Hans Ãgren

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9576892/publications.pdf

Version: 2024-02-01

		9264	16183
491	22,433	74	124
papers	citations	h-index	g-index

498	498	498	18988
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cloud droplet activation mechanisms of amino acid aerosol particles: insight from molecular dynamics simulations. Tellus, Series B: Chemical and Physical Meteorology, 2022, 65, 20476.	1.6	22
2	Simultaneous anchoring of Ni nanoparticles and single-atom Ni on BCN matrix promotes efficient conversion of nitrate in water into high-value-added ammonia. Chemical Engineering Journal, 2022, 433, 133190.	12.7	46
3	Recent Advances in Oxidation Stable Chemistry of 2D MXenes. Advanced Materials, 2022, 34, e2107554.	21.0	163
4	Thermal degradation of optical resonances in plasmonic nanoparticles. Nanoscale, 2022, 14, 433-447.	5.6	6
5	Development of 11C-Labeled ASEM Analogues for the Detection of Neuronal Nicotinic Acetylcholine Receptors (Î±7-nAChR). ACS Chemical Neuroscience, 2022, 13, 352-362.	3.5	6
6	Optical Properties of Few-Layer Ti₃CN MXene: From Experimental Observations to Theoretical Calculations. ACS Nano, 2022, 16, 3059-3069.	14.6	46
7	Ultrafast photonics applications of emerging 2D-Xenes beyond graphene. Nanophotonics, 2022, 11, 1261-1284.	6.0	65
8	Thiazoline Carbeneâ€“Cu(I)â€“Amide complexes: Efficient White Electroluminescence from Combined Monomer and Excimer Emission. ACS Applied Materials & Interfaces, 2022, 14, 15478-15493.	8.0	25
9	Odd-Number Cyclo[n]Carbons Sustaining Alternating Aromaticity. Journal of Physical Chemistry A, 2022, 126, 2445-2452.	2.5	7
10	Imaging Fluorescence Blinking of a Mitochondrial Localization Probe: Cellular Localization Probes Turned into Multifunctional Sensors. Journal of Physical Chemistry B, 2022, 126, 3048-3058.	2.6	6
11	Water molecular bridge-induced selective dual polarization in crystals for stable multi-emitters. Chemical Science, 2022, 13, 6067-6073.	7.4	3
12	Toward Novel [18F]Fluorine-Labeled Radiotracers for the Imaging of Î±-Synuclein Fibrils. Frontiers in Aging Neuroscience, 2022, 14, 830704.	3.4	5
13	Chain Length Modulated Dimerization and Cyclization of Terminal Thienyl-Blocked Oligopyrranes. Organic Letters, 2022, 24, 5428-5432.	4.6	2
14	Efficient Dye-Sensitized Solar Cells Based on a New Class of Doubly Concerted Companion Dyes. ACS Applied Materials & Interfaces, 2022, 14, 33274-33284.	8.0	28
15	X-ray absorption of molecular cationsâ€”a new challenge for electronic structure theory. Journal of Physics Condensed Matter, 2022, 34, 363002.	1.8	6
16	Recent research progress for upconversion assisted dye-sensitized solar cells. Chinese Chemical Letters, 2021, 32, 1834-1846.	9.0	28
17	Impact of molecular and packing structure on the charge-transport properties of hetero[8]circulenes. Journal of Materials Chemistry C, 2021, 9, 1451-1466.	5.5	11
18	Nucleotide Interaction with a Chitosan Layer on a Silica Surface: Establishing the Mechanism at the Molecular Level. Langmuir, 2021, 37, 1511-1520.	3.5	12

#	Article	IF	Citations
19	In silico studies of ASEM analogues targeting Î±7-nAChR and experimental verification. RSC Advances, 2021, 11, 3942-3951.	3.6	2
20	Ultraâ€Small 2D PbS Nanoplatelets: Liquidâ€Phase Exfoliation and Emerging Applications for Photoâ€Electrochemical Photodetectors. Small, 2021, 17, e2005913.	10.0	50
21	Atomistic description of plasmonic generation in alloys and core shell nanoparticles. Physical Chemistry Chemical Physics, 2021, 23, 173-185.	2.8	5
22	Breaking inversion symmetry by protonation: experimental and theoretical NEXAFS study of the diazynium ion, N₂H⁺. Physical Chemistry Chemical Physics, 2021, 23, 17166-17176.	2.8	10
23	Introducing chenodeoxycholic acid coadsorbent and strong electron-withdrawing group in indoline dyes to design high-performance solar cells: a remarkable theoretical improvement. Journal of Materials Chemistry C, 2021, 9, 5800-5807.	5.5	22
24	Manipulating crystals through photoexcitation-induced molecular realignment. Journal of Materials Chemistry C, 2021, 9, 11707-11714.	5.5	25
25	Copper confined in vesicle-like BCN cavities promotes electrochemical reduction of nitrate to ammonia in water. Journal of Materials Chemistry A, 2021, 9, 23675-23686.	10.3	42
26	Heteroâ€MXenes: Theory, Synthesis, and Emerging Applications. Advanced Materials, 2021, 33, e2004129.	21.0	150
27	PbSe Nanocrystals Produced by Facile Liquid Phase Exfoliation for Efficient UVâ€“Vis Photodetectors. Advanced Functional Materials, 2021, 31, 2010401.	14.9	35
28	Lighting up solid states using a rubber. Nature Communications, 2021, 12, 908.	12.8	21
29	Optimized Disarybisthiazole Derivatives with High Affinity to Alpha-synuclein Aggregates and Improved Pharmacokinetics. Nuklearmedizin - NuclearMedicine, 2021, 60, .	0.7	0
30	Dianthracenylazatrioxa[8]circulene: Synthesis, Characterization and Application in OLEDs. Chemistry - A European Journal, 2021, 27, 11609-11617.	3.3	7
31	Visualizing Material Processing via Photoexcitation-Controlled Organic-Phase Aggregation-Induced Emission. Research, 2021, 2021, 9862093.	5.7	13
32	Plasmonic Enhancement of Local Fields in Ultrafine Metal Nanoparticles. Journal of Physical Chemistry C, 2021, 125, 13900-13908.	3.1	6
33	Enhancing the Operability of Photoexcitation-Controlled Aggregation-Induced Emissive Molecules in the Organic Phase. Journal of Physical Chemistry Letters, 2021, 12, 6182-6189.	4.6	20
34	NIRâ€II Responsive Inorganic 2D Nanomaterials for Cancer Photothermal Therapy: Recent Advances and Future Challenges. Advanced Functional Materials, 2021, 31, 2101625.	14.9	126
35	Cryptic Sites in Tau Fibrils Explain the Preferential Binding of the AV-1451 PET Tracer toward Alzheimerâ€™s Tauopathy. ACS Chemical Neuroscience, 2021, 12, 2437-2447.	3.5	24
36	Black Phosphorus/Polymers: Status and Challenges. Advanced Materials, 2021, 33, e2100113.	21.0	53

#	Article	IF	Citations
37	Dissecting the Binding Profile of PET Tracers to Corticobasal Degeneration Tau Fibrils. ACS Chemical Neuroscience, 2021, 12, 3487-3496.	3.5	17
38	Schiff Base Zinc(II) Complexes as Promising Emitters for Blue Organic Light-Emitting Diodes. ACS Applied Electronic Materials, 2021, 3, 3436-3444.	4.3	34
39	Quadrupolar Dyes Based on Highly Polarized Coumarins. Organic Letters, 2021, 23, 6770-6774.	4.6	10
40	Direct Visualization of Nearly Free Electron States Formed by Superatom Molecular Orbitals in a Li@C₆₀ Monolayer. Journal of Physical Chemistry Letters, 2021, 12, 7812-7817.	4.6	9
41	Photoinduced Radical Emission in a Coassembly System. Angewandte Chemie - International Edition, 2021, 60, 23842-23848.	13.8	43
42	Photoinduced Radical Emission in a Coassembly System. Angewandte Chemie, 2021, 133, 24035.	2.0	8
43	Persistent radical pairs trigger nano-gold to highly efficiently and highly selectively drive the value-added conversion of nitroaromatics. Chem Catalysis, 2021, 1, 1118-1132.	6.1	10
44	Applications of Few-Layer Nb₂C MXene: Narrow-Band Photodetectors and Femtosecond Mode-Locked Fiber Lasers. ACS Nano, 2021, 15, 954-965.	14.6	176
45	Single-layer polymeric tetraoxa[8]circulene modified by s-block metals: toward stable spin qubits and novel superconductors. Nanoscale, 2021, 13, 4799-4811.	5.6	9
46	Multidimensional Structure Conformation of Persulfurated Benzene for Highly Efficient Phosphorescence. ACS Applied Materials & Interfaces, 2021, 13, 1314-1322.	8.0	13
47	Making Nitronaphthalene Fluoresce. Journal of Physical Chemistry Letters, 2021, 12, 10295-10303.	4.6	7
48	Confusion Approach Modulated Syntheses of Corrorin Parasitized Hexaphyrins(1.1.1.1.1.0) and the Oxidative Ring Cleavage Behavior. Organic Letters, 2021, 23, 8307-8311.	4.6	3
49	Two-dimensional BCN matrix inlaid with single-atom-Cu driven electrochemical nitrate reduction reaction to achieve sustainable industrial-grade production of ammonia. Applied Materials Today, 2021, 25, 101206.	4.3	31
50	Point and complex defects in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Pd</mml:mi><mml:msub><mml:mi>Se</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:m : Evolution of electronic structure and emergence of magnetism. Physical Review B, 2021, 104, .	3.2	11
51	Material-based engineering of bacteria for cancer diagnosis and therapy. Applied Materials Today, 2021, 25, 101212.	4.3	4
52	Shape Preserving Single Crystal to Amorphous to Single Crystal Polymorphic Transformation Is Possible. Journal of the American Chemical Society, 2021, 143, 20202-20206.	13.7	0
53	A Facile Approach for Elementalâ€Doped Carbon Quantum Dots and Their Application for Efficient Photodetectors. Small, 2021, 17, e2105683.	10.0	16
54	A Facile Approach for Elementalâ€Doped Carbon Quantum Dots and Their Application for Efficient Photodetectors (Small 52/2021). Small, 2021, 17, .	10.0	0

#	Article	IF	Citations
55	Nâ€Confused Phlorinâ€Prodigiosin Chimera: mesoâ€Aryl Oxidation and Ï€â€Extension Triggered by Peripheral Coordination. Angewandte Chemie - International Edition, 2020, 59, 1537-1541.	13.8	32
56	The effect of molecular structure on the properties of quinoxaline-based molecules for OLED applications. Dyes and Pigments, 2020, 173, 108008.	3.7	34
57	Hydrophobic boron organic polymers: Ultra-high capacity of enrichment and storage for chloroform. Chemical Engineering Journal, 2020, 385, 123827.	12.7	11
58	Expanded N-Confused Phlorin: A Platform for a Multiply Fused Polycyclic Ring System via Oxidation within the Macrocycle. Journal of the American Chemical Society, 2020, 142, 17195-17205.	13.7	23
59	Twisted-Planar-Twisted expanded porphyrinoid dimer as a rudimentary reaction-based methanol indicator. Nature Communications, 2020, 11, 5289.	12.8	20
60	Structure and tuneable luminescence in polymeric zinc compounds based on 3-(3-pyridyl)-5-(4-pyridyl)-1,2,4-triazole. Polyhedron, 2020, 191, 114768.	2.2	19
61	Ultraefficient Singlet Oxygen Generation from Manganese-Doped Cesium Lead Chloride Perovskite Quantum Dots. ACS Nano, 2020, 14, 12596-12604.	14.6	20
62	Integrating Timeâ€Resolved Imaging Information by Singleâ€Luminophore Dual Thermally Activated Delayed Fluorescence. Angewandte Chemie - International Edition, 2020, 59, 17018-17025.	13.8	58
63	Can attachment of tert-butyl substituents to methoxycarbazole moiety induce efficient TADF in diphenylsulfone-based blue OLED emitters?. Organic Electronics, 2020, 86, 105894.	2.6	6
64	A Fully Conjugated Planar Heterocyclic [9]Circulene. Journal of the American Chemical Society, 2020, 142, 14058-14063.	13.7	28
65	Two-Dimensional Gold Halides: Novel Semiconductors with Giant Spinâ€“Orbit Splitting and Tunable Optoelectronic Properties. Journal of Physical Chemistry Letters, 2020, 11, 9759-9765.	4.6	3
66	Huge upconversion luminescence enhancement by a cascade optical field modulation strategy facilitating selective multispectral narrow-band near-infrared photodetection. Light: Science and Applications, 2020, 9, 184.	16.6	60
67	Efficient Ambient Electrocatalytic Ammonia Synthesis by Nanogold Triggered via Boron Clusters Combined with Carbon Nanotubes. ACS Applied Materials & Interfaces, 2020, 12, 42821-42831.	8.0	27
68	When are Antiaromatic Molecules Paramagnetic?. Journal of Physical Chemistry C, 2020, 124, 21027-21035.	3.1	18
69	First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids. Physical Chemistry Chemical Physics, 2020, 22, 22314-22323.	2.8	32
70	Aromaticity of Even-Number Cyclo[n]carbons (n = 6â€“100). Journal of Physical Chemistry A, 2020, 124, 10849-10855.	2.5	30
71	Deciphering the unusual fluorescence in weakly coupled bis-nitro-pyrrolo[3,2-b]pyrroles. Communications Chemistry, 2020, 3, .	4.5	37
72	N-Confused Hexapyrrolic Phlorinoid with NIR Absorption: Synthesis, Fusion, Oxidation, and Copper(II) Coordination. Organic Letters, 2020, 22, 9648-9652.	4.6	9

#	Article	IF	Citations
73	Computational design of two-photon active organic molecules for infrared responsive materials. Journal of Materials Chemistry C, 2020, 8, 9867-9873.	5.5	7
74	Potassium ions promote electrochemical nitrogen reduction on nano-Au catalysts triggered by bifunctional boron supramolecular assembly. Journal of Materials Chemistry A, 2020, 8, 13086-13094.	10.3	44
75	BCN-Encapsulated Nano-nickel Synergistically Promotes Ambient Electrochemical Dinitrogen Reduction. ACS Applied Materials & Interfaces, 2020, 12, 31419-31430.	8.0	33
76	Plasmonic nano-shells: atomistic discrete interaction versus classic electrodynamics models. Physical Chemistry Chemical Physics, 2020, 22, 13467-13473.	2.8	14
77	Rational Synthesis of 5,5,5â€Tricyclic Fused Thiaâ€heptaphyrin (1.1.1.1.1.1.0) From a Helical Oligopyrrin Hybrid. Chemistry - an Asian Journal, 2020, 15, 1285-1289.	3.3	4
78	The carbon and oxygen K-edge NEXAFS spectra of CO⁺. Physical Chemistry Chemical Physics, 2020, 22, 16215-16223.	2.8	26
79	Dualâ€Phase Thermally Activated Delayed Fluorescence Luminogens: A Material for Timeâ€Resolved Imaging Independent of Probe Pretreatment and Probe Concentration. Angewandte Chemie, 2020, 132, 7618-7624.	2.0	7
80	Interlayerâ€Sensitized Linear and Nonlinear Photoluminescence of Quasiâ€2D Hybrid Perovskites Using Aggregationâ€Induced Enhanced Emission Active Organic Cation Layers. Advanced Functional Materials, 2020, 30, 1909375.	14.9	21
81	Benzoselenophenylpyridine platinum complexes: green versus red phosphorescence towards hybrid OLEDs. Dalton Transactions, 2020, 49, 3393-3397.	3.3	19
82	Engineering stable radicals using photochromic triggers. Nature Communications, 2020, 11, 945.	12.8	25
83	Dualâ€Phase Thermally Activated Delayed Fluorescence Luminogens: A Material for Timeâ€Resolved Imaging Independent of Probe Pretreatment and Probe Concentration. Angewandte Chemie - International Edition, 2020, 59, 7548-7554.	13.8	46
84	Computational Insight into the Binding Profile of the Second-Generation PET Tracer PI2620 with Tau Fibrils. ACS Chemical Neuroscience, 2020, 11, 900-908.	3.5	29
85	Compressing a Nonâ€Planar Aromatic Heterocyclic [7]Helicene to a Planar Hetero[8]Circulene. Chemistry - A European Journal, 2020, 26, 4935-4940.	3.3	28
86	Free Energy Profile and Kinetics of Coupled Folding and Binding of the Intrinsically Disordered Protein p53 with MDM2. Journal of Chemical Information and Modeling, 2020, 60, 1551-1558.	5.4	28
87	A Fluorescenceâ€“Phosphorescenceâ€“Phosphorescence Tripleâ€Channel Emission Strategy for Fullâ€Color Luminescence. Small, 2020, 16, e1906475.	10.0	45
88	Computational Protocol for Precise Prediction of Dye-Sensitized Solar Cell Performance. Journal of Physical Chemistry C, 2020, 124, 3980-3987.	3.1	28
89	Antiâ€Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydroâ€diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. Angewandte Chemie - International Edition, 2020, 59, 5144-5150.	13.8	17
90	Two-dimensional MXenes: From morphological to optical, electric, and magnetic properties and applications. Physics Reports, 2020, 848, 1-58.	25.6	594

#	Article	IF	Citations
91	Antiâ€Aromatic versus Induced Paratropicity: Synthesis and Interrogation of a Dihydroâ€diazatrioxa[9]circulene with a Proton Placed Directly above the Central Ring. Angewandte Chemie, 2020, 132, 5182-5188.	2.0	8
92	Flexible diphenylsulfone versus rigid dibenzothiophene-dioxide as acceptor moieties in donor-acceptor-donor TADF emitters for highly efficient OLEDs. Organic Electronics, 2020, 83, 105733.	2.6	11
93	Molecular Phosphorescence in Polymer Matrix with Reversible Sensitivity. ACS Applied Materials & Interfaces, 2020, 12, 20765-20774.	8.0	68
94	Structural stability of single-layer PdSe₂ with pentagonal puckered morphology and its nanotubes. Physical Chemistry Chemical Physics, 2020, 22, 8289-8295.	2.8	26
95	Structure, stability and electronic properties of one-dimensional tetrathia- and tetraselena[8]circulene-based materials: a comparative DFT study. New Journal of Chemistry, 2020, 44, 6872-6882.	2.8	5
96	X-Ray Absorption Spectrum of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msubsup><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn><mml:mo>+</mml:mo></mml:msubsup></mml:math> Molecular Ion. Physical Review Letters, 2020, 124, 203001.	7.8	36
97	Furans and Their Benzo Derivatives: Structure. , 2020, , 190-190.		1
98	Microlens array enhanced upconversion luminescence at low excitation irradiance. Nanoscale, 2019, 11, 14070-14078.	5.6	41
99	Structure and excitation-dependent emission of novel zinc complexes with pyridyltriazoles. RSC Advances, 2019, 9, 22143-22152.	3.6	18
100	Impact of heteroatoms (S, Se, and Te) on the aromaticity of heterocirculenes. New Journal of Chemistry, 2019, 43, 12178-12190.	2.8	10
101	Cyclo[18]carbon: Insight into Electronic Structure, Aromaticity, and Surface Coupling. Journal of Physical Chemistry Letters, 2019, 10, 6701-6705.	4.6	103
102	Spontaneous Decomposition of Fluorinated Phosphorene and Its Stable Structure. Journal of Physical Chemistry Letters, 2019, 10, 7086-7092.	4.6	5
103	Extended Discrete Interaction Model: Plasmonic Excitations of Silver Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 28867-28880.	3.1	20
104	Change in the emission saturation and kinetics of upconversion nanoparticles under different light irradiations. Optical Materials, 2019, 97, 109389.	3.6	5
105	Enhanced Sampling Simulations of Ligand Unbinding Kinetics Controlled by Protein Conformational Changes. Journal of Chemical Information and Modeling, 2019, 59, 3910-3918.	5.4	14
106	Fast upconversion super-resolution microscopy with 10 Î¼s per pixel dwell times. Nanoscale, 2019, 11, 1563-1569.	5.6	43
107	Crystal Multiâ€Conformational Control Through Deformable Carbonâ€Sulfur Bond for Singletâ€Triplet Emissive Tuning. Angewandte Chemie - International Edition, 2019, 58, 4328-4333.	13.8	82
108	Free Energy Profile for Penetration of Pittsburgh Compound-B into the Amyloid Î² Fibril. ACS Chemical Neuroscience, 2019, 10, 1783-1790.	3.5	9

#	Article	IF	Citations
109	Highly Controllable Synthesis and DFT Calculations of Double/Triple-Halide CsPbX3 (X = Cl, Br, I) Perovskite Quantum Dots: Application to Light-Emitting Diodes. Nanomaterials, 2019, 9, 172.	4.1	21
110	Destabilization of amyloid fibrils on interaction with MoS₂-based nanomaterials. RSC Advances, 2019, 9, 1613-1624.	3.6	18
111	Decomposition of molecular properties. Physical Chemistry Chemical Physics, 2019, 21, 2251-2270.	2.8	4
112	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	3.0	26
113	Quasiparticle electronic structure and optical spectra of single-layer and bilayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>PdSe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml: : Proximity and defect-induced band gap renormalization. Physical Review B, 2019, 99, .	3.2	49
114	pH-dependent X-ray Photoelectron Chemical Shifts and Surface Distribution of Cysteine in Aqueous Solution. Journal of Physical Chemistry B, 2019, 123, 3776-3785.	2.6	3
115	Crystal Multiâ€Conformational Control Through Deformable Carbonâ€Sulfur Bond for Singletâ€Triplet Emissive Tuning. Angewandte Chemie, 2019, 131, 4372-4377.	2.0	28
116	Skeletal Rearrangement of Twisted Thiaâ€Norhexaphyrin: Multiply Annulated Polypyrrolic Aromatic Macrocycles. Angewandte Chemie - International Edition, 2019, 58, 5925-5929.	13.8	26
117	Regioselectively Halogenated Expanded Porphyrinoids as Building Blocks for Constructing Porphyrinâ€“Porphyrinoid Heterodyads with Tunable Energy Transfer. Journal of the American Chemical Society, 2019, 141, 5294-5302.	13.7	38
118	Cross-interaction of tau PET tracers with monoamine oxidase B: evidence from in silico modelling and in vivo imaging. European Journal of Nuclear Medicine and Molecular Imaging, 2019, 46, 1369-1382.	6.4	74
119	Aromaticity and photophysics of tetrasila- and tetragerma-annelated tetrathienylenes as new representatives of the hetero[8]circulene family. Physical Chemistry Chemical Physics, 2019, 21, 9246-9254.	2.8	19
120	Novel Zinc Complex with an Ethylenediamine Schiff Base for High-Luminance Blue Fluorescent OLED Applications. Journal of Physical Chemistry C, 2019, 123, 11850-11859.	3.1	56
121	Recoil-induced ultrafast molecular rotation probed by dynamical rotational Doppler effect. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4877-4882.	7.1	16
122	On the decay time of upconversion luminescence. Nanoscale, 2019, 11, 4959-4969.	5.6	76
123	A three-dimensional ratiometric sensing strategy on unimolecular fluorescenceâ€“thermally activated delayed fluorescence dual emission. Nature Communications, 2019, 10, 731.	12.8	80
124	Resonant x-ray second-harmonic generation in atomic gases. Physical Review A, 2019, 100, .	2.5	3
125	Computational study of aromaticity, 1H NMR spectra and intermolecular interactions of twisted thia-norhexaphyrin and its multiply annulated polypyrrolic derivatives. Physical Chemistry Chemical Physics, 2019, 21, 25334-25343.	2.8	5
126	Effect of Familial Mutations on the Interconversion of Î±-Helix to Î²-Sheet Structures in an Amyloid-Forming Peptide: Insight from Umbrella Sampling Simulations. ACS Chemical Neuroscience, 2019, 10, 1347-1354.	3.5	16

#	Article	IF	Citations
127	Multiply Wrapped Porphyrin Dyes with a Phenothiazine Donor: A High Efficiency of 11.7% Achieved through a Synergetic Coadsorption and Cosensitization Approach. ACS Applied Materials & Interfaces, 2019, 11, 5046-5054.	8.0	83
128	Mechanism for the Extremely Efficient Sensitization of Yb³⁺Luminescence in CsPbCl₃ Nanocrystals. Journal of Physical Chemistry Letters, 2019, 10, 487-492.	4.6	55
129	Multi-channel electroluminescence of CdTe/CdS core-shell quantum dots implemented into a QLED device. Dyes and Pigments, 2019, 162, 647-653.	3.7	23
130	Mechanistic Insight into the Binding Profile of DCVJ and Î±-Synuclein Fibril Revealed by Multiscale Simulations. ACS Chemical Neuroscience, 2019, 10, 610-617.	3.5	18
131	Divalent Pseudorotaxane with Polarized Plugâ€“Socket and Padlock Functions. Organic Letters, 2018, 20, 1487-1490.	4.6	7
132	Different Positron Emission Tomography Tau Tracers Bind to Multiple Binding Sites on the Tau Fibril: Insight from Computational Modeling. ACS Chemical Neuroscience, 2018, 9, 1757-1767.	3.5	69
133	Dirac Magnons in Honeycomb Ferromagnets. Physical Review X, 2018, 8, .	8.9	106
134	Near infrared harvesting dye-sensitized solar cells enabled by rare-earth upconversion materials. Dalton Transactions, 2018, 47, 8526-8537.	3.3	48
135	Optical tuning of tetrabenzo[8]circulene derivatives through pseudorotational conformational isomerization. Dyes and Pigments, 2018, 151, 372-379.	3.7	5
136	Contribution of TADF and exciplex emission for efficient â€œwarm-whiteâ€•OLEDs. Journal of Materials Chemistry C, 2018, 6, 1543-1550.	5.5	64
137	One-step solvothermal synthesis of high-emissive amphiphilic carbon dots via rigidity derivation. Chemical Science, 2018, 9, 1323-1329.	7.4	71
138	A protected excitation-energy reservoir for efficient upconversion luminescence. Nanoscale, 2018, 10, 250-259.	5.6	41
139	Photon Upconversion Kinetic Nanosystems and Their Optical Response. Laser and Photonics Reviews, 2018, 12, 1700144.	8.7	42
140	Dynamics and self-assembly of bio-functionalized gold nanoparticles in solution: Reactive molecular dynamics simulations. Nano Research, 2018, 11, 1757-1767.	10.4	29
141	Overtone Vibrational Transition-Induced Lanthanide Excited-State Quenching in Yb³⁺/Er³⁺-Doped Upconversion Nanocrystals. ACS Nano, 2018, 12, 10572-10575.	14.6	29
142	Free Energy Landscape for Alpha-Helix to Beta-Sheet Interconversion in Small Amyloid Forming Peptide under Nanoconfinement. Journal of Physical Chemistry B, 2018, 122, 9654-9664.	2.6	16
143	Anti-Kashaâ€™s Rule Emissive Switching Induced by Intermolecular H-Bonding. Chemistry of Materials, 2018, 30, 8008-8016.	6.7	75
144	Strong Topological States and High Charge Carrier Mobility in Tetraoxa[8]circulene Nanosheets. Journal of Physical Chemistry C, 2018, 122, 22216-22222.	3.1	25

#	Article	IF	Citations
145	Low toxic Cu2GeS3/InP quantum dot sensitized infrared solar cells. Journal of Renewable and Sustainable Energy, 2018, 10, .	2.0	9
146	Identification of tautomeric intermediates of a novel thiazolylazonaphthol dye â€“ A density functional theory study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 324-332.	3.9	4
147	Unusual binding-site-specific photophysical properties of a benzothiazole-based optical probe in amyloid beta fibrils. Physical Chemistry Chemical Physics, 2018, 20, 20334-20339.	2.8	10
148	Vibronic absorption spectra of the angular fused bisindolo- and biscarbazoloanthracene blue fluorophores for OLED applications. Chemical Physics, 2018, 513, 105-111.	1.9	6
149	Synthesis and photophysical properties of Zn(II) Schiff base complexes possessing strong solvent-dependent solid-state fluorescence. Polyhedron, 2018, 155, 202-208.	2.2	20
150	A theoretical study of new representatives of closed- and open-circle benzofuran and benzocyclopentadienone oligomers. New Journal of Chemistry, 2018, 42, 11493-11505.	2.8	11
151	Molecular stacking dependent phosphorescenceâ€“fluorescence dual emission in a single luminophore for self-recoverable mechanoconversion of multicolor luminescence. Chemical Communications, 2017, 53, 2661-2664.	4.1	90
152	Selective gating to vibrational modes through resonant X-ray scattering. Nature Communications, 2017, 8, 14165.	12.8	50
153	Tuning for Visible Fluorescence and Near-Infrared Phosphorescence on a Unimolecular Mechanically Sensitive Platform via Adjustable CHâ‹¯Ï€ Interaction. ACS Applied Materials & Interfaces, 2017, 9, 3865-3872.	8.0	56
154	A coreâ€“multiple shell nanostructure enabling concurrent upconversion and quantum cutting for photon management. Nanoscale, 2017, 9, 1934-1941.	5.6	26
155	Two-photon absorption of BF₂-carrying compounds: insights from theory and experiment. Physical Chemistry Chemical Physics, 2017, 19, 5705-5708.	2.8	17
156	Recent progress in quantum chemistry of hetero[8]circulenes. Molecular Physics, 2017, 115, 2218-2230.	1.7	28
157	A computational study of aromaticity and photophysical properties of unsymmetrical azatrioxa[8]circulenes. New Journal of Chemistry, 2017, 41, 2717-2723.	2.8	16
158	Atomic level simulations of the interaction of asphaltene with quartz surfaces: role of chemical modifications and aqueous environment. Materials and Structures/Materiaux Et Constructions, 2017, 50, 1.	3.1	8
159	Propagation of the Allosteric Modulation Induced by Sodium in the Î´â€Opioid Receptor. Chemistry - A European Journal, 2017, 23, 4615-4624.	3.3	20
160	Enhancing dye-sensitized solar cell efficiency through broadband near-infrared upconverting nanoparticles. Nanoscale, 2017, 9, 6711-6715.	5.6	99
161	Quantum-classical calculations of X-ray photoelectron spectra of polymersâ€”Polymethyl methacrylate revisited. Journal of Chemical Physics, 2017, 146, 124902.	3.0	4
162	Cu²⁺-Selectivity gated photochromism in Schiff-modified diarylethenes with a star-shaped structure. Journal of Materials Chemistry C, 2017, 5, 282-289.	5.5	34

#	Article	IF	Citations
163	Dye-sensitized lanthanide-doped upconversion nanoparticles. Chemical Society Reviews, 2017, 46, 4150-4167.	38.1	281
164	Substituent-sensitive fluorescence of sequentially N-alkylated tetrabenzotetraaza[8]circulenes. New Journal of Chemistry, 2017, 41, 7621-7625.	2.8	9
165	Characterization of the binding mode of the PET tracer [18F]ASEM to a chimera structure of the Î±7 nicotinic acetylcholine receptor. RSC Advances, 2017, 7, 19787-19793.	3.6	4
166	Far-Zone Resonant Energy Transfer in X-ray Photoemission as a Structure Determination Tool. Journal of Physical Chemistry Letters, 2017, 8, 2730-2734.	4.6	4
167	New WOLEDs based on Ï€-extended azatrioxa[8]circulenes. Journal of Materials Chemistry C, 2017, 5, 4123-4128.	5.5	28
168	Theory and Calculation of the Phosphorescence Phenomenon. Chemical Reviews, 2017, 117, 6500-6537.	47.7	420
169	Selective Dualâ€Channel Imaging on Cyanostyrylâ€Modified Azulene Systems with Unimolecularly Tunable Visibleâ€“Near Infrared Luminescence. Chemistry - A European Journal, 2017, 23, 7642-7647.	3.3	87
170	Solvatochromic effect in absorption and emission spectra of star-shaped bipolar derivatives of 1,3,5-triazine and carbazole. A time-dependent density functional study. Journal of Molecular Modeling, 2017, 23, 55.	1.8	11
171	A study of the water molecule using frequency control over nuclear dynamics in resonant X-ray scattering. Physical Chemistry Chemical Physics, 2017, 19, 19573-19589.	2.8	32
172	Phase angle encoded upconversion luminescent nanocrystals for multiplexing applications. Nanoscale, 2017, 9, 1676-1686.	5.6	66
173	Helical Self-Assembly-Induced Singletâ€“Triplet Emissive Switching in a Mechanically Sensitive System. Journal of the American Chemical Society, 2017, 139, 785-791.	13.7	153
174	Optimization of coreâ€“valence states of molecules. Molecular Physics, 2017, 115, 252-259.	1.7	2
175	Efficient Solar Cells Based on Porphyrin Dyes with Flexible Chains Attached to the Auxiliary Benzothiadiazole Acceptor: Suppression of Dye Aggregation and the Effect of Distortion. ACS Applied Materials & Interfaces, 2017, 9, 36875-36885.	8.0	84
176	Achieving high-efficiency emission depletion nanoscopy by employing cross relaxation in upconversion nanoparticles. Nature Communications, 2017, 8, 1058.	12.8	239
177	Effect of Alzheimer Familial Chromosomal Mutations on the Amyloid Fibril Interaction with Different PET Tracers: Insight from Molecular Modeling Studies. ACS Chemical Neuroscience, 2017, 8, 2655-2666.	3.5	8
178	Infrared-pumpâ€“x-ray-probe spectroscopy of vibrationally excited molecules. Physical Review A, 2017, 95, .	2.5	14
179	Local decomposition of imaginary polarizabilities and dispersion coefficients. Physical Chemistry Chemical Physics, 2017, 19, 20241-20250.	2.8	8
180	Gradual collapse of nuclear wave functions regulated by frequency tuned X-ray scattering. Scientific Reports, 2017, 7, 43891.	3.3	15

#	Article	IF	Citations
181	Helicity Inversion of Supramolecular Hydrogels Induced by Achiral Substituents. ACS Nano, 2017, 11, 11880-11889.	14.6	74
182	Characterization of the adsorption dynamics of trisodium citrate on gold in water solution. RSC Advances, 2017, 7, 49655-49663.	3.6	33
183	Thermal effects in systems of colloidal plasmonic nanoparticles in high-intensity pulsed laser fields [Invited]: publisherâ€™s note. Optical Materials Express, 2017, 7, 799.	3.0	2
184	Nonempirical Simulations of Inhomogeneous Broadening of Electronic Transitions in Solution: Predicting Band Shapes in One- and Two-Photon Absorption Spectra of Chalcones. Molecules, 2017, 22, 1643.	3.8	15
185	Improving the Photocurrent in Quantum-Dot-Sensitized Solar Cells by Employing Alloy PbxCd1â^'xS Quantum Dots as Photosensitizers. Nanomaterials, 2016, 6, 97.	4.1	25
186	Nanostructured Solar Cells. Nanomaterials, 2016, 6, 145.	4.1	10
187	Suppression of surface plasmon resonance in Au nanoparticles upon transition to the liquid state. Optics Express, 2016, 24, 26851.	3.4	18
188	Optical Properties of Gold Nanoclusters Functionalized with a Small Organic Compound: Modeling by an Integrated Quantum-Classical Approach. Journal of Chemical Theory and Computation, 2016, 12, 3325-3339.	5.3	9
189	First Hyperpolarizability of Collagen Using the Point Dipole Approximation. Journal of Physical Chemistry Letters, 2016, 7, 2132-2138.	4.6	5
190	Hybrid Complex Polarization Propagator/Molecular Mechanics Method for Heterogeneous Environments. Journal of Chemical Theory and Computation, 2016, 12, 2661-2667.	5.3	10
191	A Polarization Propagator for Nonlinear X-ray Spectroscopies. Journal of Physical Chemistry Letters, 2016, 7, 1991-1995.	4.6	20
192	Theoretical Study of the Adsorption Mechanism of Cystine on Au(110) in Aqueous Solution. Small, 2016, 12, 6134-6143.	10.0	12
193	Tetra- and Octapyrroles Synthesized from Confusion and Fusion Approaches. Organic Letters, 2016, 18, 5046-5049.	4.6	13
194	Elucidating the Mechanism of Zn²⁺ Sensing by a Bipyridine Probe Based on Two-Photon Absorption. Journal of Physical Chemistry B, 2016, 120, 9067-9075.	2.6	13
195	The Culprit Is in the Cave: The Core Sites Explain the Binding Profiles of Amyloid-Specific Tracers. Journal of Physical Chemistry Letters, 2016, 7, 3313-3321.	4.6	35
196	Supramolecular Assemblies: Photoresponsive Supramolecular Assemblies Based on a C3-Symmetric Benzene-1,3,5-tricarboxamide-Anchored Diarylethene (Advanced Optical Materials 6/2016). Advanced Optical Materials, 2016, 4, 810-810.	7.3	0
197	Efficient Broadband Upconversion of Nearâ€Infrared Light in Dyeâ€Sensitized Core/Shell Nanocrystals. Advanced Optical Materials, 2016, 4, 1760-1766.	7.3	104
198	Anomalously strong two-electron one-photon X-ray decay transitions in CO caused by avoided crossing. Scientific Reports, 2016, 6, 20947.	3.3	11

#	Article	IF	Citations
199	Hybrid Materials: Theoretical Study of the Adsorption Mechanism of Cystine on Au(110) in Aqueous Solution (Small 44/2016). Small, 2016, 12, 6046-6046.	10.0	0
200	Multistep Modeling Strategy To Improve the Binding Affinity Prediction of PET Tracers to AÎ²₄₂: Case Study with Styrylbenzoxazole Derivatives. ACS Chemical Neuroscience, 2016, 7, 1698-1705.	3.5	7
201	Benzoannelated aza-, oxa- and azaoxa[8]circulenes as promising blue organic emitters. Physical Chemistry Chemical Physics, 2016, 18, 28040-28051.	2.8	54
202	Multicolor Photoluminescence Including White-Light Emission by a Single Hostâ€“Guest Complex. Journal of the American Chemical Society, 2016, 138, 13541-13550.	13.7	233
203	Theoretical study of the binding profile of an allosteric modulator NS-1738 with a chimera structure of the Î±7 nicotinic acetylcholine receptor. Physical Chemistry Chemical Physics, 2016, 18, 28003-28009.	2.8	6
204	Enhanced Photocurrent Density by Spin-Coated NiO Photocathodes for N-Annulated Perylene-Based p-Type Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2016, 8, 19393-19401.	8.0	24
205	Coupled electron-nuclear dynamics in resonant<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>Ïƒ</mml:mi><mml:mo>â†'</mml:mo> Raman scattering of CO molecules. Physical Review A, 2016, 93, .	2.8	13
206	Granular superconductor in a honeycomb lattice as a realization of bosonic Dirac material. Physical Review B, 2016, 93, .	3.2	22
207	Landau-like states in neutral particles. Physical Review B, 2016, 93, .	3.2	3
208	A High Affinity Red Fluorescence and Colorimetric Probe for Amyloid Î² Aggregates. Scientific Reports, 2016, 6, 23668.	3.3	90
209	Modeling Rayleigh Scattering of Aerosol Particles. Journal of Physical Chemistry B, 2016, 120, 4296-4301.	2.6	11
210	Decoration of gold nanoparticles with cysteine in solution: reactive molecular dynamics simulations. Nanoscale, 2016, 8, 12929-12938.	5.6	26
211	Photoresponsive Supramolecular Assemblies Based on a C₃â€Symmetric Benzeneâ€1,3,5â€tricarboxamideâ€Anchored Diarylethene. Advanced Optical Materials, 2016, 4, 840-847.	7.3	36
212	First-Principles Simulations of One- and Two-Photon Absorption Band Shapes of the Bis(BF₂) Core Complex. Journal of Physical Chemistry B, 2016, 120, 2323-2332.	2.6	28
213	Plasmon-enhanced two-photon-induced isomerization for highly-localized light-based actuation of inorganic/organic interfaces. Nanoscale, 2016, 8, 4194-4202.	5.6	16
214	An experimental and theoretical study of coreâ€“valence double ionisation of acetaldehyde (ethanal). Physical Chemistry Chemical Physics, 2016, 18, 2535-2547.	2.8	3
215	Hyperpolarizabilities of extended molecular mechanical systems. Physical Chemistry Chemical Physics, 2016, 18, 8710-8722.	2.8	14
216	Simulation of Gold Functionalization with Cysteine by Reactive Molecular Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 272-276.	4.6	43

#	Article	IF	Citations
217	Morphology Tuning of Self-Assembled Perylene Monoimide from Nanoparticles to Colloidosomes with Enhanced Excimeric NIR Emission for Bioimaging. ACS Applied Materials & Interfaces, 2016, 8, 2336-2347.	8.0	26
218	Quantum mechanics capacitance molecular mechanics modeling of core-electron binding energies of methanol and methyl nitrite on Ag(111) surface. Journal of Chemical Physics, 2016, 145, 024703.	3.0	7
219	Hostâ€“Guest Interactionâ€Mediated Construction of Hydrogels and Nanovesicles for Drug Delivery. Small, 2015, 11, 5901-5906.	10.0	31
220	Efficiency Enhanced Colloidal Mn-Doped Type II Core/Shell ZnSe/CdS Quantum Dot Sensitized Hybrid Solar Cells. Journal of Nanomaterials, 2015, 2015, 1-9.	2.7	11
221	Residues remote from the binding pocket control the antagonist selectivity towards the corticotropin-releasing factor receptor-1. Scientific Reports, 2015, 5, 8066.	3.3	17
222	Toward assessment of density functionals for vibronic coupling in twoâ€photon absorption: A case study of 4â€nitroaniline. Journal of Computational Chemistry, 2015, 36, 1124-1131.	3.3	12
223	Effect of bridging group configuration on photophysical and photovoltaic performance in dye-sensitized solar cells. Journal of Materials Chemistry A, 2015, 3, 14325-14333.	10.3	23
224	Surface-Altered Protonation Studied by Photoelectron Spectroscopy and Reactive Dynamics Simulations. Journal of Physical Chemistry Letters, 2015, 6, 807-811.	4.6	13
225	Highly sensitive detection of low-level water content in organic solvents and cyanide in aqueous media using novel solvatochromic AIEE fluorophores. RSC Advances, 2015, 5, 12191-12201.	3.6	78
226	DFT simulation of the heteroannelated octatetraenes vibronic spectra with the Franckâ€“Condon and Herzbergâ€“Teller approaches including Duschinsky effect. Chemical Physics, 2015, 459, 65-71.	1.9	22
227	Relation between Nonlinear Optical Properties of Pushâ€“Pull Molecules and Metric of Charge Transfer Excitations. Journal of Chemical Theory and Computation, 2015, 11, 4182-4188.	5.3	39
228	Molecular mechanisms for the adhesion of chitin and chitosan to montmorillonite clay. RSC Advances, 2015, 5, 54580-54588.	3.6	22
229	Frequency-dependent force fields for QMMM calculations. Physical Chemistry Chemical Physics, 2015, 17, 7800-7812.	2.8	11
230	Molecular dynamics simulations indicate that DNA bases using graphene nanopores can be identified by their translocation times. RSC Advances, 2015, 5, 9389-9395.	3.6	12
231	Dropping a Droplet of Cysteine Molecules on a Rutile (110) Interface: Reactive versus Nonreactive Classical Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2015, 119, 6703-6712.	3.1	16
232	Energy-Cascaded Upconversion in an Organic Dye-Sensitized Core/Shell Fluoride Nanocrystal. Nano Letters, 2015, 15, 7400-7407.	9.1	341
233	Sterically hindered diarylethenes with a benzobis(thiadiazole) bridge: photochemical and kinetic studies. Journal of Materials Chemistry C, 2015, 3, 8665-8674.	5.5	9
234	Investigation of the Binding Profiles of AZD2184 and Thioflavin T with Amyloid-Î²(1â€“42) Fibril by Molecular Docking and Molecular Dynamics Methods. Journal of Physical Chemistry B, 2015, 119, 11560-11567.	2.6	48

#	Article	IF	Citations
235	Photochromic Diarylethenes with Heterocyclic Aromatic Rings: Correlation between Thermal Bistability and Geometrical Characters of Transition States. Journal of Physical Chemistry A, 2015, 119, 9140-9147.	2.5	14
236	Systematic Investigations on the Roles of the Electron Acceptor and Neighboring Ethynylene Moiety in Porphyrins for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 21956-21965.	8.0	76
237	Synthesis of a Neo-Confused Octaphyrin and the Formation of Its Mononuclear Complexes. Organic Letters, 2015, 17, 4806-4809.	4.6	31
238	Pyrimidine-2-carboxylic Acid as an Electron-Accepting and Anchoring Group for Dye-Sensitized Solar Cells. ACS Applied Materials & Interfaces, 2015, 7, 26355-26359.	8.0	23
239	Porphyrins Containing a Triphenylamine Donor and up to Eight Alkoxy Chains for Dye-Sensitized Solar Cells: A High Efficiency of 10.9%. ACS Applied Materials & Interfaces, 2015, 7, 27976-27985.	8.0	137
240	Einsteinâ€“Bohr recoiling double-slit gedanken experiment performed at the molecular level. Nature Photonics, 2015, 9, 120-125.	31.4	66
241	Toward Fully Nonempirical Simulations of Optical Band Shapes of Molecules in Solution: A Case Study of Heterocyclic Ketoimine Difluoroborates. Journal of Physical Chemistry A, 2015, 119, 5145-5152.	2.5	39
242	Light upconverting coreâ€“shell nanostructures: nanophotonic control for emerging applications. Chemical Society Reviews, 2015, 44, 1680-1713.	38.1	483
243	A new Dâ€“Aâ€“Ï€â€“A type organic sensitizer based on substituted dihydroindolo [2,3-b] carbazole and DPP unit with a bulky branched alkyl chain for highly efficient DSCs. Journal of Materials Chemistry A, 2015, 3, 3777-3784.	10.3	25
244	LanthanideâEDoped Fluoride Core/Multishell Nanoparticles for Broadband Upconversion of Infrared Light. Advanced Optical Materials, 2015, 3, 575-582.	7.3	50
245	Acylation of dipyrromethanes at the Î± and Î² positions and further development of fluorescent Zn2+ probes. Sensors and Actuators B: Chemical, 2015, 206, 291-302.	7.8	24
246	Enhanced Upconversion Luminescence in Yb3+/Tm3+-Codoped Fluoride Active Core/Active Shell/Inert Shell Nanoparticles through Directed Energy Migration. Nanomaterials, 2014, 4, 55-68.	4.1	76
247	Site-selective photoemission from delocalized valence shells induced by molecular rotation. Nature Communications, 2014, 5, 3816.	12.8	16
248	Microsecond Molecular Dynamics Simulations Provide Insight into the Allosteric Mechanism of the Gs Protein Uncoupling from the Î²2Adrenergic Receptor. Journal of Physical Chemistry B, 2014, 118, 141212122505008.	2.6	10
249	Neoâ€Fused Hexaphyrin: A Molecular Puzzle Containing an Nâ€Linked Pentaphyrin. Angewandte Chemie - International Edition, 2014, 53, 14069-14073.	13.8	52
250	Computational studies of DNA sequencing with solid-state nanopores: key issues and future prospects. Frontiers in Chemistry, 2014, 2, 5.	3.6	13
251	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	14.6	1,166
252	Principles of phosphorescent organic light emitting devices. Physical Chemistry Chemical Physics, 2014, 16, 1719-1758.	2.8	398

#	Article	IF	Citations
253	A near-infrared â€œonâ€“offâ€•fluorescent and colourimetric cyanide chemodosimeter based on phenothiazine with applications in living cell imaging. RSC Advances, 2014, 4, 59809-59816.	3.6	14
254	Two-Photon Absorption of Metal-Assisted Chromophores. Journal of Chemical Theory and Computation, 2014, 10, 5630-5639.	5.3	14
255	Theoretical studies on the dynamics of DNA fragment translocation through multilayer graphene nanopores. RSC Advances, 2014, 4, 50494-50502.	3.6	17
256	Cosensitizers for simultaneous filling up of both absorption valleys of porphyrins: a novel approach for developing efficient panchromatic dye-sensitized solar cells. Chemical Communications, 2014, 50, 15609-15612.	4.1	99
257	Simultaneous Multiple Wavelength Upconversion in a Coreâ€“Shell Nanoparticle for Enhanced Near Infrared Light Harvesting in a Dye-Sensitized Solar Cell. ACS Applied Materials & Interfaces, 2014, 6, 18018-18025.	8.0	77
258	Non-linear optical properties of molecules in heterogeneous environments: a quadratic density functional/molecular mechanics response theory. Physical Chemistry Chemical Physics, 2014, 16, 8981.	2.8	18
259	Photovoltaic properties of bis(octyloxy)benzo-[c][1,2,5]thiadiazole sensitizers based on an N,N-diphenylthiophen-2-amine donor. Journal of Materials Chemistry C, 2014, 2, 4063-4072.	5.5	18
260	Theoretical study on passivation of small CdS clusters. Molecular Physics, 2014, 112, 674-682.	1.7	3
261	SERS and MD simulation studies of a kinase inhibitor demonstrate the emergence of a potential drug discovery tool. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10416-10421.	7.1	37
262	A Musclelike [2](2)Rotaxane: Synthesis, Performance, and Molecular Dynamics Simulations. Journal of Organic Chemistry, 2014, 79, 6996-7004.	3.2	28
263	Studies of pH-Sensitive Optical Properties of the deGFP1 Green Fluorescent Protein Using a Unique Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 3492-3502.	5.3	5
264	A Hybrid Density Functional Theory/Molecular Mechanics Approach for Linear Response Properties in Heterogeneous Environments. Journal of Chemical Theory and Computation, 2014, 10, 989-1003.	5.3	39
265	Molecular dynamics simulation of strong interaction mechanisms at wet interfaces in clayâ€“polysaccharide nanocomposites. Journal of Materials Chemistry A, 2014, 2, 9541-9547.	10.3	27
266	Red turn-on fluorescent phenazine-cyanine chemodosimeters for cyanide anion in aqueous solution and its application for cell imaging. Sensors and Actuators B: Chemical, 2014, 203, 833-847.	7.8	51
267	Effects of Graphene Nanopore Geometry on DNA Sequencing. Journal of Physical Chemistry Letters, 2014, 5, 1602-1607.	4.6	54
268	Size-Tunable and Monodisperse Tm³⁺/Gd³⁺-Doped Hexagonal NaYbF₄ Nanoparticles with Engineered Efficient Near Infrared-to-Near Infrared Upconversion for In Vivo Imaging. ACS Applied Materials & Interfaces, 2014, 6, 13884-13893.	8.0	128
269	Engineering Topochemical Polymerizations Using Block Copolymer Templates. Journal of the American Chemical Society, 2014, 136, 13381-13387.	13.7	65
270	Role of Protonation State and Solvation on the pH Dependent Optical Properties of Bromocresol Green. Journal of Chemical Theory and Computation, 2014, 10, 3958-3968.	5.3	3

#	Article	IF	Citations
271	2-Diphenylaminothiophene as the donor of porphyrin sensitizers for dye-sensitized solar cells. New Journal of Chemistry, 2014, 38, 3227-3235.	2.8	47
272	Chelation-Induced Quenching of Two-Photon Absorption of Azacrown Ether Substituted Distyryl Benzene for Metal Ion Sensing. Journal of Chemical Theory and Computation, 2014, 10, 778-788.	5.3	12
273	Molecular Structure â€“ Optical Property Relationships for a Series of Non-Centrosymmetric Two-photon Absorbing Push-Pull Triarylamine Molecules. Scientific Reports, 2014, 4, 4447.	3.3	55
274	Comparative computational IR, Raman and phosphorescence study of Ru- and Rh-based complexes. Molecular Physics, 2013, 111, 1526-1538.	1.7	6
275	Structural and Electronic Properties of Poly(9,9-dialkylfluorene)-Based Alternating Copolymers in Solution: An NMR Spectroscopy and Density Functional Theory Study. Journal of Physical Chemistry C, 2013, 117, 17969-17982.	3.1	15
276	pH-Induced Modulation of One- and Two-Photon Absorption Properties in a Naphthalene-Based Molecular Probe. Journal of Chemical Theory and Computation, 2013, 9, 3660-3669.	5.3	12
277	Substituent effects on the photophysical properties of fluorescent 2-benzoylmethylenequinoline difluoroboranes: A combined experimental and quantum chemical study. Dyes and Pigments, 2013, 99, 957-965.	3.7	42
278	Dioxygen spectra and bioactivation. International Journal of Quantum Chemistry, 2013, 113, 1847-1867.	2.0	41
279	Unimolecular Photoconversion of Multicolor Luminescence on Hierarchical Self-Assemblies. Journal of the American Chemical Society, 2013, 135, 5175-5182.	13.7	144
280	Chirality Control for in Situ Preparation of Gold Nanoparticle Superstructures Directed by a Coordinatable Organogelator. Journal of the American Chemical Society, 2013, 135, 9174-9180.	13.7	68
281	Theoretical study on key factors in DNA sequencing with graphene nanopores. RSC Advances, 2013, 3, 2445.	3.6	41
282	Photothermal-responsive [2]rotaxanes. RSC Advances, 2013, 3, 2341.	3.6	12
283	Amyloid Fibril-Induced Structural and Spectral Modifications in the Thioflavin-T Optical Probe. Journal of Physical Chemistry Letters, 2013, 4, 70-77.	4.6	29
284	Cross-Linked Polysaccharide Assemblies in Marine Gels: An Atomistic Simulation. Journal of Physical Chemistry Letters, 2013, 4, 2637-2642.	4.6	25
285	Resonant and Nonresonant Hyperpolarizabilities of Spatially Confined Molecules: A Case Study of Cyanoacetylene. Journal of Chemical Theory and Computation, 2013, 9, 3463-3472.	5.3	27
286	A theoretical study revealing the promotion of lightâ€absorbing carbon particles solubilization by natural surfactants in nanosized water droplets. Atmospheric Science Letters, 2013, 14, 86-90.	1.9	4
287	Spin-spin and spin-orbit interactions in nanographene fragments: A quantum chemistry approach. Journal of Chemical Physics, 2012, 136, 104702.	3.0	37
288	Binding Mechanism and Magnetic Properties of a Multifunctional Spin Label for Targeted EPR Imaging of Amyloid Proteins: Insight from Atomistic Simulations and First-Principles Calculations. Journal of Chemical Theory and Computation, 2012, 8, 4766-4774.	5.3	8

#	Article	IF	Citations
289	Color modeling of protein optical probes. Physical Chemistry Chemical Physics, 2012, 14, 1107-1112.	2.8	40
290	Raman Scattering at Resonant or Near-Resonant Conditions: A Generalized Short-Time Approximation. Chinese Journal of Chemical Physics, 2012, 25, 31-47.	1.3	1
291	Encapsulation Influence on EPR Parameters of Spin-Labels: 2,2,6,6-Tetramethyl-4-methoxypiperidine-1-oxyl in Cucurbit[8]uril. Journal of Chemical Theory and Computation, 2012, 8, 257-263.	5.3	19
292	NMR Spinâ€"Spin Coupling Constants in Polymethine Dyes as Polarity Indicators. Chemistry - A European Journal, 2012, 18, 11677-11684.	3.3	14
293	Use of colloidal upconversion nanocrystals for energy relay solar cell light harvesting in the near-infrared region. Journal of Materials Chemistry, 2012, 22, 16709.	6.7	101
294	The Role of Molecular Conformation and Polarizable Embedding for One- and Two-Photon Absorption of Disperse Orange 3 in Solution. Journal of Physical Chemistry B, 2012, 116, 8169-8181.	2.6	40
295	Type-II colloidal quantum dot sensitized solar cells with a thiourea based organic redox couple. Journal of Materials Chemistry, 2012, 22, 6032.	6.7	41
296	Luminescent Color Conversion on Cyanostilbeneâ€Functionalized Quantum Dots via Inâ€situ Photoâ€Tuning. Advanced Materials, 2012, 24, 4020-4024.	21.0	93
297	Experimental and theoretical study of IR and Raman spectra of tetraoxa[8]circulenes. Vibrational Spectroscopy, 2012, 61, 156-166.	2.2	51
298	Density Functional Theory/Molecular Mechanics Approach for Electronic g-Tensors of Solvated Molecules. Journal of Physical Chemistry B, 2011, 115, 4350-4358.	2.6	20
299	Molecular dynamics simulations of a branched tetradecasaccharide substrate in the active site of a xyloglucanendo-transglycosylase. Molecular Simulation, 2011, 37, 1001-1013.	2.0	9
300	Density Functional Restrictedâ€"Unrestricted/Molecular Mechanics Theory for Hyperfine Coupling Constants of Molecules in Solution. Journal of Chemical Theory and Computation, 2011, 7, 3261-3271.	5.3	18
301	Density Functional Theory Study of Photophysical Properties of Iridium(III) Complexes with Phenylisoquinoline and Phenylpyridine Ligands. Journal of Physical Chemistry C, 2011, 115, 20724-20731.	3.1	74
302	A molecular dynamics study of the thermal response of crystalline cellulose Iβ. Cellulose, 2011, 18, 207-221.	4.9	39
303	Modeling solvatochromism of Nile red in water. International Journal of Quantum Chemistry, 2011, 111, 1521-1530.	2.0	21
304	Theoretical Study of Phosphorescence of Iridium Complexes with Fluorineâ€Substituted Phenylpyridine Ligands. European Journal of Inorganic Chemistry, 2011, 2011, 2517-2524.	2.0	82
305	Computational protocols for prediction of solute NMR relative chemical shifts. A case study of <scp>L</scp>â€tryptophan in aqueous solution. Journal of Computational Chemistry, 2011, 32, 2853-2864.	3.3	25
306	IR, Raman and UVâ€"vis spectra of the Ru(II) cyano complexes studied by DFT. Molecular Simulation, 2011, 37, 670-677.	2.0	5

#	Article	IF	Citations
307	Spin-flip time dependent density functional theory applied to excited states with single, double, or mixed electron excitation character. Journal of Chemical Physics, 2010, 133, 114104.	3.0	88
308	Experimental and theoretical study of core-valence double photoionization of OCS. Physical Review A, 2010, 82, .	2.5	14
309	X-ray absorption spectra of graphene from first-principles simulations. Physical Review B, 2010, 82, .	3.2	78
310	Fluorescence and FTIR Spectra Analysis of Trans-A2B2-Substituted Di- and Tetra-Phenyl Porphyrins. Materials, 2010, 3, 4446-4475.	2.9	47
311	Auger effect in the presence of strong x-ray pulses. Physical Review A, 2010, 81, .	2.5	38
312	Valence photoionization of the LiCl monomer and dimer. Physical Review A, 2010, 81, .	2.5	8
313	Recoil splitting of x-ray-induced optical fluorescence. Physical Review A, 2010, 81, .	2.5	5
314	Impact Ionization and Auger Recombination Rates in Semiconductor Quantum Dots. Journal of Physical Chemistry C, 2010, 114, 3743-3747.	3.1	29
315	Ultrasmall Monodisperse NaYF₄:Yb³⁺/Tm³⁺ Nanocrystals with Enhanced Near-Infrared to Near-Infrared Upconversion Photoluminescence. ACS Nano, 2010, 4, 3163-3168.	14.6	586
316	Surface-Active cis-Pinonic Acid in Atmospheric Droplets: A Molecular Dynamics Study. Journal of Physical Chemistry Letters, 2010, 1, 769-773.	4.6	88
317	Modeling the Structure and Absorption Spectra of Stilbazolium Merocyanine in Polar and Nonpolar Solvents Using Hybrid QM/MM Techniques. Journal of Physical Chemistry B, 2010, 114, 13349-13357.	2.6	52
318	Breakdown of the first hyperpolarizability/bond-length alternation parameter relationship. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 16453-16458.	7.1	84
319	Controlling yield and morphology for gold nanorods in a seed-mediated synthesis method for cell imaging. , 2010, , .		0
320	Theoretical design of phosphorescence parameters for organic electro-luminescence devices based on iridium complexes. Chemical Physics, 2009, 358, 245-257.	1.9	73
321	Multifocus Structures of Ultrashort Self-Focusing Laser Beam Observed in a Three-Photon Fluorescent Medium. IEEE Journal of Quantum Electronics, 2009, 45, 816-824.	1.9	5
322	Theoretical Study of the Cyclometalated Iridium(III) Complexes Used as Chromophores for Organic Light-Emitting Diodes. Journal of Physical Chemistry A, 2009, 113, 726-735.	2.5	111
323	Stimulated Rayleighâ€“Bragg Scattering From a Two-Photon Absorbing CdSeâ€“CdSâ€“ZnS Quantum-Rods System: Optical Power Limiting and Phase-Conjugation. IEEE Journal of Quantum Electronics, 2008, 44, 894-901.	1.9	2
324	A metal-wire/quantum-dot composite metamaterial with negative Îµ and compensated optical loss. Applied Physics Letters, 2008, 93, .	3.3	39

#	Article	IF	Citations
325	Degenerate Perturbation Theory for Electronic g Tensors: Leading-Order Relativistic Effects. Journal of Chemical Theory and Computation, 2008, 4, 1810-1828.	5.3	20
326	Dynamic properties and optical phase conjugation of two-photon pumped ultrashort blue stimulated emission in a chromophore solution. Physical Review A, 2008, 77, .	2.5	10
327	Optical reflection from excitonic quantum-dot multilayer structures. Applied Physics Letters, 2008, 93, 183117.	3.3	6
328	Single-photon core-valence double ionization of molecular oxygen. Physical Review A, 2008, 78, .	2.5	16
329	Dynamic photon emission from multiphoton-excited semiconductor quantum dots. Journal of Applied Physics, 2008, 103, 093703.	2.5	3
330	Symmetry-forbidden x-ray Raman scattering induced by a strong infrared-laser field. Physical Review A, 2008, 77, .	2.5	13
331	A QUANTUM MECHANICAL â€" ELECTRODYNAMICAL APPROACH TO NONLINEAR PROPERTIES: APPLICATION TO OPTICAL POWER LIMITING WITH PLATINUM-ORGANIC COMPOUNDS. Journal of Nonlinear Optical Physics and Materials, 2007, 16, 157-169.	1.8	3
332	Dynamics of the damping oscillator formed by the collective generation of surface polaritons for extraordinary light transmission through subwavelength hole arrays in thin metal films. Physical Review B, 2007, 76, .	3.2	2
333	Radiative emission from multiphoton-excited semiconductor quantum dots. Journal of Applied Physics, 2007, 101, 063712.	2.5	2
334	Selective excitation of surface-polariton Bloch waves for efficient transmission of light through a subwavelength hole array in a thin metal film. Physical Review B, 2007, 76, .	3.2	11
335	Light-Matter Interaction of Strong Laser Pulses in the Micro-, Nano-, and Pico-second Regimes. Materials Research Society Symposia Proceedings, 2007, 1015, 1.	0.1	0
336	Dynamic interpretation of resonant x-ray Raman scattering: Ethylene and benzene. Physical Review A, 2007, 76, .	2.5	24
337	Recipe of Polarized One-Electron Potential Optimization for Development of Polarizable Force Fields. Journal of Chemical Theory and Computation, 2007, 3, 1947-1959.	5.3	18
338	Surface-plasmon-assisted electromagnetic field enhancement in semiconductor quantum dots. Applied Physics A: Materials Science and Processing, 2007, 87, 167-169.	2.3	2
339	Time-dependent density functional calculations of phosphorescence parameters for fac-tris(2-phenylpyridine) iridium. Chemical Physics, 2007, 333, 157-167.	1.9	154
340	Complete band gaps in three-dimensional quantum dot photonic crystals. Physical Review B, 2006, 74, .	3.2	7
341	Theoretical study of phosphorescence in dye doped light emitting diodes. Journal of Chemical Physics, 2006, 125, 234704.	3.0	38
342	Modeling of multi-photon-induced photoluminescence from organic fluorophores and metal-coated semiconductor nanoparticles. , 2006, , .		1

#	Article	IF	Citations
343	Heisenberg Exchange in Dinuclear Manganese Complexes:â€‰ A Density Functional Theory Study. Journal of Chemical Theory and Computation, 2006, 2, 981-989.	5.3	37
344	Density functional theory study of vibronic structure of the first absorption Qx band in free-base porphin. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 308-323.	3.9	70
345	Room-temperature photoluminescence of doped 4H-SiC film grown on AlN/Si(100). Applied Physics A: Materials Science and Processing, 2006, 86, 145-149.	2.3	4
346	Multiphoton excitation of quantum dots by ultrashort and ultraintense laser pulses. Applied Physics Letters, 2006, 88, 221114.	3.3	13
347	Femtosecond nuclear motion ofHClprobed by resonant x-ray Raman scattering in the Cl1sregion. Physical Review A, 2006, 73, .	2.5	63
348	Evaluation of low-scaling methods for calculation of phosphorescence parameters. Journal of Chemical Physics, 2006, 124, 114106.	3.0	37
349	Nanoscale excitonic-plasmonic optical waveguiding by metal-coated quantum dots. , 2006, , .		0
350	ResonantLII,IIIx-ray Raman scattering from HCl. Physical Review A, 2006, 74, .	2.5	10
351	Theoretical study of triplet state properties of free-base porphin. Chemical Physics, 2005, 312, 299-309.	1.9	44
352	Theoretical DFT study of phosphorescence from porphyrins. Chemical Physics, 2005, 315, 215-239.	1.9	94
353	Ab initio calculations of vibronic activity in phosphorescence microwave double resonance spectra of p-dichlorobenzene. Theoretical Chemistry Accounts, 2005, 113, 15-27.	1.4	10
354	The principles of infrared-x-ray pump-probe spectroscopy. Applications on proton transfer in core-ionized water dimers. Journal of Chemical Physics, 2005, 122, 094319.	3.0	39
355	Infraredâ€“x-ray pump-probe spectroscopy of the NO molecule. Physical Review A, 2005, 72, .	2.5	31
356	Phase-sensitive x-ray absorption driven by strong infrared fields. Physical Review A, 2005, 71, .	2.5	11
357	A comparison of density-functional-theory and coupled-cluster frequency-dependent polarizabilities and hyperpolarizabilities. Molecular Physics, 2005, 103, 439-450.	1.7	74
358	Chemical and electronic structures of liquid methanol from x-ray emission spectroscopy and density functional theory. Physical Review B, 2005, 71, .	3.2	87
359	Singletâ€“triplet transitions in three-atomic molecules studied by time-dependent MCSCF and density functional theory. Molecular Physics, 2004, 102, 1391-1406.	1.7	24
360	Role of electronic localization and charge-vibrational coupling in resonant photoelectron spectra of polymers: Application to poly(para-phenylenevinylene). Physical Review B, 2004, 69, .	3.2	16

#	Article	IF	Citations
361	Generalization of the duration-time concept for interpreting high-resolution resonant photoemission spectra. Physical Review A, 2004, 69, .	2.5	25
362	Two-color phase-sensitive x-ray pump-probe spectroscopy. Physical Review A, 2004, 70, .	2.5	11
363	Local structures of liquid water studied by x-ray emission spectroscopy. Physical Review B, 2004, 69, .	3.2	83
364	Profile of resonant photoelectron spectra versus the spectral function width and photon frequency detuning. Physical Review A, 2004, 70, .	2.5	3
365	Spectral profiles of two-photon absorption: Coherent versus two-step two-photon absorption. Materials Research Society Symposia Proceedings, 2004, 846, DD1.2.1.	0.1	1
366	Solvent effects on optically detected magnetic resonance in triplet spin labels. Theoretical Chemistry Accounts, 2004, 111, 168-175.	1.4	12
367	Sign Change of Hyperpolarizabilities of Solvated Water, Revised:Â Effects of Equilibrium and Nonequilibrium Solvationâ€. Journal of Physical Chemistry A, 2004, 108, 8961-8965.	2.5	21
368	Calculations of two-photon absorption cross sections by means of density-functional theory. Chemical Physics Letters, 2003, 374, 446-452.	2.6	136
369	CASSCF calculations of triplet state properties: applications to benzene derivatives. Molecular Physics, 2003, 101, 2103-2114.	1.7	30
370	Influence of electron-acceptor strength on the resonant two-photon absorption cross sections of diphenylaminofluorene-based chromophores. Physical Chemistry Chemical Physics, 2003, 5, 3869-3873.	2.8	41
371	Dynamical properties of X-ray Raman scattering. Physical Chemistry Chemical Physics, 2003, 5, 1-11.	2.8	25
372	Density functional theory of nonlinear triplet response properties with applications to phosphorescence. Journal of Chemical Physics, 2003, 119, 11024-11034.	3.0	79
373	Restricted density functional theory of linear time-dependent properties in open-shell molecules. Journal of Chemical Physics, 2003, 119, 34-46.	3.0	91
374	Restricted density-functional linear response theory calculations of electronic g-tensors. Journal of Chemical Physics, 2003, 119, 10489-10496.	3.0	26
375	Fine and hyperfine structure in three low-lying3Î£+states of molecular hydrogen. Molecular Physics, 2003, 101, 2335-2346.	1.7	6
376	Ab initio study of nonhomogeneous broadening of the zero-field splitting of triplet guest molecules in diluted glasses. Journal of Chemical Physics, 2003, 119, 3120-3129.	3.0	14
377	Geometrical information on core-excited states obtained from interference quenching of vibrational states in resonant x-ray photoemission. Physical Review A, 2003, 67, .	2.5	9
378	Effects of dipole alignment and channel interference on two-photon absorption cross sections of two-dimensional charge-transfer systems. Journal of Chemical Physics, 2002, 117, 11102-11106.	3.0	73

#	Article	IF	Citations
379	Theory and first principles calculations of dissociative resonant photoionization: The evolution of atomic peaks and holes. Journal of Chemical Physics, 2002, 116, 629-645.	3.0	11
380	Doppler interference in dissociative resonant photoemission. Physical Review A, 2002, 66, .	2.5	14
381	Activation of Triplet Dioxygen by Glucose Oxidase:â€‰ Spinâ^'Orbit Coupling in the Superoxide Ion. Journal of Physical Chemistry B, 2002, 106, 3742-3750.	2.6	71
382	General theory for pulse propagation in two-photon active media. Journal of Chemical Physics, 2002, 117, 6214-6220.	3.0	31
383	Ab initiostudy of the Cu2pand3score-level XPS spectra of copper phthalocyanine. Physical Review B, 2002, 66, .	3.2	29
384	Relativistic effects on linear and nonlinear polarizabilities studied by effective-core potential, Douglasâ€"Kroll, and Diracâ€"Hartreeâ€"Fock response theory. Journal of Chemical Physics, 2002, 116, 6914-6923.	3.0	60
385	Density Functional Theory Calculations of Electron Paramagnetic Resonance Parameters of a Nitroxide Spin Label in Tissue Factor and Factor VIIa Protein Complex. Journal of Physical Chemistry B, 2002, 106, 12354-12360.	2.6	19
386	A coupled-cluster study of lanthanum trihalide structures. Dalton Transactions RSC, 2002, , 4603-4606.	2.3	8
387	Density-functional theory of linear and nonlinear time-dependent molecular properties. Journal of Chemical Physics, 2002, 117, 9630-9645.	3.0	359
388	An ab initio method for computing multi-atom resonant photoemission. Chemical Physics Letters, 2002, 354, 100-108.	2.6	13
389	X-Ray Emission Spectroscopy of Hydrogen Bonding and Electronic Structure of Liquid Water. Physical Review Letters, 2002, 89, 137402.	7.8	242
390	Ab initio modeling of excited state absorption of polyenes. Physical Chemistry Chemical Physics, 2001, 3, 2567-2575.	2.8	35
391	Nitrogen bonding structure in carbon nitride thin films studied by soft x-ray spectroscopy. Applied Physics Letters, 2001, 79, 4348-4350.	3.3	114
392	Theoretical study of the near-edge CuLx-ray absorption spectrum of copper phthalocyanine. Physical Review B, 2001, 63, .	3.2	39
393	Role of the cavity field in nonlinear optical response in the condensed phase. Journal of Chemical Physics, 2001, 114, 3105-3108.	3.0	28
394	Effects of Ï€ centers and symmetry on two-photon absorption cross sections of organic chromophores. Journal of Chemical Physics, 2001, 114, 9813-9820.	3.0	193
395	Simulations of vibronic profiles in two-photon absorption. Chemical Physics Letters, 2000, 330, 447-456.	2.6	178
396	X-ray Raman scattering under pulsed excitation. Journal of Chemical Physics, 2000, 112, 5593-5603.	3.0	8

#	Article	IF	Citations
397	Continuum modeling of multi-mode vibronic excitations in near-edge x-ray absorption fine structure spectra. Journal of Chemical Physics, 2000, 113, 3734-3740.	3.0	5
398	Modeling of dynamic molecular solvent properties using local and cavity field approaches. Journal of Chemical Physics, 2000, 112, 1868-1875.	3.0	42
399	Resonant x-ray Raman Scattering involving avoided crossings in the final-state potential-energy curves. Physical Review A, 2000, 62, .	2.5	14
400	Hydrogen Bonding to Tyrosyl Radical Analyzed by Ab Initio g-Tensor Calculations. Journal of Physical Chemistry A, 2000, 104, 5149-5153.	2.5	64
401	Electronic and vibronic contributions to two-photon absorption of molecules with multi-branched structures. Journal of Chemical Physics, 2000, 113, 7055-7061.	3.0	226
402	Theoretical calculations of excited state absorption. Physical Chemistry Chemical Physics, 2000, 2, 5357-5363.	2.8	37
403	Vibrational contributions to solute molecular properties obtained through a semiclassical model employing ellipsoidal cavities. Journal of Chemical Physics, 1999, 110, 7960-7965.	3.0	10
404	Core ionization energies of carbonâ€“nitrogen molecules and solids. Journal of Chemical Physics, 1999, 111, 9678-9686.	3.0	36
405	Duration of x-ray Raman scattering. Physical Review A, 1999, 59, 380-389.	2.5	91
406	Large two-photon absorption cross sections in two-dimensional, charge-transfer, cumulene-containing aromatic molecules. Journal of Chemical Physics, 1999, 111, 7758-7765.	3.0	98
407	Bond-Length-Dependent Core Hole Localization Observed in Simple Hydrocarbons. Physical Review Letters, 1999, 83, 1315-1318.	7.8	19
408	Solvent effects on the polarizabilities and hyperpolarizabilities of conjugated polymers. Journal of Chemical Physics, 1999, 111, 9853-9858.	3.0	30
409	Spin uncoupling in molecular hydrogen activation by platinum clusters. Journal of Molecular Catalysis A, 1999, 149, 179-195.	4.8	34
410	Resonant X-ray Raman scattering. Physics Reports, 1999, 312, 87-330.	25.6	435
411	Internal and external heavy-atom effects on phosphorescence radiative lifetimes calculated using a mean-field spinâ€“orbit Hamiltonian. Chemical Physics Letters, 1999, 310, 215-221.	2.6	65
412	Spin uncoupling in ethylene activation by palladium and platinum atoms. International Journal of Quantum Chemistry, 1999, 72, 581-596.	2.0	10
413	Cubic Optical Response of Molecules in a Nonequilibrium and Equilibrium Solvation Model. Journal of Physical Chemistry A, 1999, 103, 8375-8383.	2.5	11
414	Orientational Probing of Multilayer 2-Mercaptobenzoxazole through NEXAFS:Â An Experimental and Theoretical Study. Journal of Physical Chemistry A, 1999, 103, 4641-4648.	2.5	17

#	Article	IF	Citations
415	Measurements of core hole localization in x-ray Raman scattering. JETP Letters, 1998, 67, 1064-1068.	1.4	10
416	Some recent developments of high-order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	2.0	33
417	Response theory calculations of the singletâ€“triplet transition probabilities in the HOCl molecule. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2061-2067.	1.7	14
418	Saturation of the Optical Band Gap and Properties of Five-Membered Heteroaromatic Oligomers. Journal of Physical Chemistry B, 1998, 102, 1710-1712.	2.6	24
419	Response to â€œComment on â€˜The hyperpolarizability of trans-butadiene: A critical test case for quantum chemical modelsâ€™â€‰â€•[J. Chem. Phys. 108, 4355 (1998)]. Journal of Chemical Physics, 1998, 108, 4358-4360.	3.0	6
420	Soft and hard x-ray Raman scattering by oriented symmetrical molecules: Selection rules, interference, and dephasing mechanisms. Journal of Chemical Physics, 1998, 109, 5060-5069.	3.0	5
421	A semiclassical approximation model for properties of molecules in solution. Journal of Chemical Physics, 1998, 109, 3589-3595.	3.0	37
422	A theoretical study of the near-edge x-ray absorption spectra of some larger amino acids. Journal of Chemical Physics, 1998, 109, 1456-1464.	3.0	66
423	Dielectric and optical properties of pure liquids by means ofab initioreaction field theory. Physical Review E, 1998, 57, 4778-4785.	2.1	15
424	Nonlinear optical response of molecules in a nonequilibrium solvation model. Journal of Chemical Physics, 1998, 109, 5576-5584.	3.0	58
425	Spin uncoupling in surface chemisorption of unsaturated hydrocarbons. Journal of Chemical Physics, 1998, 108, 1193-1205.	3.0	94
426	Vibrational corrections to static and dynamic hyperpolarizabilities of pure liquids: Calculations on methanol. Journal of Chemical Physics, 1998, 109, 3580-3588.	3.0	20
427	Some recent developments of highâ€order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	2.0	3
428	Femtosecond Dissociation of Core-Excited HCl Monitored by Frequency Detuning. Physical Review Letters, 1997, 79, 3150-3153.	7.8	166
429	Collapse of vibrational structure in spectra of resonant x-ray Raman scattering. Physical Review A, 1997, 56, 256-264.	2.5	61
430	The hyperpolarizability of trans-butadiene: A critical test case for quantum chemical models. Journal of Chemical Physics, 1997, 106, 1827-1835.	3.0	25
431	Acetonitrile: A critical test case for solvent induced hyperpolarizabilities obtained by the reaction field model. Journal of Chemical Physics, 1997, 107, 9535-9541.	3.0	28
432	Collision-induced b1Î£g+â€“a1 Î”g, b1Î£g+â€“X3 Î£g- and a1Î”gâ€“X3Î£g - transition probabilities in molecular oxygen. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2231-2239.	1.7	74

#	Article	IF	Citations
433	Excitation-energy-dependent resonant photoemission: C1s-Ï€*spectra of carbon monoxide. Physical Review A, 1997, 56, 4665-4674.	2.5	38
434	Ab initio calculations of the polarizability and the hyperpolarizability of C60. Journal of Chemical Physics, 1997, 106, 8788-8791.	3.0	64
435	Restoration of selection rules in nonadiabatic resonant inelastic x-ray scattering. Journal of Experimental and Theoretical Physics, 1997, 85, 20-26.	0.9	13
436	Simulations of resonant X-ray emission spectra of molecules. Applied Physics A: Materials Science and Processing, 1997, 65, 115-122.	2.3	5
437	Nuclear dynamics in X-ray Raman scattering. Applied Physics A: Materials Science and Processing, 1997, 65, 123-130.	2.3	9
438	Direct SCF direct static-exchange calculations of electronic spectra. Theoretical Chemistry Accounts, 1997, 97, 14-40.	1.4	171
439	Cubic response functions in the multiconfiguration selfâ€consistent field approximation. Journal of Chemical Physics, 1996, 105, 6401-6419.	3.0	96
440	Response Theory and Calculations of Spin-Orbit Coupling Phenomena in Molecules. Advances in Quantum Chemistry, 1996, , 71-162.	0.8	137
441	Paramagnetic Exchange Spin-Catalysis of theCisâ^'TransIsomerization of Substituted Ethylenes. The Journal of Physical Chemistry, 1996, 100, 8308-8315.	2.9	12
442	Response theory for static and dynamic polarizabilities of excited states. Journal of Chemical Physics, 1996, 105, 581-587.	3.0	46
443	Magnetic hyperpolarizabilities in a cubic response formulation. Theoretica Chimica Acta, 1996, 93, 235-241.	0.8	14
444	Spin-catalysis phenomena. International Journal of Quantum Chemistry, 1996, 57, 519-532.	2.0	45
445	Magnetic phosphorescence of molecular oxygen. A study of the b1Î£g+-X3Î£gâ^' transition probability using multiconfiguration response theory. Chemical Physics, 1996, 208, 299-311.	1.9	57
446	X-ray resonant scattering involving dissociative states. Physical Review A, 1996, 54, 379-393.	2.5	95
447	Quenching of Symmetry Breaking in Resonant Inelastic X-Ray Scattering by Detuned Excitation. Physical Review Letters, 1996, 77, 5035-5038.	7.8	116
448	A Configuration Interaction Study of the (O₂)₂Dimer. Spectroscopy Letters, 1996, 29, 677-695.	1.0	14
449	Spin-orbit coupling in the intersystem crossing of the ring-opened oxirane biradical. International Journal of Quantum Chemistry, 1995, 55, 23-34.	2.0	12
450	Response theory calculations of singlet-triplet transitions in molecular nitrogen. Chemical Physics, 1995, 190, 11-29.	1.9	23

#	Article	IF	Citations
451	Core electron chemical shifts in conjugated molecules and polymers. Journal of Chemical Physics, 1995, 103, 5848-5859.	3.0	14
452	Sign change of hyperpolarizabilities of solvated water. Journal of Chemical Physics, 1995, 102, 9362-9367.	3.0	100
453	Solvent induced polarizabilities and hyperpolarizabilities of paraâ€nitroaniline studied by reaction field linear response theory. Journal of Chemical Physics, 1994, 100, 8240-8250.	3.0	169
454	Resonant inelastic x-ray scattering with symmetry-selective excitation. Physical Review A, 1994, 49, 4378-4389.	2.5	154
455	Phosphorescence of aromatic molecules. Journal of Molecular Structure, 1994, 311, 185-197.	3.6	6
456	The interpretation of the Wulf absorption band of ozone. Chemical Physics Letters, 1994, 217, 531-538.	2.6	53
457	The Vegard-Kaplan band and the phosphorescent decay of N2. Chemical Physics Letters, 1994, 231, 387-394.	2.6	8
458	Radiative lifetimes of triplet spin sublevels of the azabenzenes. Chemical Physics, 1994, 181, 291-304.	1.9	12
459	On the interpretation of the external heavy atom effect on singlet-triplet transitions. Chemical Physics, 1994, 181, 15-28.	1.9	50
460	Response theory calculations of the vibronically induced 1A1gâ^'1B2u two-photon spectrum of benzene. Chemical Physics Letters, 1993, 209, 513-518.	2.6	30
461	The vibronically induced phosphorescence in benzene. Chemical Physics, 1993, 175, 245-254.	1.9	47
462	Calculation of xâ€ray emission spectra of molecules and polymers by the Greenâ€™s function method. Journal of Chemical Physics, 1993, 99, 2821-2828.	3.0	12
463	Dipole hyperpolarizability surfaces of ammonia. Journal of Chemical Physics, 1993, 99, 9815-9819.	3.0	13
464	Spinâ€“orbit coupling constants in a multiconfiguration linear response approach. Journal of Chemical Physics, 1992, 96, 2118-2126.	3.0	90
465	Multiconfigurational quadratic response functions for singlet and triplet perturbations: The phosphorescence lifetime of formaldehyde. Journal of Chemical Physics, 1992, 97, 9178-9187.	3.0	148
466	High resolution xâ€ray photoelectron spectroscopy study of Cr(CO)6in the gas phase. Journal of Chemical Physics, 1992, 96, 8770-8780.	3.0	32
467	The second-order energy contribution from the spin-orbit interaction operator to the potential energy curve of Cr2. International Journal of Quantum Chemistry, 1992, 41, 729-731.	2.0	5
468	Calculation of time autocorrelation and spectral functions using locally expanded potentials. International Journal of Quantum Chemistry, 1992, 42, 365-401.	2.0	2

#	Article	IF	Citations
469	The core electron shake phenomenon. International Journal of Quantum Chemistry, 1992, 42, 685-718.	2.0	18
470	Excited state structures and vibronic spectra of H2CO+, HDCO+, and D2CO+ using molecular gradient and Hessian techniques. Journal of Chemical Physics, 1991, 95, 5906-5917.	3.0	14
471	Doubly charged valence states of formaldehyde, acetaldehyde, acetone, and formamide studied by means of photon excited Auger electron spectroscopy and ab initio calculations. Journal of Chemical Physics, 1991, 95, 5187-5197.	3.0	31
472	A theoretical study of xâ€ray photoelectron spectra of model molecules for polymethylmethacrylate. Journal of Chemical Physics, 1991, 95, 2965-2974.	3.0	80
473	Interaction between theory and experiment in molecular core electron spectroscopies. International Journal of Quantum Chemistry, 1991, 39, 455-486.	2.0	13
474	MCSCF/MCLRStudies of potential energy surfaces, spectra, and properties of theX1A1anda3B2states of ozone. International Journal of Quantum Chemistry, 1991, 40, 475-490.	2.0	28
475	Vibronic emission from short-lived core-hole states: Theory and applications for the water molecule. Physical Review A, 1989, 40, 187-206.	2.5	88
476	An efficient method for calculating molecular radiative intensities in the VUV and soft X-ray wavelength regions. Physica Scripta, 1989, 40, 745-750.	2.5	45
477	Selfâ€consistent reaction field calculations of photoelectron binding energies for solvated molecules. Journal of Chemical Physics, 1989, 90, 6422-6435.	3.0	40
478	Efficient optimization of large scale MCSCF wave functions with a restricted step algorithm. Journal of Chemical Physics, 1987, 87, 451-466.	3.0	112
479	A diabatic model for photoionization. Application to the inner valence xâ€ray photoelectron spectrum of acetylene. Journal of Chemical Physics, 1986, 85, 6270-6275.	3.0	14
480	Theoretical studies of I.R. intensities in Zn2+OH2and Mg2+OH2. Molecular Physics, 1986, 57, 857-863.	1.7	5
481	Origin of phase transition shifts of ionization energies in water. Molecular Physics, 1985, 55, 901-922.	1.7	19
482	Direct restricted-step MCSCF calculations on the structure and spectrum of cyclobutadiene. International Journal of Quantum Chemistry, 1985, 28, 237-246.	2.0	0
483	Origin of Fine Structure in the Vicinity of the K-edges in the CO Electron Energy Loss Spectra. Physica Scripta, 1984, 30, 55-58.	2.5	37
484	Application of the potential model for ESCA shifts to core-hole state geometric relaxation. Chemical Physics Letters, 1981, 83, 149-150.	2.6	11
485	SCF and limited CI calculations for assignment of the Auger spectrum and of the satellites in the soft X-ray spectrum of H2O. Chemical Physics Letters, 1975, 35, 336-344.	2.6	113
486	The X-ray emission spectrum of water. Journal of Physics B: Atomic and Molecular Physics, 1975, 8, L18-L19.	1.6	41

#	Article	IF	Citations
487	Properties and Spectroscopies. , 0, , 125-312.		3
488	Syntheses of thiophene appended N-confused phlorin isomers. Journal of Porphyrins and Phthalocyanines, 0, , A-G.	0.8	1
489	Synthesis, characterization, and spectroscopic properties of 2â€(3,5,6â€trichloroâ€1,4â€benzoquinonâ€2â€yl)â€neoâ€fused hexaphyrin. Bulletin of the Korean Chemical Society, 0, , .	1.9	0
490	Less is more: On the effect of benzannulation on solid-state emission of difluoroborates. Journal of Materials Chemistry C, 0, , .	5.5	6
491	Electronic and Optical Properties of C₁₆S₈ and C₁₆S₄Se₄ Molecules and Crystals. New Journal of Chemistry, 0, , .	2.8	1