical study of bis(N-(5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl)ethanimidamido)M complexes (M) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tt 50 Chemistry, 2016, 1080, 16-22.	1.1	1
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3873	Computing UV/vis spectra using a combined molecular dynamics and quantum chemistry approach: bis-triazin-pyridine (BTP) ligands studied in solution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 7728-7736.	1.3	21
3874	Broad temperature range of cubic blue phase present in simple binary mixture systems containing rodlike Schiff base mesogens with tolane moiety. <i>Soft Matter</i> , 2016, 12, 3110-3120.	1.2	11
3875	Ionisation and (de-)protonation energies of gas-phase amino acids from an optimally tuned range-separated hybrid functional. <i>Molecular Physics</i> , 2016, 114, 1218-1224.	0.8	11
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3879	Evaluation of Range-Corrected Density Functionals for the Simulation of Pyridinium-Containing Molecular Crystals. <i>Journal of Physical Chemistry A</i> , 2016, 120, 939-947.	1.1	23
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3881	Experimental and computational studies of 4-(Trifluoromethyl)pyridine-2-carboxylic acid. <i>Journal of Molecular Structure</i> , 2016, 1111, 55-60.	1.8	8
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3883	Spectroscopic and TD-DFT studies on the turn-off fluorescent chemosensor based on anthraldehyde N(4) cyclohexyl thiosemicarbazone for the selective recognition of fluoride and copper ions. <i>Polyhedron</i> , 2016, 109, 7-18.	1.0	43
3884	Dipole properties of PH <sub>3</sub> , PF <sub>3</sub> , PF <sub>5</sub> , PCl <sub>3</sub> , SiCl <sub>4</sub> , GeCl <sub>4</sub> , and SnCl <sub>4</sub> . <i>Molecular Physics</i> , 2016, 114, 1657-1663.	0.8	4
3885	Investigating the role of the $\pi$ -bridge characteristics in donor- $\pi$ -spacer-acceptor type dyes for solar cell application: a theoretical study. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	5
3886	Electronic Structure Properties of Two-Dimensional $\pi$ -Conjugated Polymers. <i>Macromolecules</i> , 2016, 49, 1305-1312.	2.2	32
3887	Plasmon-enhanced two-photon-induced isomerization for highly-localized light-based actuation of inorganic/organic interfaces. <i>Nanoscale</i> , 2016, 8, 4194-4202.	2.8	16
3888	Theoretical study and design of highly efficient platinum( $\text{II}$ ) complexes bearing tetradentate ligands for OLED. <i>RSC Advances</i> , 2016, 6, 11648-11656.	1.7	37
3889	Distinct molecule adsorption behaviors on warped nanographene C <sub>80</sub> H <sub>30</sub> : A theoretical study. <i>Carbon</i> , 2016, 100, 428-434.	5.4	20
3890	Computational design of benzo [1,2-b:4,5-b'] dithiophene based thermally activated delayed fluorescent materials. <i>Dyes and Pigments</i> , 2016, 127, 189-196.	2.0	9
3891	Computer Modeling of Halogen Bonds and Other $\pi$ -Hole Interactions. <i>Chemical Reviews</i> , 2016, 116, 5155-5187.	23.0	537
3892	Supramolecular complexes involving non-symmetric viologen cations and hexacyanoferrate( $\text{II}$ ) anions. A spectroscopic, crystallographic and computational study. <i>RSC Advances</i> , 2016, 6, 575-585.	1.7	17
3893	Effect of polyfluorination on self-assembling and electronic properties of thioalkyl-porphyrines. <i>Journal of Porphyrins and Phthalocyanines</i> , 2016, 20, 223-233.	0.4	15
3894	A comparative IR/Raman, X-ray and computational study of diethylzinc pyridine complexes. <i>Journal of Organometallic Chemistry</i> , 2016, 806, 77-82.	0.8	7
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3897	Neutral, heteroleptic copper(I)-4H-imidazolates complexes: synthesis and characterization of their structural, spectral and redox properties. <i>Dalton Transactions</i> , 2016, 45, 4835-4842.	1.6	21
3898	Intrinsic Properties of Two Benzodithiophene-Based Donor-Acceptor Copolymers Used in Organic Solar Cells: A Quantum-Chemical Approach. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1051-1064.	1.1	8
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3901	Theoretical insight into the stereometric effect of bisPC71BM on polymer cell performance. <i>Science Bulletin</i> , 2016, 61, 139-147.	4.3	19
3902	Theoretical investigation on ESIPT mechanism of a new fluorescent sensor in different solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 159, 30-34.	2.0	13
3903	Computational benchmark for calculation of silane and siloxane thermochemistry. <i>Journal of Molecular Modeling</i> , 2016, 22, 35.	0.8	21
3904	Electronic structures of hydrogen functionalized carbon nanotube: Density functional theory (DFT) study. <i>Solid State Sciences</i> , 2016, 55, 138-143.	1.5	15
3905	Dynamics of Isolated 1,8-Naphthalimide and N-Methyl-1,8-naphthalimide: An Experimental and Computational Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 2089-2095.	1.1	23
3906	Theoretical investigation on ratiometric two-photon fluorescent probe for $\text{Zn}^{2+}$ detection based on ICT mechanism. <i>Journal of Molecular Structure</i> , 2016, 1114, 65-77.	1.8	7
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3915	Synthesis, spectral analysis and quantum chemical studies on molecular geometry of (2E,6E)-2,6-bis(2-chlorobenzylidene)cyclohexanone: Experimental and theoretical approaches. <i>Journal of Molecular Structure</i> , 2016, 1116, 9-21.	1.8	8
3916	Magnetic circular dichroism of chlorofullerenes: Experimental and computational study. <i>Chemical Physics Letters</i> , 2016, 647, 117-121.	1.2	9
3917	Understanding anionic Chugaev elimination in pericyclic tetracene formation. <i>Tetrahedron</i> , 2016, 72, 1686-1689.	1.0	3
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3921	Kohn-Sham calculations of NMR shifts for paramagnetic 3d metal complexes: protocols, delocalization error, and the curious amide proton shifts of a high-spin iron(II) macrocycle complex. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21051-21068.	1.3	37
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3923	Vibrationally resolved optical spectra and ultrafast electronic relaxation dynamics of diamantane. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8701-8709.	1.3	7
3924	Theoretical investigation of [Ru(tpy) <sub>2</sub> ] <sup>2+</sup> , [Ru(tpy)(bpy)(H <sub>2</sub> O)] <sup>2+</sup> and [Ru(tpy)(bpy)(Cl)] <sup>+</sup> complexes in acetone revisited: Inclusion of strong spin-orbit couplings to quantum chemistry calculations. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650001.	1.8	1
3925	Theoretical study on thermal cis-to-trans isomerization of BF <sub>2</sub> -coordinated azo compounds of the para-substitution with electron donating groups. <i>Dyes and Pigments</i> , 2016, 129, 100-108.	2.0	15
3926	Charge generation in organic photovoltaics: a review of theory and computation. <i>Molecular Systems Design and Engineering</i> , 2016, 1, 10-24.	1.7	86
3927	Diverse Optimal Molecular Libraries for Organic Light-Emitting Diodes. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1942-1952.	2.3	15
3928	Photo-induced alignment behaviour of polymerisable liquid crystals on bisazide in a polymer matrix. <i>Liquid Crystals</i> , 2016, 43, 910-919.	0.9	5
3929	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. <i>Chemical Reviews</i> , 2016, 116, 4937-4982.	23.0	408
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3931	Three-photon circular dichroism: towards a generalization of chiroptical non-linear light absorption. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4174-4184.	1.3	10

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3933	How Bond Length Alternation and Thermal Disorder Affect the Optical Excitation Energies of $\pi$ -Conjugated Chains: A Combined Density Functional Theory and Molecular Dynamics Study. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1872-1882.	2.3	10
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3935	Solvent Effects on Electronic Excitations of an Organic Chromophore. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1853-1861.	2.3	57
3936	Optical absorption and emission properties of benzene-expanded Janus AT nucleobase analogues: A DFT study. <i>Structural Chemistry</i> , 2016, 27, 1175-1187.	1.0	4
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3939	Fluorescent DNA probes at liquid/liquid interfaces studied by surface second harmonic generation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2981-2992.	1.3	16
3940	Theoretical assessment of the electro-optical features of the group III nitrides (B <sub>12</sub> N <sub>12</sub> , Al <sub>12</sub> N <sub>12</sub> and Tl <sub>12</sub> N <sub>12</sub> ) overlayers on 10 transition metals (Li, Na and K). <i>Applied Surface Science</i> , 2016, 363, 197-208.	3.1	83
3941	Electronic and optical properties of the Au <sub>22</sub> [1,8-bis(diphenylphosphino) octane] <sub>6</sub> nanoclusters disclosed by DFT and TD-DFT calculations. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	12
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3946	Vibrational analysis on the revised potential energy curve of the low-barrier hydrogen bond in photoactive yellow protein. <i>Computational and Structural Biotechnology Journal</i> , 2016, 14, 16-19.	1.9	6
3947	Comparing the ion affinity of two ionophores: Theoretical study of alkali earth metal ion $\rightarrow$ "nano tubular cyclic peptide complexes. <i>Journal of Molecular Liquids</i> , 2016, 214, 101-110.	2.3	6
3948	Structure and Absolute Configuration of Pseudohygrophorones A <sub>12</sub> and B <sub>12</sub> , Alkyl Cyclohexenone Derivatives from <i>Hygrophorus abieticola</i> (Basidiomycetes). <i>Journal of Natural Products</i> , 2016, 79, 74-80.	1.5	21
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3951	Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices. <i>Journal of Materials Chemistry C</i> , 2016, 4, 1009-1018.	2.7	99
3952	A computational approach to the resonance Raman spectrum of doxorubicin in aqueous solution. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	14
3953	Solvatofluorochromic, non-centrosymmetric $\pi$ -expanded diketopyrrolopyrrole. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 2025-2033.	1.5	12
3954	Hydrogen bonding inside and outside carbon nanotubes: HF dimer as a case study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2417-2427.	1.3	11
3955	Quantum chemical theory calculations on the mechanism of the homogeneous, unimolecular gas-phase elimination kinetics of selected diazirines. <i>Computational and Theoretical Chemistry</i> , 2016, 1078, 23-29.	1.1	4
3956	Calculation of low bandgap homopolymers: Comparison of TD-DFT methods with experimental oligomer series. <i>Chemical Physics Letters</i> , 2016, 645, 169-173.	1.2	26
3957	Experimental and computational evaluation of the barrier to torsional rotation in a butadiyne-linked porphyrin dimer. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 5264-5274.	1.3	57
3958	Coumarin-based donor-acceptor organic dyes for a dye-sensitized solar cell: photophysical properties and electron injection mechanism. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	23
3959	Benchmark <i>ab Initio</i> Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 444-454.	2.3	99
3960	( <i>Z</i> )-1,2-Di(1-pyrenyl)disilene: Synthesis, Structure, and Intramolecular Charge-Transfer Emission. <i>Journal of the American Chemical Society</i> , 2016, 138, 758-761.	6.6	44
3961	Solvent effects on excited-state electron-transfer rate of pyrene-labeled deoxyuridine: A theoretical study. <i>Chemical Physics Letters</i> , 2016, 644, 25-30.	1.2	5
3962	Excited-state localization and energy transfer in pyrene core dendrimers with fluorene/carbazole as the dendrons and acetylene as the linkages. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4134-4143.	1.3	6
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3964	Computational insights into the photophysical and electroluminescence properties of homoleptic fac-Ir(C <sup>N</sup> ) <sub>3</sub> complexes employing different phenyl-derivative-featuring phenylimidazole-based ligands for promising phosphors in OLEDs. <i>Dalton Transactions</i> , 2016, 45, 3034-3047.	1.6	7
3965	Protonated thiophene-based oligomers as formed within zeolites: understanding their electron delocalization and aromaticity. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2080-2086.	1.3	17
3966	Warning to Theoretical Structure Elucidation of Endohedral Metallofullerenes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1275-1283.	1.5	29
3967	Calculation on frequency and temperature properties of birefringence of nematic liquid crystal 5CB in terahertz band. <i>Chemical Physics Letters</i> , 2016, 645, 205-209.	1.2	17

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3973	Unexpected multiple activated steps in the excited state decay of some bis(phenylethynyl)-fluorenes and -anthracenes. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 285-294.	1.3	3
3974	Chelation behavior of various flavonols and transfer of flavonol-chelated zinc(II) to alanyl aspartic dipeptide: A PCM/DFT investigation. <i>Journal of Molecular Structure</i> , 2016, 1107, 278-290.	1.8	7
3975	Lycopene, oxidative cleavage derivatives and antiradical activity. <i>Computational and Theoretical Chemistry</i> , 2016, 1077, 92-98.	1.1	13
3976	Systematic study on the TD-DFT calculated electronic circular dichroism spectra of chiral aromatic nitro compounds: A comparison of B3LYP and CAM-B3LYP. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 155, 95-102.	2.0	46
3977	Influence of intermolecular hydrogen bonding and solvent effects on the excited-state properties of a photoactive yellow protein chromophore compound. <i>Journal of Alloys and Compounds</i> , 2016, 659, 82-89.	2.8	6
3978	Interactions of zinc octacarboxyphthalocyanine with selected amino acids and with albumin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 155, 54-60.	2.0	9
3979	N-Alkylthienopyrroledione versus benzothiadiazole pulling units in push-pull copolymers used for photovoltaic applications: density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 1017-1024.	1.3	15
3980	5,7-Bis(2-arylethenyl)-6H-1,4-diazepine-2,3-dicarbonitriles: synthesis, and experimental and theoretical evaluation of the effects of substituents at 5,6,7-positions on the molecular configuration and spectral properties. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 1138-1146.	1.5	10
3981	Computational study of new azo dyes with different anchoring groups for dye-sensitised solar cells. <i>Molecular Physics</i> , 2016, 114, 650-662.	0.8	18
3982	Theoretical study on the mechanism of the gas-phase elimination kinetics of alkyl chloroformates. <i>Molecular Physics</i> , 2016, 114, 719-729.	0.8	2
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3984	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <i>Molecular Physics</i> , 2016, 114, 21-33.	0.8	21
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3988	Photophysics of Auramine-O: electronic structure calculations and nonadiabatic dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 403-413.	1.3	15
3989	Investigation of substitution effect on fluorescence properties of Zn <sup>2+</sup> -selective ratiometric fluorescent compounds: 2-(2-Hydroxyphenyl)benzimidazole derivatives. <i>Talanta</i> , 2016, 146, 575-584.	2.9	22
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4930	Phenothiazine derivatives as an easily accessible emitter for green light-emitting electrochemical cells. <i>Journal of Luminescence</i> , 2018, 197, 383-388.	1.5	18
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4957	Deviation from the <i>trans</i> -Effect in Ligand-Exchange Reactions of Zeise's Ions PtCl <sub>3</sub> (C <sub>2</sub> H <sub>4</sub> ) <sup>+</sup> with Heavier Halides (Br <sup>+</sup> ,) Tj ETQq1 1 0.784314 rgt	0.7	1
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4974	Chiomagnetic nanoparticles and gels. <i>Science</i> , 2018, 359, 309-314.	6.0	201
4975	Negative influence of p <i>K<sub>a</sub></i> on activation energy barrier: A case study for double proton transfer reaction in inorganic acid dimers. <i>Journal of Computational Chemistry</i> , 2018, 39, 993-998.	1.5	4
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5053	Electronically excited states of carbazole-modified ortho-phenylenes. <i>Chemical Physics Letters</i> , 2018, 693, 95-100.	1.2	1
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5060	A simple multi-responsive system based on aldehyde functionalized amino-boranes. <i>Chemical Science</i> , 2018, 9, 1902-1911.	3.7	99
5061	Can TDDFT Describe Excited Electronic States of Naphthol Photoacids? A Closer Look with EOM-CCSD. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 867-876.	2.3	27
5062	The effect of twisted $D_{4h}$ configuration on electron transfer and photo-physics characteristics. <i>Molecular Physics</i> , 2018, 116, 1179-1191.	0.8	2
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5064	Photophysics and peripheral ring size dependent aggregate emission of cross-conjugated enediynes: applications to white light emission and vapor sensing. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4167-4180.	1.3	7
5065	Structuring Conjugated Polymers and Polyelectrolytes Through Self-Assembly. <i>Materials and Energy</i> , 2018, , 67-114.	2.5	0
5066	Computational simulation of vibrationally resolved spectra for spin-forbidden transitions. <i>Chirality</i> , 2018, 30, 850-865.	1.3	15
5067	Computational study of the chemical reactivity of the Blue-M1 intermediate melanoidin. <i>Computational and Theoretical Chemistry</i> , 2018, 1134, 22-29.	1.1	39
5068	The consequences of two distinct reaction coordinates in the decomposition of the ethylamine cation conformers. <i>Chemical Physics Letters</i> , 2018, 701, 165-170.	1.2	0
5069	Unconventional Synthesis of a Cu <sup>I</sup> Rotaxane with a Superacceptor Stopper: Ultrafast Excited-State Dynamics and Near-Infrared Luminescence. <i>Chemistry - A European Journal</i> , 2018, 24, 10422-10433.	1.7	9



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5080	A combined theoretical and experimental study of the ultrafast photophysics of Rhodamine B. <i>Molecular Physics</i> , 2018, 116, 2162-2171.	0.8	7
5081	Theoretical Development of Near-Infrared Bioluminescent Systems. <i>Chemistry - A European Journal</i> , 2018, 24, 9340-9352.	1.7	9
5082	An experimental and DFT study of the packing and structure of dithenoylmethane monocarbonylphosphine Rhodium(I) complex [Rh((C <sub>4</sub> H <sub>3</sub> S)COCHCO(C <sub>4</sub> H <sub>3</sub> S))(CO)(PPh <sub>3</sub> )]. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 83, 33-41.	1.3	0
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5084	<sup>35</sup> Cl Nuclear Magnetic Resonance Analysis of Pentacoordinate Titanium <i>n</i> -Butoxide Derivatives. <i>Chemistry Letters</i> , 2018, 47, 183-185.	0.7	1
5085	Synthesis and properties of new heterocyclic betaines: 4-Aryl-5-(methoxycarbonyl)-2-oxo-3-(pyridin-1-ium-1-yl)-2,3-dihydro-1 H -pyrrol-3-ides. <i>Tetrahedron</i> , 2018, 74, 2466-2474.	1.0	11
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5090	1,2,3- versus 1,2-Indeno Ring Fusions Influence Structure Property and Chirality of Corannulene Bowls. <i>Journal of Organic Chemistry</i> , 2018, 83, 3979-3986.	1.7	12
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5092	Electron transfer and charge transport of photoelectric material in external electric field. <i>Journal of Luminescence</i> , 2018, 199, 278-284.	1.5	7
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5103	Local structure and hydrogen bond characteristics of imidazole molecules for proton conduction in acid and base proton-conducting composite materials. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10311-10318.	1.3	23
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5105	Radical Ions of 3-Styryl-quinoxalin-2-one Derivatives Studied by Pulse Radiolysis in Organic Solvents. <i>Journal of Physical Chemistry B</i> , 2018, 122, 4051-4066.	1.2	6

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5107	Investigation on the performance of PCM/TD-DFT functionals (standard pure, hybrid and long-range) Tj ETQq1 1 0.784314 rgBT /Over 1-(2,5-dimethylfuran-3-yl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one dye in different solvents. <i>Journal of Molecular Structure</i> , 2018, 1164, 289-296.	1.8	6
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5117	Transition metal doping: a new and effective approach for remarkably high nonlinear optical response in aluminum nitride nanocages. <i>New Journal of Chemistry</i> , 2018, 42, 6976-6989.	1.4	61
5118	Effect of phosphorus on the electronic and optical properties of naphthoxaphospholes: theoretical investigation. <i>Molecular Physics</i> , 2018, 116, 1581-1588.	0.8	4
5119	<i>para</i> -Aminosalicylic acid in the treatment of manganese toxicity. Complexation of $\text{Mn}^{2+}$ with 4-amino-2-hydroxybenzoic acid and its <i>N</i> -acetylated metabolite. <i>New Journal of Chemistry</i> , 2018, 42, 8035-8049.	1.4	14
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5121	Theoretical Study of Electron Transfer Properties of Squaraine Dyes for Dye Sensitized Solar Cell. <i>IOP Conference Series: Materials Science and Engineering</i> , 2018, 299, 012058.	0.3	2
5122	Computational studies of the nonlinear optical properties of organometallic complexes. <i>Coordination Chemistry Reviews</i> , 2018, 375, 389-409.	9.5	40
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5130	Electronic structures and photophysical properties of phosphorescent platinum (II) complexes with tridentate C <sup>N</sup> *N cyclometalated ligands. <i>Applied Organometallic Chemistry</i> , 2018, 32, e3929.	1.7	8
5131	Dispersion interactions in oligomerization of metal diketonates: a DFT evaluation. <i>Chemical Papers</i> , 2018, 72, 829-839.	1.0	9
5132	Correlating cluster size and NLO response of complexes aggregated with bifurcated metal bonds: a DFT study. <i>Structural Chemistry</i> , 2018, 29, 119-127.	1.0	1
5133	UV absorbers for cellulosic apparels: A computational and experimental study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 355-361.	2.0	9
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5136	A theoretical study of structural, opto-electronic and nonlinear properties of arylboroxine derivatives. <i>Indian Journal of Physics</i> , 2018, 92, 57-68.	0.9	2
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5140	Quantum modeling of ultrafast photoinduced charge separation. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 013002.	0.7	29
5141	Experimental and theoretical investigation of fluorescence solvatochromism of dialkoxyphenyl-pyrene molecules. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 3258-3264.	1.3	13

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5143	Adsorption modes of molecular iodine on defected boron nitrides: A DFT study. <i>Applied Surface Science</i> , 2018, 434, 604-612.	3.1	16
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5149	Xylaropyrones B and C, new $\beta$ -pyrones from the endophytic fungus <i>Xylaria</i> sp. SC1440. <i>Natural Product Research</i> , 2018, 32, 1525-1531.	1.0	11
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5155	Quantum dynamical studies of ultrafast charge separation in nanostructured organic polymer materials: Effects of vibronic interactions and molecular packing. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25502.	1.0	30
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5161	Effect of hydrogen-bonded interactions on the energetics and spectral properties of the astromolecule aminoacetonitrile. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25459.	1.0	1
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5163	Effect of methyl substituents on the electronic transitions in simple meso-aniline-BODIPY based dyes: RI-CC2 and TD-CAM-B3LYP computational investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 239-245.	2.0	18
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5165	A series of bowl-shaped PDI dimers designed for organic photovoltaic cells through engineering N-annulated bridge towards potential alternatives of PDI bridged dimer acceptors. <i>Dyes and Pigments</i> , 2018, 148, 394-404.	2.0	17
5166	Solvatochromic isocyanonaphthalene dyes as ligands for silver(I) complexes, their applicability in silver(I) detection and background reduction in biolabelling. <i>Sensors and Actuators B: Chemical</i> , 2018, 255, 2555-2567.	4.0	12
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5172	A computational study of photonic materials based on Ni bis(dithiolene) fused with benzene, possessing gigantic second hyperpolarizabilities. <i>Journal of Materials Chemistry C</i> , 2018, 6, 91-110.	2.7	14
5173	Novel water soluble cationic Au(I) complexes with cyclic PNNP ligand as building blocks for heterometallic supramolecular assemblies with anionic hexarhenium cluster units. <i>Journal of Luminescence</i> , 2018, 196, 485-491.	1.5	16
5174	Shortfall of B3LYP in Reproducing NMR <sup>1</sup> J <sub>CH</sub> Couplings in Some Isomeric Epoxy Structures with Strong Stereoelectronic Effects: A Benchmark Study on DFT Functionals. <i>ChemPhysChem</i> , 2018, 19, 631-642.	1.0	12
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5179	Unusual response to environmental polarity in a nonlinear-optical benzylidene-type chromophore containing a 1,3-bis(dicyanomethylidene)indane acceptor fragment. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 404-413.	1.3	5
5180	Linear and Nonlinear Optical Properties of Tricyanopropylidene-Based Merocyanine Dyes: Synergistic Experimental and Theoretical Investigations. <i>ChemPhysChem</i> , 2018, 19, 187-197.	1.0	28
5181	Computational design of quadrupolar donor-acceptor-donor molecules with near-infrared light-harvesting capabilities. <i>Dyes and Pigments</i> , 2018, 149, 882-892.	2.0	11
5182	Emission properties of Si-based styryl-carbazole derivatives: Role of meta- and para-vinyl substituents and silicon atom. <i>Journal of Luminescence</i> , 2018, 196, 57-63.	1.5	4
5183	The effect of different $\pi$ -bridge configuration on bi-anchored triphenylamine and phenyl modified triphenylamine based dyes for dye sensitized solar cell (DSSC) application: A theoretical approach. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 79, 235-253.	1.3	24
5184	Investigating the excited state optical properties and origin of large Stokes shift in Benz[c,d]indole N-Heteroarene BF <sub>2</sub> dyes with ab initio tools. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2018, 178, 472-480.	1.7	22
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5717	Different reactivity to glutathione but similar tumor cell toxicity of chalcones and their quinolinone analogues. <i>Medicinal Chemistry Research</i> , 2019, 28, 1448-1460.	1.1	15



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7593	Refined standards for simulating UV $\rightarrow$ vis absorption spectra of acceptors in organic solar cells by TD-DFT. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2021, 407, 113087.	2.0	9
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8115	A Highly Strained All-Phenylene Conjoined Bismacrocyclic. <i>Angewandte Chemie</i> , 2021, 133, 17508-17512.	1.6	11
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8183	Hydricity of 3d Transition Metal Complexes from Density Functional Theory: A Benchmarking Study. <i>Molecules</i> , 2021, 26, 4072.	1.7	19
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8187	Towards the development of antioxidant-wrapped graphene-based fluorescent nanomaterials having theranostic potentials: A combined experimental and theoretical study. <i>Carbon Trends</i> , 2021, 4, 100042.	1.4	1
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8203	[Ag <sub>23</sub> Pd <sub>2</sub> (PPh <sub>3</sub> ) <sub>10</sub> Cl <sub>7</sub> ]: A new family of synthesizable bi-icosahedral superatomic molecules. <i>Journal of Chemical Physics</i> , 2021, 155, 024302.	1.2	15
8204	Water-Soluble BODIPY-Based fluorescent probe for BSA and HSA detection. <i>Journal of Molecular Liquids</i> , 2022, 345, 117031.	2.3	19
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8217	The Quest to Simulate Excited-State Dynamics of Transition Metal Complexes. <i>Jacs Au</i> , 2021, 1, 1116-1140.	3.6	30
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8221	Synthesis, characterization and DFT calculations of linear and NLO properties of novel (Z)-5-benzylidene-3-N(4-methylphenyl)-2-thioxothiazolidin-4-one. <i>Journal of Sulfur Chemistry</i> , 2021, 42, 645-663.	1.0	15
8222	Remarkable electronic and NLO properties of bimetallic superalkali clusters: a DFT study. <i>Journal of Nanostructure in Chemistry</i> , 2022, 12, 529-545.	5.3	16
8223	Benchmarking of Density Functionals for <i>&lt;i&gt;Z&lt;/i&gt;</i> -Azoarene Half-Lives via Automated Transition State Search. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6474-6485.	1.1	8
8224	Comparison in optoelectronic properties of triphenylamine-imidazole or imidazole as donor for dye-sensitized solar cell: theoretical approach. <i>Journal of Molecular Modeling</i> , 2021, 27, 225.	0.8	3
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8226	O- <i>isopropylferrocenesulfonate</i> : Synthesis of Polysubstituted Derivatives and Electrochemical Study. <i>European Journal of Inorganic Chemistry</i> , 2021, 2021, 3165-3176.	1.0	8
8227	Understanding the molecular mechanism of the chlorine atom transfer between ammonia and hypochlorous acid with electron localisation function (ELF). <i>Molecular Physics</i> , 0, , e1961035.	0.8	2
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9098	Solvent effects on excited-state relaxation dynamics of paddle-wheel BODIPY-Hexaoxatriphenylene conjugates: Insights from non-adiabatic dynamics simulations. <i>Chinese Journal of Chemical Physics</i> , 2022, 35, 117-128.	0.6	0
9099	Peri- <i>Acenoacene</i> for Solution Processed Distributed Feedback Laser: The Effect of 1,2-Oxaborine Doping. <i>Advanced Optical Materials</i> , 2022, 10, .	3.6	9
9100	Polycyclic Aromatic Hydrocarbons (PAHs) in Interstellar Ices: A Computational Study into How the Ice Matrix Influences the Ionic State of PAH Photoproducts. <i>ACS Earth and Space Chemistry</i> , 2022, 6, 766-774.	1.2	5
9101	Two-Photon Absorption Cooperative Effects within Multi-Dipolar Ruthenium Complexes: The Decisive Influence of Charge Transfers. <i>Molecules</i> , 2022, 27, 1493.	1.7	0
9102	Design of a D- $\pi$ -A framework with various auxiliary acceptors on optoelectronic and charge transfer properties for efficient dyes in DSSCs: A DFT/TD-DFT study. <i>Journal of Computational Electronics</i> , 2022, 21, 361-377.	1.3	1
9103	Optimized nonlinear optical (NLO) response of silicon carbide nanosheet by alkali metals doping: a DFT insight. <i>European Physical Journal Plus</i> , 2022, 137, 1.	1.2	23
9104	Quantum chemical designing of novel fullerene-free acceptor molecules for organic solar cell applications. <i>Journal of Molecular Modeling</i> , 2022, 28, 67.	0.8	8
9105	Approximate functionals in hypercomplex Kohn-Sham theory. <i>Electronic Structure</i> , 2022, 4, 014011.	1.0	3
9106	The Excited State and Charge Transfer of Two Nonfullerene Acceptors from First-Principles Many-Body Green's Function Theory. <i>Journal of Chemistry</i> , 2022, 2022, 1-8.	0.9	0
9107	Comparison of semi-empirical and density functional approaches for the colour and constitution of anthraquinone dyes using X-ray structure. <i>Coloration Technology</i> , 2022, 138, 417-426.	0.7	0
9108	Fewest switches surface hopping with Baek-An couplings. <i>Open Research Europe</i> , 0, 1, 49.	2.0	10
9109	Theoretical insights into the nonlinear optical properties of cyclotriphosphazene (P <sub>3</sub> N <sub>3</sub> Cl <sub>6</sub> ), tris(4-hydroxyphenyl) ethane and their various inorganic-organic hybrid derivatives. <i>Journal of Materials Science</i> , 2022, 57, 6971-6987.	1.7	11
9110	Quasi-Relativistic Calculation of EPR $\langle i \rangle g \langle i \rangle$ Tensors with Derivatives of the Decoupling Transformation, Gauge-Including Atomic Orbitals, and Magnetic Balance. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2246-2266.	2.3	16
9111	Asymmetric Tandem Conjugate Addition and Reaction with Carbocations on Unsaturated Heterocycles. <i>Advanced Synthesis and Catalysis</i> , 2022, 364, 1337-1344.	2.1	2
9112	Organic Electronics from Nature: Computational Investigation of the Electronic and Optical Properties of the Isomers of Bixin and Norbixin Present in the Achiote Seeds. <i>Molecules</i> , 2022, 27, 2138.	1.7	0
9113	Anticooperativity of Multiple Halogen Bonds and Its Effect on Stoichiometry of Cocrystals of Perfluorinated Iodobenzenes. <i>Crystal Growth and Design</i> , 2022, 22, 2644-2653.	1.4	14
9114	Electronic Structure Changes of an Aromatic Amine Photoacid along the Förster Cycle. <i>Angewandte Chemie</i> , 0, , .	1.6	0

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9116	Photophysical and Electrochemical Properties of Push-Pull Oligo(ferrocenyl-phenyleneethynylene)s: Supramolecular Orders in Molecular Films. <i>Langmuir</i> , 2022, 38, 4077-4089.	1.6	1
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9118	Theoretical Modeling of Absorption and Fluorescent Characteristics of Cyanine Dyes. <i>Photochem</i> , 2022, 2, 202-216.	1.3	5
9119	Photoinduced bond oscillations in ironpentacarbonyl give delayed synchronous bursts of carbonmonoxide release. <i>Nature Communications</i> , 2022, 13, 1337.	5.8	2
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9122	Perylene-Based Linear Nonalternant Nanoribbons with Bright Emission and Ambipolar Redox Behavior. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	19
9123	Evidence for Participation of 4f and 5d Orbitals in Lanthanide Metal-Ligand Bonding and That Y(III) Has Less of This Complex-Stabilizing Ability. A Thermodynamic, Spectroscopic, and DFT Study of Their Complexation by the Nitrogen Donor Ligand TPEN. <i>Inorganic Chemistry</i> , 2022, 61, 4627-4638.	1.9	11
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9128	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. <i>Magnetochemistry</i> , 2022, 8, 36.	1.0	7
9129	Excited states of chlorophyll <i>a</i> and <i>b</i> in solution by time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2022, 156, 124111.	1.2	2
9130	Femtosecond Spectroscopy and Nonlinear Optical Properties of aza-BODIPY Derivatives in Solution. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	4
9131	Synthesis of Polysubstituted Ferrocenesulfoxides. <i>Molecules</i> , 2022, 27, 1798.	1.7	4
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9134	Intersystem Crossings in Late-Row Elements: A Perspective. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3039-3046.	2.1	11
9135	Determining the Energy Gap between the S <sub>1</sub> and T <sub>1</sub> States of Thermally Activated Delayed Fluorescence Molecular Systems Using Transient Fluorescence Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2507-2515.	2.1	12
9136	Estimating Phosphorescent Emission Energies in Ir <sup>III</sup> Complexes Using Large-Scale Quantum Computing Simulations**. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	3
9137	One-Shot Approach for Enforcing Piecewise Linearity on Hybrid Functionals: Application to Band Gap Predictions. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3066-3071.	2.1	10
9138	Synthesis and Self-Assembly of Benzoperylene Benzimidazoles: Tunable Morphology with Aggregation-Induced Enhanced Emission. <i>Chemistry - an Asian Journal</i> , 2022, 17, .	1.7	1
9139	Computational analysis of carbazole-based newly efficient D- $\pi$ -A organic spacer dye derivatives for dye-sensitized solar cells. <i>Structural Chemistry</i> , 2022, 33, 1097-1107.	1.0	7
9140	Designing Special Nonmetallic Superalkalis Based on a Cage-like Adamantane Complexant. <i>Frontiers in Chemistry</i> , 2022, 10, 853160.	1.8	3
9141	Basis Set Dependence of Optical Rotation Calculations with Different Choices of Gauge. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1861-1870.	1.1	5
9142	Electronically Excited Complex Formation in Magnesium Cluster-Halogen Atom Reactions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1848-1860.	1.1	1
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9145	Relative Populations and IR Spectra of Cu <sub>38</sub> Cluster at Finite Temperature Based on DFT and Statistical Thermodynamics Calculations. <i>Frontiers in Chemistry</i> , 2022, 10, 841964.	1.8	3
9146	Super-Exchange Charge Transfer in One-Photon and Two-Photon Absorption of Multibranched Compounds. <i>ACS Omega</i> , 2022, 7, 9743-9753.	1.6	1
9147	Density Functional Theory Study of Carbamoyl-Substituted Dihydroazulene/Vinylheptafulvene Derivatives and Solvent Effects. <i>Journal of Physical Chemistry C</i> , 2022, 126, 4815-4825.	1.5	1
9148	Spectroscopic characterization of the a <sup>3</sup> state of aluminum monofluoride. <i>Journal of Chemical Physics</i> , 2022, 156, 124306.	1.2	2
9149	Stealth Luminescent Organic Nanoparticles Made from Quadrupolar Dyes for Two-Photon Bioimaging: Effect of End-Groups and Core. <i>Molecules</i> , 2022, 27, 2230.	1.7	0
9150	Perylene-Based Linear Nonalternant Nanoribbons with Bright Emission and Ambipolar Redox Behavior. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	2

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9152	Donor functionalized perylene and different ĩ€-spacer based sensitizers for dye-sensitized solar cell applications â€” a theoretical approach. <i>Journal of Molecular Modeling</i> , 2022, 28, 102.	0.8	6
9153	Electronic Structure Changes of an Aromatic Amine Photoacid along the Frster Cycle. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	6
9154	A Benchmark Protocol for DFT Approaches and Data-Driven Models for Halide-Water Clusters. <i>Molecules</i> , 2022, 27, 1654.	1.7	5
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9163	Theoretical prediction of pH-dependent electronic spectra in aqueous solution: A combinational application of QM/MM calculations and constant-pH simulations with configuration-selection scheme. <i>Chemical Physics Letters</i> , 2022, 798, 139624.	1.2	0
9164	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2331-2340.	2.3	6
9165	How the Interplay among Conformational Disorder, Solvation, Local, and Charge-Transfer Excitations Affects the Absorption Spectrum and Photoinduced Dynamics of Perylene Diimide Dimers: A Molecular Dynamics/Quantum Vibronic Approach. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3718-3736.	2.3	12
9166	Quantum chemical study of end-capped acceptor and bridge on triphenyl diamine based molecules to enhance the optoelectronic properties of organic solar cells. <i>Polymer</i> , 2022, 245, 124675.	1.8	26
9167	NBO technique as a descriptor of aromaticity. <i>Computational and Theoretical Chemistry</i> , 2022, 1210, 113637.	1.1	5
9168	Highly Deepâ€”Blue Luminescent Twisted Diphenylamino Terphenyl Emitters by Bromineâ€”Lithium Exchange Borylationâ€”Suzuki Sequence. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	6

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9170	Light- and pH-dependent structural changes in cyanobacteriochrome AnPixJg2. <i>Photochemical and Photobiological Sciences</i> , 2022, 21, 447-469.	1.6	6
9171	Machine learned calibrations to high-throughput molecular excited state calculations. <i>Journal of Chemical Physics</i> , 2022, 156, 134116.	1.2	5
9172	Guanosine Dianions Hydrated by One to Four Water Molecules. <i>Journal of Physical Chemistry Letters</i> , 2022, , 3230-3236.	2.1	4
9173	Improving Results by Improving Densities: Density-Corrected Density Functional Theory. <i>Journal of the American Chemical Society</i> , 2022, 144, 6625-6639.	6.6	45
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9176	Effect of Electron Donating/Withdrawing Groups on Molecular Photoswitching of Functionalized Hemithioindigo Derivatives: a Computational Multireference Study. <i>ChemPhotoChem</i> , 2022, 6, .	1.5	4
9177	Enhancement in non-linear optical properties of carbon nitride (C <sub>2</sub> N) by doping superalkali (Li <sub>3</sub> O): A DFT study. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113654.	1.1	18
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9180	Insight into the spatial interaction of D- $\pi$ -A bridge derived cyanines and nitroreductase for fluorescent cancer hypoxia detection. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 273, 121031.	2.0	0
9181	Depicting the role of end-capped acceptors to amplify the photovoltaic properties of benzothiadiazole core-based molecules for high-performance organic solar cell applications. <i>Computational and Theoretical Chemistry</i> , 2022, 1211, 113669.	1.1	14
9182	Nonlinear optical response of some Boron-dipyrromethene dyes: An experimental and theoretical investigation. <i>Materials Chemistry and Physics</i> , 2022, 283, 126057.	2.0	2
9183	Quantum chemical approach to study TIPSTAP derivatives with anticipated minimized crystal roughness for photovoltaic application with estimated PCE of over 20%. <i>Solar Energy</i> , 2022, 237, 96-107.	2.9	13
9184	Aggregation induced emission (AIE)-active ferrocene conjugated linear $\pi$ -extended multi donor- $\pi$ -acceptor (D-D $\pi^2$ - $\pi$ -A) chromophores: Synthesis, structural, theoretical, linear and nonlinear optical studies. <i>Dyes and Pigments</i> , 2022, 201, 110193.	2.0	17
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9188	Theoretical investigation of the influence of ĩ€-spacer on photovoltaic performances in carbazole-based dyes for dye-sensitized solar cells applications. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 428, 113870.	2.0	30
9189	The ionized states of 6,6-dimethylfulvene; the vibrational energy levels studied by photoionization, configuration interaction and density functional calculations. <i>Chemical Physics Letters</i> , 2022, 796, 139558.	1.2	0
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9192	Shedding light on the second order nonlinear optical responses of commercially available acidic azo dyes for laser applications. <i>Dyes and Pigments</i> , 2022, 202, 110284.	2.0	8
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9194	Luminescence of Reichardt's dye in polyelectrolyte-modified saponite colloids. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2022, 642, 128663.	2.3	1
9195	Experimental and theoretical gas-phase absorption spectra of thionated uracils. <i>Chemical Physics</i> , 2022, 558, 111500.	0.9	4
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9199	A spectroscopic study of benzonitrile. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2022, 283, 108159.	1.1	3
9200	Low-lying electronic states of ethanol investigated by theoretical and synchrotron radiation methods. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2022, 285, 108170.	1.1	1
9201	Neolignans from <i>Myristica fragrans</i> seeds, revision of their absolute configurations, reduction products and biological activities. <i>Phytochemistry</i> , 2022, 199, 113174.	1.4	1
9202	Studies on spectro photophysical properties of PBBO-laser dye. <i>Journal of Molecular Structure</i> , 2022, 1259, 132660.	1.8	0
9203	Electronic structure, optical properties, and electron dynamics in organic dye-sensitized TiO <sub>2</sub> interfaces by local hybrid density functionals. <i>Chemical Physics</i> , 2022, 559, 111521.	0.9	2
9204	Intermolecular hydrogen-bonding-induced fluorescence of 3-hydroxyisonicotinaldehyde in different pH media. <i>Journal of Luminescence</i> , 2022, 247, 118878.	1.5	5



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9206	Spectral characterization of the main pigments in the plant photosynthetic apparatus by theory and experiment. <i>Chemical Physics</i> , 2022, 559, 111517.	0.9	9
9207	Attochemistry of hydrogen bonded amide and thioamide model complexes in protein following vertical ionization. <i>Chemical Physics</i> , 2022, 559, 111508.	0.9	1
9208	Effects of linkage between donors on photoinduced charge transfer in one-photon and two-photon absorption of Donor- $\pi$ -Donor- $\pi$ -Acceptor conjugates. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 275, 121179.	2.0	2
9209	New insights into ferric iron-facilitated UV254 photolytic defluorination of perfluorooctanoic acid (PFOA): Combined experimental and theoretical study. <i>Journal of Hazardous Materials</i> , 2022, 434, 128865.	6.5	10
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9212	Two nickel (II) complexes with side chain isomeric ligands: L-leucine and L-isoleucine to study non-covalent interactions and metal-ligand bonding. <i>Journal of Molecular Structure</i> , 2022, 1261, 132898.	1.8	2
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9214	Synthesis, photophysical, electrochemical and computational studies of novel 2-aminoimidazolones with D- $\pi$ -A framework. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 429, 113918.	2.0	5
9215	Theoretical and experimental investigation of 1,4-dihydropyridine-based hexahydroquinoline-3-carboxylates: Photophysics and bovine serum albumin binding studies. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2022, 429, 113915.	2.0	3
9216	Conformational Dynamics in Excited States and Photophysical Properties of Meso-Substituted Nitro Derivatives of Octaethylporphyrin and Their Zn Complexes. <i>Optics and Spectroscopy (English) Tj ETQq1 1 0.784314.gBT /Overlock 10</i>		
9217	Fast Approximate but Accurate QM/MM Interactions for Polarizable Embedding. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 344-356.	2.3	6
9218	Linear and second-order nonlinear optical properties of non-fullerene acceptor derivatives with A $\pi$ -D $\pi$ -A structure. <i>International Journal of Quantum Chemistry</i> , 2022, 122, .	1.0	0
9219	The Density Functional Theory Account of Interplaying Long-Range Exchange and Dispersion Effects in Supramolecular Assemblies of Aromatic Hydrocarbons with Spin. <i>Molecules</i> , 2022, 27, 45.	1.7	1
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9224	Investigation of OLED and TADF Properties of Phenazine Based Compounds. <i>Journal of the Institute of Science and Technology</i> , 2021, 11, 2926-2936.	0.3	1
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9804	<a href="http://www.w3.org/1998/Math/MathML">http://www.w3.org/1998/Math/MathML</a> altimg="si129.svg" display="inline" id="d1e2003"><mml:mrow><mml:mi mathvariant="normal">O</mml:mi><mml:mo linebreak="goodbreak" linebreakstyle="after">^{\cdot}</mml:mo><mml:mi mathvariant="normal">M</mml:mi><mml:mo linebreak="goodbreak" linebreakstyle="after">=</mml:mo><mml:mrow><mml:mo>\{</mml:mo><mml:mi mathvariant="normal">Ti</mml:mi><mml:mo>,</mml:mo><mml:mi>Si</mml:mi></mml:mrow></mml:math>	1.3	4
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10059	TDDFT versus <i>GW</i> /BSE Methods for Prediction of Light Absorption and Emission in a TADF Emitter. <i>Journal of Physical Chemistry A</i> , 2022, 126, 9627-9643.	1.1	1
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10061	Interexcited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 271-292.	2.3	5

#	ARTICLE	IF	CITATIONS
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10064	Câ€O Bond Activation in Mononuclear Lanthanide Oxocarbonyl Complexes OLn( $\bar{I}$ - <sup>2</sup> -CO) (Ln =) Tj ETQq0 0 0 rgBT /Overlock 1.9	1.9	0
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10068	<scp>SVECV</scp>â€f12: A composite scheme for accurate and costâ€effective evaluation of reaction barriers. <scp>ll</scp>. Benchmarking using Karton's <scp>BH28</scp> barrier heights database. <i>International Journal of Quantum Chemistry</i> , 2023, 123, .	1.0	3
10069	Absolute excited state molecular geometries revealed by resonance Raman signals. <i>Nature Communications</i> , 2022, 13, .	5.8	3
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10075	Computational Study of New Small Molecules based Thiophene as Donor Materials for Bulk Heterojunction Photovoltaic Cells. <i>Journal of Fluorescence</i> , 2023, 33, 553-563.	1.3	3
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10078	Characterization of excited states in time-dependent density functional theory using localized molecular orbitals. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	1
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10096	Effect of acetylene linkage on solvatochromism of betaine consisting of 1-methylpyridinium and phenolate units. <i>Results in Chemistry</i> , 2023, 5, 100784.	0.9	0
10097	Experimental and Computational Study of Triphenylamine Dyes for Photovoltaic Cell Applications. <i>EPL Applied Physics</i> , 0, , .	0.3	0
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10155	Probing Colossal Carbon Rings. <i>Journal of Physical Chemistry A</i> , 2023, 127, 1168-1178.	1.1	3
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10166	Design of A type carbon nano hoops with enhanced nonlinear optical response: a size-dependent effect study. <i>New Journal of Chemistry</i> , 2023, 47, 5390-5398.	1.4	3
10167	Communication of molecular fluorophores with other photoluminescence centres in carbon dots. <i>Nanoscale</i> , 2023, 15, 4022-4032.	2.8	8
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10179	Modulation of chiral spectral deflection by van der Waals force-induced molecular electropolarization in catenane oligomers. <i>RSC Advances</i> , 2023, 13, 11055-11061.	1.7	1
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10183	Creating intense and refined NLO responses by utilizing dual donor structural designs in A-D-D-A type organic switches: computed device parameters. <i>Structural Chemistry</i> , 2023, 34, 2021-2038.	1.0	8
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