TheoDORE: A toolbox for a detailed and automated anal computations

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Citation Report

#	Article	IF	Citations
1	Enhanced Rigidity Changes Ultraviolet Absorption: Effect of a Merocyanine Binder on G-Quadruplex Photophysics. Journal of Physical Chemistry Letters, 2020, 11, 10212-10218.	2.1	10
2	Analysis and visualization of energy densities. II. Insights from linear-response time-dependent density functional theory calculations. Physical Chemistry Chemical Physics, 2020, 22, 26852-26864.	1.3	12
3	Spatial Anisotropy of Charge Transfer at Perfluoropentaceneâ€“Pentacene (001) Single-Crystal Interfaces and its Relevance for Thin Film Devices. ACS Applied Materials & Interfaces, 2020, 12, 53547-53556.	4.0	9
4	Multiscale Conformational Sampling Reveals Excited-State Locality in DNA Self-Repair Mechanism. Journal of Physical Chemistry A, 2020, 124, 9133-9140.	1.1	6
5	Excimer Intermediates en Route to Long-Lived Charge-Transfer States in Single-Stranded Adenine DNA as Revealed by Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 7483-7488.	2.1	21
6	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. Inorganic Chemistry, 2020, 59, 14666-14678.	1.9	23
7	Exciton Isolation in Cross-Pentacene Architecture. Journal of the American Chemical Society, 2020, 142, 17393-17402.	6.6	15
8	Ground- and Excited-State Properties of Iron(II) Complexes Linked to Organic Chromophores. Inorganic Chemistry, 2020, 59, 14746-14761.	1.9	28
9	Modulating Excited Charge-Transfer States of G-Quartet Self-Assemblies by Earth Alkaline Cations and Hydration. Journal of Physical Chemistry A, 2020, 124, 8101-8111.	1.1	4
10	Electronic structure software. Journal of Chemical Physics, 2020, 153, 070401.	1.2	34
11	Stacking Effects on Anthraquinone/DNA Charge-Transfer Electronically Excited States. Molecules, 2020, 25, 5927.	1.7	5
12	Charge Separation and Charge Transfer in the Low-Lying Excited States of Pentacene. Journal of Physical Chemistry C, 2020, 124, 24653-24666.	1.5	25
13	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. Chemical Science, 2020, 11, 7685-7693.	3.7	9
14	Potential energy surfaces of charge transfer states. Molecular Physics, 2020, 118, e1776903.	0.8	9
15	A New Benchmark Set for Excitation Energy of Charge Transfer States: Systematic Investigation of Coupled Cluster Type Methods. Journal of Chemical Theory and Computation, 2020, 16, 4213-4225.	2.3	48
16	Multiâ€Tier Electronic Structure Analysis of Sita's Mo and W Complexes Capable of Thermal or Photochemical N₂Splitting. European Journal of Inorganic Chemistry, 2020, 2020, 1506-1518.	1.0	10
17	A systematic analysis of excitonic properties to seek optimal singlet fission: the BN-substitution patterns in tetracene. Journal of Materials Chemistry C, 2020, 8, 7793-7804.	2.7	22
18	pysisyphus: Exploring potential energy surfaces in ground and excited states. International Journal of Quantum Chemistry, 2021, 121, e26390.	1.0	29

#	Article	IF	Citations
19	Fullerene Desymmetrization as a Means to Achieve Singleâ€Enantiomer Electron Acceptors with Maximized Chiroptical Responsiveness. Advanced Materials, 2021, 33, e2004115.	11.1	35
20	Improved Description of Charge-Transfer Potential Energy Surfaces via Spin-Component-Scaled CC2 and ADC(2) Methods. Journal of Chemical Theory and Computation, 2021, 17, 439-449.	2.3	14
21	Probing solvents effects on the absorption spectrum of oxo-centered carbonyl-triruthenium clusters. Polyhedron, 2021, 194, 114944.	1.0	2
22	Tetradentate N^NÂ°N^N-type luminophores for Pt(II) complexes: Synthesis, photophysical and quantum-chemical investigation. Inorganica Chimica Acta, 2021, 518, 120090.	1.2	10
23	Platinum and palladium complexes of tridentate â^'C^N^N (phen-ide)-pyridine-thiazol ligands â€“ A case study involving spectroelectrochemistry, photoluminescence spectroscopy and TD-DFT calculations. Inorganica Chimica Acta, 2021, 518, 120093.	1.2	18
24	Suppressing dimer formation by increasing conformational freedom in multi-carbazole thermally activated delayed fluorescence emitters. Journal of Materials Chemistry C, 2021, 9, 189-198.	2.7	25
25	Ultrafast photochemistry of a molybdenum carbonylâ€“nitrosyl complex with a triazacyclononane coligand. Physical Chemistry Chemical Physics, 2021, 23, 24187-24199.	1.3	2
26	Higher MLCT lifetime of carbene iron(<scp>ii</scp>) complexes by chelate ring expansion. Chemical Communications, 2021, 57, 7541-7544.	2.2	24
27	Conjugation- and Aggregation-Directed Design of Covalent Organic Frameworks as White-Light-Emitting Diodes. Journal of the American Chemical Society, 2021, 143, 1061-1068.	6.6	75
28	Ultrafast and long-time excited state kinetics of an NIR-emissive vanadium(<scp>iii</scp>) complex I: synthesis, spectroscopy and static quantum chemistry. Chemical Science, 2021, 12, 10780-10790.	3.7	28
29	The importance of finite temperature and vibrational sampling in the absorption spectrum of a nitro-functionalized Ru(<scp>ii</scp>) water oxidation catalyst. Physical Chemistry Chemical Physics, 2021, 23, 17724-17733.	1.3	2
30	Ultrafast and long-time excited state kinetics of an NIR-emissive vanadium(<scp>iii</scp>) complex II. Elucidating triplet-to-singlet excited-state dynamics. Chemical Science, 2021, 12, 10791-10801.	3.7	24
31	Distinct photodynamics of Îº-N and Îº-C pseudoisomeric iron(<scp>ii</scp>) complexes. Chemical Communications, 2021, 57, 6640-6643.	2.2	23
32	Influence of the Environment on Shaping the Absorption of Monomeric Infrared Fluorescent Proteins. Journal of Physical Chemistry B, 2021, 125, 2231-2240.	1.2	1
33	Effect of varying the TD-lc-DFTB range-separation parameter on charge and energy transfer in a model pentacene/buckminsterfullerene heterojunction. Journal of Chemical Physics, 2021, 154, 054102.	1.2	9
34	Deciphering excited state properties utilizing algebraic diagrammatic construction schemes of decreasing order. Journal of Computational Chemistry, 2021, 42, 793-800.	1.5	3
35	Deciphering the Chemical Basis of Fluorescence of a Seleniumâ€Labeled Uracil Probe when Bound at the Bacterial Ribosomal Aâ€Site. Chemistry - A European Journal, 2021, 27, 4927-4931.	1.7	3
36	Elucidating the Electronic Structure of a Delayed Fluorescence Emitter via Orbital Interactions, Excitation Energy Components, Charge-Transfer Numbers, and Vibrational Reorganization Energies. Journal of Physical Chemistry Letters, 2021, 12, 2712-2720.	2.1	35

#	Article	IF	Citations
37	Applicability of DFT functionals for evaluating the first hyperpolarizability of phenol blue in solution. Journal of Chemical Physics, 2021, 154, 094501.	1.2	6
38	Assessing challenging intraâ€•and <scp>interâ€molecular chargeâ€transfer</scp> excitations energies with <scp>doubleâ€hybrid</scp> density functionals. Journal of Computational Chemistry, 2021, 42, 970-981.	1.5	22
39	How the Size and Density of Charge-Transfer Excitons Depend on Heterojunctionâ€™s Architecture. Journal of Physical Chemistry C, 2021, 125, 5458-5474.	1.5	6
40	Unexpectedly Long Lifetime of the Excited State of Benzothiadiazole Derivative and Its Adducts with Lewis Acids. Molecules, 2021, 26, 2030.	1.7	5
41	Quantum Dynamics of Exciton Transport and Dissociation in Multichromophoric Systems. Annual Review of Physical Chemistry, 2021, 72, 591-616.	4.8	31
42	Embelinâ€™s Versatile Photochemistry Makes It a Potent Photosensitizer for Photodynamic Therapy. Journal of Physical Chemistry B, 2021, 125, 3527-3537.	1.2	2
43	Exploitation of Baird Aromaticity and Clarâ€™s Rule for Tuning the Triplet Energies of Polycyclic Aromatic Hydrocarbons. Chemistry, 2021, 3, 532-549.	0.9	15
44	The orbital picture of the first dipole hyperpolarizability from many-body response theory. Journal of Chemical Physics, 2021, 154, 184109.	1.2	7
45	Chasing unphysical TD-DFT excited states in transition metal complexes with a simple diagnostic tool. Journal of Chemical Physics, 2021, 154, 204102.	1.2	8
46	Visualisation of Chemical Shielding Tensors (VIST) to Elucidate Aromaticity and Antiaromaticity**. European Journal of Organic Chemistry, 2021, 2021, 2529-2539.	1.2	16
47	Reference Energies for Intramolecular Charge-Transfer Excitations. Journal of Chemical Theory and Computation, 2021, 17, 3666-3686.	2.3	51
48	Quantum chemical investigation of the ground- and excited-state acidities of a dihydroxyfuranoflavylium cation. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	2
49	Learning the Exciton Properties of Azo-dyes. Journal of Physical Chemistry Letters, 2021, 12, 5957-5962.	2.1	4
50	Competition between the Photothermal Effect and Emission in Potential Phototherapy Agents. Journal of Physical Chemistry B, 2021, 125, 8733-8741.	1.2	7
51	On the Low-Lying Electronically Excited States of Azobenzene Dimers: Transition Density Matrix Analysis. Molecules, 2021, 26, 4245.	1.7	9
52	An efficient Fock space multi-reference coupled cluster method based on natural orbitals: Theory, implementation, and benchmark. Journal of Chemical Physics, 2021, 155, 014105.	1.2	4
53	Self-assembly of rylene-decorated guanine ribbons on graphene surface for optoelectronic applications: a theoretical study. Nanotechnology, 2021, 32, 435405.	1.3	2
54	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518

#	Article	IF	Citations
55	A Ruthenium(II) Water Oxidation Catalyst Containing a pH-Responsive Ligand Framework. Inorganic Chemistry, 2021, 60, 13299-13308.	1.9	7
56	Tuning the Properties of Azadipyrromethene-Based Near-Infrared Dyes Using Intramolecular BO Chelation and Peripheral Substitutions. Inorganic Chemistry, 2021, 60, 13320-13331.	1.9	11
57	Null Exciton-Coupled Chromophoric Dimer Exhibits Symmetry-Breaking Charge Separation. Journal of the American Chemical Society, 2021, 143, 13769-13781.	6.6	57
58	Highly Emissive Biological Bilirubin Molecules: Shedding New Light on the Phototherapy Scheme. Journal of Physical Chemistry B, 2021, 125, 9213-9222.	1.2	3
59	A Series of Iron(II)â€NHC Sensitizers with Remarkable Power Conversion Efficiency in Photoelectrochemical Cells**. Chemistry - A European Journal, 2021, 27, 16260-16269.	1.7	16
60	Minimal-active-space multistate density functional theory for excitation energy involving local and charge transfer states. Npj Computational Materials, 2021, 7, .	3.5	12
61	Spectral Signatures of Oxidation States in a Manganeseâ€Oxo Cubane Water Oxidation Catalyst. Chemistry - A European Journal, 2021, 27, 17078-17086.	1.7	4
62	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(pâ€˜phenylene vinylene)s (PPVs). Open Research Europe, 0, 1, 111.	2.0	2
63	Ligand-controlled and nanoconfinement-boosted luminescence employing Pt(<scp>ii</scp>) and Pd(<scp>ii</scp>) complexes: from color-tunable aggregation-enhanced dual emitters towards self-referenced oxygen reporters. Chemical Science, 2021, 12, 3270-3281.	3.7	43
64	Functional group introduction and aromatic unit variation in a set of Ï€-conjugated macrocycles: revealing the central role of local and global aromaticity. Organic Chemistry Frontiers, 2021, 8, 4730-4745.	2.3	10
65	Influence of the crystal packing in singlet fission: one step beyond the gas phase approximation. Physical Chemistry Chemical Physics, 2021, 23, 14164-14177.	1.3	12
66	Excitonic Model for Strongly Coupled Multichromophoric Systems: The Electronic Circular Dichroism Spectra of Guanine Quadruplexes as Test Cases. Journal of Chemical Theory and Computation, 2021, 17, 405-415.	2.3	19
67	Density functional theory calculations of large systems: Interplay between fragments, observables, and computational complexity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1574.	6.2	16
68	Luminescent Pd(II) Complexes with Tridentate ^{â^’} Arylâ€pyridineâ€(benzo)thiazole Ligands. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2022, 648, e202100278.	0.6	5
69	First-principles interpretation of electron transport through single-molecule junctions using molecular dynamics of electron attached states. Molecular Physics, 2021, 119, .	0.8	2
70	Alkaline Earth Cations Binding Mode Tailors Excited-State Charge Transfer Properties of Guanine Quadruplex: A TDDFT Study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, , 120584.	2.0	0
71	The role of excited-state character, structural relaxation, and symmetry breaking in enabling delayed fluorescence activity in pushâ€“pull chromophores. Physical Chemistry Chemical Physics, 2021, 23, 26135-26150.	1.3	10
72	Low efficiency roll-off blue TADF OLEDs employing a novel acridineâ€“pyrimidine based high triplet energy host. Journal of Materials Chemistry C, 2021, 9, 17471-17482.	2.7	14

#	Article	IF	Citations
73	Charge-Transfer Landscape Manifesting the Structureâ€“Rate Relationship in the Condensed Phase Via Machine Learning. Journal of Physical Chemistry B, 2021, 125, 13267-13278.	1.2	11
74	Tuning the Quantum Chemical Properties of Flavins via Modification at C8. Journal of Physical Chemistry B, 2021, 125, 12654-12669.	1.2	7
75	Are luminescent Ru2+ chelated complexes selective coordinative sensors for the detection of heavy cations?. Physical Chemistry Chemical Physics, 2022, 24, 2309-2317.	1.3	0
76	libwfa: Wavefunction analysis tools for excited and openâ€shell electronic states. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	16
77	Energy Counterbalance to Harness Photoinduced Structural Planarization of Dibenzo[b,f]azepines toward Thermal Reversibility. Journal of the American Chemical Society, 2022, 144, 1748-1757.	6.6	15
78	Panchromatic Absorption and Oxidation of an Iron(II) Spin Crossover Complex. Inorganic Chemistry, 2022, 61, 1659-1671.	1.9	10
79	Impact of Charge-Resonance Excitations on CT-Mediated J-Type Aggregation in Singlet and Triplet Exciton States of Perylene Di-Imide Aggregates: A TDDFT Investigation. Computation, 2022, 10, 18.	1.0	4
80	Exciton interactions in helical crystals of a hydrogen-bonded eumelanin monomer. Chemical Science, 2022, 13, 2331-2338.	3.7	6
81	The overlooked NIR luminescence of Cr(ppy)₃. Chemical Communications, 2022, 58, 3701-3704.	2.2	16
82	Unraveling the acid-base characterization and solvent effects on structural and electronic properties of a bis-bidentated bridging ligand. Physical Chemistry Chemical Physics, 2022, , .	1.3	4
83	Photoinduced waterâ€“chromophore electron transfer causes formation of guanosine photodamage. Physical Chemistry Chemical Physics, 2022, 24, 8217-8224.	1.3	3
84	Excited-state proton transfer in a 2-aminopyridine dimer: a surface hopping study. Physical Chemistry Chemical Physics, 2022, 24, 7274-7292.	1.3	1
85	Charge-Transfer Excitations within Density Functional Theory: How Accurate Are the Most Recommended Approaches?. Journal of Chemical Theory and Computation, 2022, 18, 1646-1662.	2.3	30
86	Taming Disulfide Bonds with Laser Fields. Nonadiabatic Surface-Hopping Simulations in a Ruthenium Complex. Journal of Physical Chemistry Letters, 2022, 13, 1894-1900.	2.1	6
87	Organic materials repurposing, a data set for theoretical predictions of new applications for existing compounds. Scientific Data, 2022, 9, 54.	2.4	16
88	Effects of Heterocyclic Ring Fusion and Chain Elongation on Chiroptical Properties of Polyaza[9]helicene: A Computational Study. Journal of Physical Chemistry A, 2022, 126, 1412-1421.	1.1	5
89	[2.2.2.2]Paracyclophanetetraenes (PCTs): cyclic structural analogues of poly(pâ€˜phenylene vinylene)s (PPVs). Open Research Europe, 0, 1, 111.	2.0	4
90	Ligandâ€induced Donor State Destabilisation â€“ A New Route to Panchromatically Absorbing Cu(I) Complexes. Chemistry - A European Journal, 2022, , .	1.7	5

#	Article	IF	Citations
91	Deciphering the Spectral Tuning Mechanism in Proteorhodopsin: The Dominant Role of Electrostatics Instead of Chromophore Geometry. Chemistry - A European Journal, 2022, 28, .	1.7	5
92	Making optical excitations visible â€“ An exciton wavefunction extension to the time-dependent configuration interaction method. Chemical Physics, 2022, 557, 111502.	0.9	7
93	Computational Calculation of Dissolved Organic Matter Absorption Spectra. Environmental Science & Technology, 2022, 56, 491-500.	4.6	16
94	Virtual Screening of TADF Emitters for Single-Layer OLEDs. Frontiers in Chemistry, 2021, 9, 800027.	1.8	7
95	Accurate Polarization-Resolved Absorption Spectra of Organic Semiconductor Thin Films Using First-Principles Quantum-Chemical Methods: Pentacene as a Case Study. Journal of Physical Chemistry Letters, 2022, 13, 3726-3731.	2.1	11
96	Regiochemistry of Donor Dendrons Controls the Performance of Thermally Activated Delayed Fluorescence Dendrimer Emitters for High Efficiency Solutionâ€Processed Organic Lightâ€Emitting Diodes. Advanced Science, 2022, 9, e2201470.	5.6	19
97	Computerâ€Aided Design of Fluorinated Flavin Derivatives by Modulation of Intersystem Crossing and Fluorescence. ChemPhotoChem, 2022, 6, .	1.5	5
98	Activity-Based Photosensitizers with Optimized Triplet State Characteristics Toward Cancer Cell Selective and Image Guided Photodynamic Therapy. ACS Applied Bio Materials, 2022, 5, 2754-2767.	2.3	5
99	Evaluation of molecular photophysical and photochemical properties using linear response time-dependent density functional theory with classical embedding: Successes and challenges. Journal of Chemical Physics, 2022, 156, .	1.2	10
100	Vibronic effects accelerate the intersystem crossing processes of the through-space charge transfer states in the triptycene bridged acridineâ€“triazine donorâ€“acceptor molecule TpAT-tFFO. Chemical Science, 2022, 13, 7057-7066.	3.7	9
101	Twisting Enabled Charge Transfer Excitons in Epitaxially Fused Quantum Dot Molecules. Nano Letters, 2022, 22, 4912-4918.	4.5	6
102	Constructing high-performance TADF polymers from non-TADF monomers: a computational investigation. Physical Chemistry Chemical Physics, 2022, 24, 17686-17694.	1.3	6
103	Following the density evolution using real time density functional theory and density based indexes: Application to model pushâ€“pull molecules. Journal of Computational Chemistry, 2022, 43, 1464-1473.	1.5	3
104	Electronic Structure Effects Related to the Origin of the Remarkable Near-Infrared Absorption of Blastochloris viridisâ€™ Light Harvesting 1-Reaction Center Complex. Journal of Chemical Theory and Computation, 2022, 18, 4555-4564.	2.3	2
105	Nonadiabatic molecular dynamics simulations based on time-dependent density functional tight-binding method. Journal of Chemical Physics, 2022, 157, .	1.2	5
106	Towards Optimized Photoluminescent Copper(I) Phenanthroline-Functionalized Complexes: Control of the Photophysics by Symmetry-Breaking and Spinâ€“Orbit Coupling. Materials, 2022, 15, 5222.	1.3	4
107	Excited state processes in nitrile-substituted 2-(oxazolinyl)-phenols in gas and implicit solvents: A computational study. Chemical Physics Letters, 2022, 806, 139969.	1.2	1
108	Luminescent Iridium Complexes with a Sulfurated Bipyridine Ligand: PCET Thermochemistry of the Disulfide Unit and Photophysical Properties. Inorganic Chemistry, 0, , .	1.9	2

#	Article	IF	Citations
109	Highâ€Performance Blue Electroluminescence Devices Based on Linear Gold(I) Complexes as Ultrafast Triplet Exciton Harvesters. Advanced Optical Materials, 2022, 10, .	3.6	8
110	Natamycin sequesters ergosterol and interferes with substrate transport by the lysine transporter Lyp1 from yeast. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 184012.	1.4	10
111	Isoelectronic Pt(II) Complexes of Cyclometalating C^N^N Ligands with Phenyl/(Benzo)thiophenyl and Pyridyl/(Benzo)thiazolyl Moieties. Dalton Transactions, 0, , .	1.6	2
112	Excimer evolution hampers symmetry-broken charge-separated states. Chemical Science, 2022, 13, 10824-10835.	3.7	13
113	Stressing the differences in alizarin and purpurin dyes through UV-visible light absorption and¹H-NMR spectroscopies. Physical Chemistry Chemical Physics, 2022, 24, 19452-19462.	1.3	3
114	Photophysics of Anionic Bis(4Hâ€imidazolato)Cu(I) Complexes. Chemistry - A European Journal, 0, , .	1.7	3
115	Trajectory Surface Hopping for a Polarizable Embedding QM/MM Formulation. Journal of Physical Chemistry A, 2022, 126, 6780-6789.	1.1	6
116	Atomic Group Decomposition of Charge Transfer Excitation Global Indexes. Journal of Physical Chemistry A, 2022, 126, 6314-6328.	1.1	1
117	The Full d³â€“d⁵ Redox Series of Mononuclear Manganese Complexes: Geometries and Electronic Structures of [Mn(dgpy)₂]ⁿ⁺. Inorganic Chemistry, 2022, 61, 14616-14625.	1.9	5
118	Photodynamics of Gasâ€Phase Pyruvic Acid Following Light Absorption in the Actinic Region. ChemPhotoChem, 2022, 6, .	1.5	3
119	Bright Vâ€Shaped bisâ€imidazo[1,2â€a]pyridine Fluorophores with Nearâ€UV to Deepâ€Blue Emission. Chemistry - an Asian Journal, 2022, 17, .	1.7	7
120	Newton-X Platform: New Software Developments for Surface Hopping and Nuclear Ensembles. Journal of Chemical Theory and Computation, 2022, 18, 6851-6865.	2.3	18
121	Dissecting conjugation and electronic effects on the linear and non-linear optical properties of rhenium(<scp>i</scp>) carbonyl complexes. Physical Chemistry Chemical Physics, 2022, 24, 28069-28079.	1.3	2
122	Non-empirical double-hybrid density functionals as reliable tools for electronic structure calculations. Electronic Structure, 2022, 4, 043001.	1.0	4
123	A Thermally Activated Delayed Fluorescence Emitter Investigated by Timeâ€Resolved Nearâ€Infrared Spectroscopy. Chemistry - A European Journal, 2023, 29, .	1.7	4
124	A posteriori localization of manyâ€body excited states through simultaneous diagonalization. Journal of Computational Chemistry, 2023, 44, 105-116.	1.5	1
125	Effects of Size and Morphology on the Excited-State Properties of Nanoscale WO₃ Materials from First-Principles Calculations: Implications for Optoelectronic Devices. ACS Applied Nano Materials, 2022, 5, 16289-16297.	2.4	1
126	A Materials Acceleration Platform for Organic Laser Discovery. Advanced Materials, 2023, 35, .	11.1	10

#	Article	IF	Citations
127	Classification and Analysis of Molecular Excited States. , 2024, , 55-83.		3
128	Triplet Emitting C^N^C Cyclometalated Dibenzo[c,h]Acridine Pt(II) Complexes. Molecules, 2022, 27, 8054.	1.7	2
129	On the Cooperative Origin of Solvent-Enhanced Symmetry-Breaking Charge Transfer in a Covalently Bound Tetracene Dimer Leading to Singlet Fission. Journal of the American Chemical Society, 2022, 144, 23492-23504.	6.6	7
130	Intersystem Crossing and Intramolecular Triplet Excitation Energy Transfer in Spiro[9,10-dihydro-9-oxoanthracene-10,2Â´-5Â´,6Â´-benzindan] Investigated by DFT/MRCI Methods. Canadian Journal of Chemistry, 0, , .	0.6	0
131	Highly Luminescent Blue Emitter with Balanced Hybridized Locally and Chargeâ€Transfer Excitedâ€States Emission. ChemPhotoChem, 2023, 7, .	1.5	1
132	The subsystem quantum chemistry program <scp>Serenity</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	11
133	Understanding Charge Dynamics in Dense Electronic Manifolds in Complex Environments. Journal of Chemical Theory and Computation, 2023, 19, 626-639.	2.3	7
134	Theoretical Study of Charge Mobility in Crystal Porphine and a Computer Design of a Porphine-Based Semiconductive Discotic Liquid Mesophase. International Journal of Molecular Sciences, 2023, 24, 736.	1.8	1
135	Intermolecular Interactions and Charge Resonance Contributions to Triplet and Singlet Exciton States of Oligoacene Aggregates. Molecules, 2023, 28, 119.	1.7	1
136	Remote Steric Control of the Tetrahedral Coordination Geometry around Heteroleptic Copper(I) Bis(Diimine) Complexes. Molecules, 2023, 28, 983.	1.7	1
137	Effects of solvent polarity on the novel excited-state intramolecular thiol proton transfer and photophysical property compared with the oxygen proton transfer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2023, 293, 122475.	2.0	29
138	Energy Component Analysis for Electronically Excited States of Molecules: Why the Lowest Excited State Is Not Always the HOMO/LUMO Transition. Journal of Chemical Theory and Computation, 2023, 19, 2340-2352.	2.3	8
139	Room-Temperature Phosphorescence from Pd(II) and Pt(II) Complexes as Supramolecular Luminophores: The Role of Self-Assembly, Metalâ€“Metal Interactions, Spinâ€“Orbit Coupling, and Ligand-Field Splitting. Journal of the American Chemical Society, 2023, 145, 3937-3951.	6.6	20
140	Dicarbon defect in hexagonal boron nitride monolayer - a theoretical study. Canadian Journal of Chemistry, 0, , .	0.6	1
141	Excited states of <scp>orthoâ€nitrobenzaldehyde</scp> as a challenging case for singleâ€and <scp>multiâ€reference</scp> electronic structure theory. Journal of Computational Chemistry, 2023, 44, 1381-1394.	1.5	4
142	Janus-type emission from a cyclometalated iron(iii) complex. Nature Chemistry, 2023, 15, 468-474.	6.6	19
143	Effect of stacking interactions on charge transfer states in photoswitches interacting with ion channels. Physical Chemistry Chemical Physics, 2023, 25, 8331-8335.	1.3	0
144	Effect of Terminal Fluorination on Chiroptical Properties of Carbo[5â€“8]helicenes: A Systematic Computational Study at the RI-ADC(2) Level. Journal of Physical Chemistry A, 2023, 127, 2284-2294.	1.1	0

#	Article	IF	Citations
145	Biphenyl Au(III) Complexes with Phosphine Ancillary Ligands: Synthesis, Optical Properties, and Electroluminescence in Light-Emitting Electrochemical Cells. Inorganic Chemistry, 2023, 62, 4903-4921.	1.9	4
146	Classification of doubly excited molecular electronic states. Chemical Science, 2023, 14, 4012-4026.	3.7	5
147	Panchromatic light harvesting and record power conversion efficiency for carboxylic/cyanoacrylic Fe(<scp>ii</scp>) NHC co-sensitized FeSSCs. Chemical Science, 2023, 14, 4288-4301.	3.7	10
148	Effect of Fluorine Substitution on Absorption and Emission Properties of Figureâ€eightâ€shaped [5]Helicene Dimer : A Computational Study at RIâ€MP2/RIâ€ADC(2) Level. ChemPhysChem, 0, , .	1.0	0
149	An Expedited Route to Optical and Electronic Properties at Finite Temperature via Unsupervised Learning. Molecules, 2023, 28, 3411.	1.7	3
157	Multistate Energy Decomposition Analysis of Molecular Excited States. Jacs Au, 2023, 3, 1800-1819.	3.6	3
159	Solar cells: Organic photovoltaic solar cells. , 2023, , 247-263.		0
160	DNA photostability. , 2023, , 311-336.		0
176	Keeping the chromophores crossed: evidence for null exciton splitting. Chemical Society Reviews, 2023, 52, 6664-6679.	18.7	6
193	Visualizing and characterizing excited states from time-dependent density functional theory. Physical Chemistry Chemical Physics, 2024, 26, 3755-3794.	1.3	2