Patrick Norman

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2965405/publications.pdf

Version: 2024-02-01

		57719	74108
202	7,474	44	75
papers	citations	h-index	g-index

223	223	223	5406
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
2	Electronic and vibronic contributions to two-photon absorption of molecules with multi-branched structures. Journal of Chemical Physics, 2000, 113, 7055-7061.	1.2	226
3	Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. Chemical Reviews, 2018, 118, 7208-7248.	23.0	214
4	Near-resonant absorption in the time-dependent self-consistent field and multiconfigurational self-consistent field approximations. Journal of Chemical Physics, 2001, 115, 10323.	1.2	197
5	Nonlinear response theory with relaxation: The first-order hyperpolarizability. Journal of Chemical Physics, 2005, 123, 194103.	1.2	178
6	Solvent-Induced Two-Photon Absorption of a Pushâ^'Pull Moleculeâ€. Journal of Physical Chemistry A, 2000, 104, 4718-4722.	1.1	161
7	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. Physical Review A, 2012, 85, .	1.0	137
8	Polarization Propagator for X-Ray Spectra. Physical Review Letters, 2006, 97, 143001.	2.9	111
9	A perspective on nonresonant and resonant electronic response theory for time-dependent molecular properties. Physical Chemistry Chemical Physics, 2011, 13, 20519.	1.3	109
10	Large two-photon absorption cross sections in two-dimensional, charge-transfer, cumulene-containing aromatic molecules. Journal of Chemical Physics, 1999, 111, 7758-7765.	1.2	98
11	Asymmetric-Lanczos-Chain-Driven Implementation of Electronic Resonance Convergent Coupled-Cluster Linear Response Theory. Journal of Chemical Theory and Computation, 2012, 8, 1616-1628.	2.3	98
12	Cubic response functions in the multiconfiguration selfâ€consistent field approximation. Journal of Chemical Physics, 1996, 105, 6401-6419.	1.2	96
13	Density-functional theory calculations of optical rotatory dispersion in the nonresonant and resonant frequency regions. Journal of Chemical Physics, 2004, 120, 5027-5035.	1.2	81
14	X-ray absorption spectra from the resonant-convergent first-order polarization propagator approach. Physical Review A, 2006, 74, .	1.0	75
15	A Palette of Fluorescent Thiopheneâ€Based Ligands for the Identification of Protein Aggregates. Chemistry - A European Journal, 2015, 21, 15133-15137.	1.7	74
16	Quadratic response functions in the relativistic four-component Kohn-Sham approximation. Journal of Chemical Physics, 2008, 128, 024105.	1.2	71
17	Electric and magnetic properties of fullerenes. Journal of Chemical Physics, 1998, 109, 572-577.	1.2	70
18	Cubic Nonlinear Optical Properties of Platinum-Terminated Polyynediyl Chains. Inorganic Chemistry, 2008, 47, 9946-9957.	1.9	66

#	Article	IF	Citations
19	Ab initio calculations of the polarizability and the hyperpolarizability of C60. Journal of Chemical Physics, 1997, 106, 8788-8791.	1.2	64
20	On the Efficiency of Algorithms for Solving Hartreeâ€“Fock and Kohnâ€“Sham Response Equations. Journal of Chemical Theory and Computation, 2011, 7, 1610-1630.	2.3	64
21	Complex polarization propagator calculations of magnetic circular dichroism spectra. Journal of Chemical Physics, 2008, 128, 094103.	1.2	63
22	Electronic circular dichroism spectra from the complex polarization propagator. Journal of Chemical Physics, 2007, 126, 134102.	1.2	61
23	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.	1.2	60
24	A simple polyol-free synthesis route to Gd2O3 nanoparticles for MRI applications: an experimental and theoretical study. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	59
25	Non-linear electric and magnetic properties obtained from cubic response functions in the random phase approximation. Chemical Physics, 1996, 203, 23-42.	0.9	58
26	Nonlinear optical response of molecules in a nonequilibrium solvation model. Journal of Chemical Physics, 1998, 109, 5576-5584.	1.2	58
27	Ab initio calculations of three-photon absorption. Chemical Physics Letters, 2003, 375, 233-239.	1.2	58
28	The A and B Terms of Magnetic Circular Dichroism Revisited. Journal of Physical Chemistry A, 2008, 112, 9615-9618.	1.1	55
29	On the Influence of Water on the Electronic Structure of Firefly Oxyluciferin Anions from Absorption Spectroscopy of Bare and Monohydrated Ions in Vacuo. Journal of the American Chemical Society, 2013, 135, 6485-6493.	6.6	55
30	Structure-to-property relations for two-photon absorption of hydrocarbon oligomers. Chemical Physics Letters, 1998, 296, 8-18.	1.2	54
31	Carbon X-ray absorption spectra of fluoroethenes and acetone: A study at the coupled cluster, density functional, and static-exchange levels of theory. Journal of Chemical Physics, 2013, 138, 124311.	1.2	53
32	Self-interaction-corrected time-dependent density-functional-theory calculations of x-ray-absorption spectra. Physical Review A, 2007, 76, .	1.0	52
33	Efficient Calculations of Molecular Linear Response Properties for Spectral Regions. Journal of Chemical Theory and Computation, 2014, 10, 2449-2455.	2.3	51
34	Bottom-Up Hierarchical Self-Assembly of Chiral Porphyrins through Coordination and Hydrogen Bonds. Journal of the American Chemical Society, 2015, 137, 15795-15808.	6.6	51
35	Cubic response functions in the random phase approximation. Chemical Physics Letters, 1995, 242, 7-16.	1.2	50
36	Tuning the Work Function of Graphene-on-Quartz with a High Weight Molecular Acceptor. Journal of Physical Chemistry C, 2014, 118, 4784-4790.	1.5	50

#	Article	IF	Citations
37	Theoretical study of linear and nonlinear absorption in platinum-organic compounds. Chemical Physics, 2002, 285, 207-220.	0.9	49
38	Polarization propagator calculations of the polarizability tensor at imaginary frequencies and long-range interactions for the noble gases and n-alkanes. Journal of Chemical Physics, 2003, 118, 9167-9174.	1.2	48
39	Damped Response Theory in Combination with Polarizable Environments: The Polarizable Embedding Complex Polarization Propagator Method. Journal of Chemical Theory and Computation, 2014, 10, 1164-1171.	2.3	48
40	Beyond the electric-dipole approximation: A formulation and implementation of molecular response theory for the description of absorption of electromagnetic field radiation. Journal of Chemical Physics, 2015, 142, 244111.	1.2	48
41	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	1.2	47
42	Response theory for static and dynamic polarizabilities of excited states. Journal of Chemical Physics, 1996, 105, 581-587.	1.2	46
43	Effects of vibration on the polarizability and the first and second hyperpolarizabilities of HF, HCl, and HBr. Journal of Chemical Physics, 1999, 111, 3042-3050.	1.2	46
44	Communication: A reduced-space algorithm for the solution of the complex linear response equations used in coupled cluster damped response theory. Journal of Chemical Physics, 2013, 139, 211102.	1.2	45
45	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
46	Modeling of dynamic molecular solvent properties using local and cavity field approaches. Journal of Chemical Physics, 2000, 112, 1868-1875.	1.2	42
47	Few-states models for three-photon absorption. Journal of Chemical Physics, 2004, 121, 2020-2029.	1.2	41
48	Time-dependent density functional theory for resonant properties: resonance enhanced Raman scattering from the complex electric-dipole polarizability. Physical Chemistry Chemical Physics, 2009, 11, 4539.	1.3	40
49	Resonant Inelastic X-ray Scattering Amplitudes and Cross Sections in the Algebraic Diagrammatic Construction/Intermediate State Representation (ADC/ISR) Approach. Journal of Chemical Theory and Computation, 2017, 13, 5552-5559.	2.3	40
50	Relativistic four-component static-exchange approximation for core-excitation processes in molecules. Physical Review A, 2006, 73, .	1.0	39
51	Near-edge x-ray absorption and natural circular dichroism spectra of L-alanine: A theoretical study based on the complex polarization propagator approach. Journal of Chemical Physics, 2007, 127, 165104.	1.2	38
52	Origin of DNA-Induced Circular Dichroism in a Minor-Groove Binder. Journal of the American Chemical Society, 2017, 139, 14947-14953.	6.6	38
53	A semiclassical approximation model for properties of molecules in solution. Journal of Chemical Physics, 1998, 109, 3589-3595.	1.2	37
54	Theoretical calculations of excited state absorption. Physical Chemistry Chemical Physics, 2000, 2, 5357-5363.	1.3	37

#	Article	IF	Citations
55	Evaluation of low-scaling methods for calculation of phosphorescence parameters. Journal of Chemical Physics, 2006, 124, 114106.	1.2	37
56	Computational study of the Rayleigh light scattering properties of atmospheric pre-nucleation clusters. Physical Chemistry Chemical Physics, 2014, 16, 10883-10890.	1.3	37
57	XABOOM: An X-ray Absorption Benchmark of Organic Molecules Based on Carbon, Nitrogen, and Oxygen 1s â†' Ï€* Transitions. Journal of Chemical Theory and Computation, 2021, 17, 1618-1637.	2.3	37
58	Relative Stability of the L_a and L_b Excited States in Adenine and Guanine: Direct Evidence from TD-DFT Calculations of MCD Spectra. Journal of Physical Chemistry Letters, 2014, 5, 1806-1811.	2.1	36
59	Binding modes of a core-extended metalloporphyrin to human telomeric DNA G-quadruplexes. Organic and Biomolecular Chemistry, 2015, 13, 2453-2463.	1.5	36
60	Ab initio modeling of excited state absorption of polyenes. Physical Chemistry Chemical Physics, 2001, 3, 2567-2575.	1.3	35
61	Electric dipole polarizabilities and C6 dipole-dipole dispersion coefficients for sodium clusters and C60. Journal of Chemical Physics, 2006, 125, 124306.	1.2	35
62	Non-additivity of polarizabilities and van der Waals C6 coefficients of fullerenes. Journal of Chemical Physics, 2013, 138, 114107.	1.2	34
63	Toward a Molecular Understanding of the Detection of Amyloid Proteins with Flexible Conjugated Oligothiophenes. Journal of Physical Chemistry A, 2014, 118, 9820-9827.	1.1	34
64	VeloxChem: A Pythonâ€driven densityâ€functional theory program for spectroscopy simulations in highâ€performance computing environments. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1457.	6.2	34
65	Some recent developments of high-order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	1.0	33
66	Excited state polarizabilities in solution obtained by cubic response theory: Calculations on para-, ortho-, and meta-nitroaniline. Journal of Chemical Physics, 1998, 109, 6351-6357.	1.2	33
67	Linear complex polarization propagator in a four-component Kohnâ€“Sham framework. Journal of Chemical Physics, 2010, 133, 064105.	1.2	33
68	Resonance Raman Spectra of TNT and RDX Using Vibronic Theory, Excited-State Gradient, and Complex Polarizability Approximations. Journal of Physical Chemistry A, 2012, 116, 7862-7872.	1.1	33
69	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103.	1.2	33
70	Complex polarization propagator method for calculation of dispersion coefficients of extended Ï€-conjugated systems: The C6 coefficients of polyacenes and C60. Journal of Chemical Physics, 2005, 123, 124312.	1.2	32
71	Calculations of dynamic hyperpolarizabilities for small and medium-sized molecules. , 2001, , 1-62.		31
72	Surface-Enhanced Raman Scattering Due to Charge-Transfer Resonances: A Time-Dependent Density Functional Theory Study of Ag₁₃-4-Mercaptopyridine. Journal of Physical Chemistry C, 2016, 120, 20721-20735.	1.5	31

#	Article	IF	Citations
73	Single determinant calculations of excited state polarizabilities. Chemical Physics, 1997, 224, 201-214.	0.9	30
74	Solvent effects on the polarizabilities and hyperpolarizabilities of conjugated polymers. Journal of Chemical Physics, 1999, 111, 9853-9858.	1.2	30
75	Requirements of first-principles calculations of X-ray absorption spectra of liquid water. Physical Chemistry Chemical Physics, 2016, 18, 566-583.	1.3	30
76	Static polarizabilities and C6 dispersion coefficients using the algebraic-diagrammatic construction scheme for the complex polarization propagator. Journal of Chemical Physics, 2017, 146, .	1.2	30
77	Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. Chemical Science, 2020, 11, 4180-4193.	3.7	29
78	Acetonitrile: A critical test case for solvent induced hyperpolarizabilities obtained by the reaction field model. Journal of Chemical Physics, 1997, 107, 9535-9541.	1.2	28
79	Resonance enhanced Raman scattering from the complex electric-dipole polarizability: A theoretical study on N2. Chemical Physics Letters, 2009, 468, 119-123.	1.2	28
80	Two-photon absorption in five-membered heteroaromatic oligomers. Optics Communications, 1999, 168, 297-303.	1.0	27
81	Probing single-walled carbon nanotube defect chemistry using resonance Raman spectroscopy. Carbon, 2014, 67, 17-26.	5.4	27
82	K- and L-edge X-ray absorption spectrum calculations of closed-shell carbon, silicon, germanium, and sulfur compounds using damped four-component density functional response theory. Physical Chemistry Chemical Physics, 2016, 18, 13591-13603.	1.3	27
83	QM/MM-MD Simulations of Conjugated Polyelectrolytes: A Study of Luminescent Conjugated Oligothiophenes for Use as Biophysical Probes. Journal of Physical Chemistry A, 2014, 118, 3419-3428.	1.1	26
84	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	1.2	26
85	Character and spectra of triplet states in short polyenes. Chemical Physics, 1995, 194, 19-31.	0.9	25
86	The hyperpolarizability of trans-butadiene: A critical test case for quantum chemical models. Journal of Chemical Physics, 1997, 106, 1827-1835.	1.2	25
87	Binding sites for luminescent amyloid biomarkers from non-biased molecular dynamics simulations. Chemical Communications, 2018, 54, 3030-3033.	2.2	25
88	Suppressing depolarization by tail substitution in an organic supramolecular ferroelectric. Physical Chemistry Chemical Physics, 2019, 21, 2069-2079.	1.3	25
89	Excited state properties through cubic response theory: polarizabilities of benzene and naphthalene. Chemical Physics Letters, 1997, 268, 337-344.	1.2	24
90	Molecular length dependence of optical properties of hydrocarbon oligomers. Chemical Physics Letters, 1998, 285, 160-163.	1.2	24

#	Article	IF	Citations
91	Onsager Reaction Field Description of Optical Properties of Octupolar Molecules in Solution. Journal of the American Chemical Society, 1998, 120, 11188-11189.	6.6	24
92	Saturation of the Optical Band Gap and Properties of Five-Membered Heteroaromatic Oligomers. Journal of Physical Chemistry B, 1998, 102, 1710-1712.	1.2	24
93	Rotationally averaged linear absorption spectra beyond the electric-dipole approximation. Molecular Physics, 2017, 115, 63-74.	0.8	24
94	Response theory calculations of singlet-triplet transitions in molecular nitrogen. Chemical Physics, 1995, 190, 11-29.	0.9	23
95	C6dipole-dipole dispersion coefficients for then-alkanes: Test of an additivity procedure. Physical Review A, 2004, 69, .	1.0	23
96	Quadratic response functions in the time-dependent four-component Hartree-Fock approximation. Journal of Chemical Physics, 2004, 121, 6145-6154.	1.2	23
97	Theoretical Simulations of Clamping Levels in Optical Power Limiting. Journal of Physical Chemistry B, 2006, 110, 20912-20916.	1.2	22
98	Molecular dynamics effects on luminescence properties of oligothiophene derivatives: a molecular mechanicsâ€“response theory study based on the CHARMM force field and density functional theory. Physical Chemistry Chemical Physics, 2011, 13, 17532.	1.3	22
99	Sign Change of Hyperpolarizabilities of Solvated Water, Revised:Â Effects of Equilibrium and Nonequilibrium Solvationâ€. Journal of Physical Chemistry A, 2004, 108, 8961-8965.	1.1	21
100	TD-DFT Investigation of the Magnetic Circular Dichroism Spectra of Some Purine and Pyrimidine Bases of Nucleic Acids. Journal of Physical Chemistry A, 2015, 119, 5476-5489.	1.1	21
101	Vibrational corrections to static and dynamic hyperpolarizabilities of pure liquids: Calculations on methanol. Journal of Chemical Physics, 1998, 109, 3580-3588.	1.2	20
102	Size, Order, and Dimensional Relations for Silicon Cluster Polarizabilities. Journal of Physical Chemistry A, 2002, 106, 395-399.	1.1	20
103	Nuclear spin circular dichroism. Journal of Chemical Physics, 2014, 140, 134103.	1.2	20
104	DNA Electronic Circular Dichroism on the Inter-Base Pair Scale: An Experimentalâ€“Theoretical Case Study of the AT Homo-Oligonucleotide. Journal of Physical Chemistry Letters, 2015, 6, 355-359.	2.1	20
105	A Polarization Propagator for Nonlinear X-ray Spectroscopies. Journal of Physical Chemistry Letters, 2016, 7, 1991-1995.	2.1	20
106	Geometry optimization of core electron excited molecules. Computational and Theoretical Chemistry, 1997, 401, 107-115.	1.5	19
107	Relativistic contributions to single and double core electron ionization energies of noble gases. Journal of Chemical Physics, 2011, 135, 054310.	1.2	19
108	Naphthodithiophene Diimide Based Chiral Ï€â€Conjugated Nanopillar Molecules. Angewandte Chemie - International Edition, 2021, 60, 24543-24548.	7.2	19

#	Article	IF	Citations
109	The hypermagnetizability of molecular oxygen. Journal of Chemical Physics, 1997, 106, 8552-8563.	1.2	18
110	Complex Polarization Propagator Approach in the Restricted Open-Shell, Self-Consistent Field Approximation: The Near K-Edge X-ray Absorption Fine Structure Spectra of Allyl and Copper Phthalocyanine. Journal of Physical Chemistry B, 2011, 115, 5096-5102.	1.2	18
111	Hyperpolarizability depolarization ratios of nitroanilines. Journal of Chemical Physics, 1997, 107, 9063-9066.	1.2	17
112	Nonlinear optical susceptibilities of fullerenes in the condensed phase. Physical Review B, 2000, 61, 3060-3066.	1.1	17
113	Relativistic effects on linear and non-linear polarizabilities of the furan homologues. Computational and Theoretical Chemistry, 2003, 633, 237-246.	1.5	17
114	On circular dichroism and the separation between chromophore and chiral center: The near carbon Kâ€edge Xâ€ray absorption and circular dichroism spectra of noradrenaline and <scp>L</scp>â€DOPA. Chirality, 2009, 21, E13-9.	1.3	17
115	The magnetic circular dichroism spectrum of the C₆₀ fullerene. Molecular Physics, 2013, 111, 1401-1404.	0.8	17
116	Generalized integral-screening for efficient calculations of nonlinear optical properties of large molecules. Journal of Chemical Physics, 1998, 108, 7973-7979.	1.2	16
117	X-ray absorption and natural circular dichroism spectra of C84: A theoretical study using the complex polarization propagator approach. Journal of Chemical Physics, 2008, 128, 234304.	1.2	16
118	Near sulfur L-edge X-ray absorption spectra of methanethiol in isolation and adsorbed on a Au(111) surface: a theoretical study using the four-component static exchange approximation. Physical Chemistry Chemical Physics, 2010, 12, 5596.	1.3	16
119	Predicting near-UV electronic circular dichroism in nucleosomal DNA by means of DFT response theory. Physical Chemistry Chemical Physics, 2015, 17, 21866-21879.	1.3	16
120	Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	6.2	16
121	Dielectric and optical properties of pure liquids by means ofab initioreaction field theory. Physical Review E, 1998, 57, 4778-4785.	0.8	15
122	The Cottonâ€“Mouton effect of gaseous CO2, N2O, OCS, and CS2. A cubic response multiconfigurational self-consistent field study. Journal of Chemical Physics, 2001, 114, 8372-8381.	1.2	15
123	Two-photon absorption in the relativistic four-component Hartreeâ€“Fock approximation. Journal of Chemical Physics, 2005, 122, 114106.	1.2	15
124	Noradrenaline and a Thiol Analogue on Gold Surfaces: An Infrared Reflectionâ^'Absorption Spectroscopy, X-ray Photoelectron Spectroscopy, and Near-Edge X-ray Absorption Fine Structure Spectroscopy Study. Journal of Physical Chemistry C, 2011, 115, 165-175.	1.5	15
125	Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution. Photochemical and Photobiological Sciences, 2017, 16, 1415-1423.	1.6	15
126	Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. Physical Chemistry Chemical Physics, 2019, 21, 17410-17422.	1.3	15

#	Article	IF	Citations
127	Kinetic Monte Carlo simulations of organic ferroelectrics. Physical Chemistry Chemical Physics, 2019, 21, 1375-1383.	1.3	15
128	Magnetic hyperpolarizabilities in a cubic response formulation. Theoretica Chimica Acta, 1996, 93, 235-241.	0.9	14
129	Role of noncollinear magnetization for the first-order electric-dipole hyperpolarizability at the four-component Kohnâ€“Sham density functional theory level. Journal of Chemical Physics, 2009, 130, 024109.	1.2	14
130	Rayleigh light scattering properties of atmospheric molecular clusters consisting of sulfuric acid and bases. Physical Chemistry Chemical Physics, 2015, 17, 15701-15709.	1.3	14
131	Distinct Electrostatic Interactions Govern the Chiro-Optical Properties and Architectural Arrangement of Peptideâ€“Oligothiophene Hybrid Materials. Macromolecules, 2017, 50, 7102-7110.	2.2	14
132	Tau Protein Binding Modes in Alzheimerâ€™s Disease for Cationic Luminescent Ligands. Journal of Physical Chemistry B, 2021, 125, 11628-11636.	1.2	14
133	Effects of Ï€-stacking interactions on the near carbon K-edge x-ray absorption fine structure: A theoretical study of the ethylene pentamer and the phthalocyanine dimer. Journal of Chemical Physics, 2009, 130, 104305.	1.2	13
134	A theoretical and experimental study of non-linear absorption properties of substituted 2,5-di-(phenylethynyl)thiophenes and structurally related compounds. Molecular Physics, 2009, 107, 629-641.	0.8	13
135	Atomic ‹i›C‹/i› ‹sub›6‹/sub› dispersion coefficients: a four-component relativistic Kohnâ€“Sham study. Molecular Physics, 2012, 110, 2535-2541.	0.8	13
136	A combined MD/QM and experimental exploration of conformational richness in branched oligothiophenes. Physical Chemistry Chemical Physics, 2014, 16, 24841-24852.	1.3	13
137	Spectroscopic signatures of topological and diatom-vacancy defects in single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2014, 16, 1479-1486.	1.3	13
138	A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion. Physical Chemistry Chemical Physics, 2016, 18, 13267-13279.	1.3	13
139	Binding Modes and Selectivity of Ruthenium Complexes to Human Telomeric DNA Gâ€Quadruplexes. Chemistry - A European Journal, 2018, 24, 15577-15588.	1.7	13
140	Algebraic-diagrammatic construction scheme for the polarization propagator including ground-state coupled-cluster amplitudes. II. Static polarizabilities. Journal of Chemical Physics, 2019, 150, 174105.	1.2	13
141	X-ray absorption spectrum simulations of hexagonal ice. Journal of Chemical Physics, 2019, 150, 034501.	1.2	13
142	Microscopic Theory of Nonlinear Optics. Challenges and Advances in Computational Chemistry and Physics, 2006, , 1-49.	0.6	12
143	Phenylboronic Ester- and Phenylboronic Acid-Terminated Alkanethiols on Gold Surfaces. Journal of Physical Chemistry C, 2012, 116, 796-806.	1.5	12
144	Assessing frequency-dependent site polarisabilities in linear response polarisable embedding. Molecular Physics, 2017, 115, 39-47.	0.8	12

#	Article	IF	Citations
145	A quantum-mechanical perspective on linear response theory within polarizable embedding. Journal of Chemical Physics, 2017, 146, 234101.	1.2	12
146	Elucidating DNA binding of dithienylethenes from molecular dynamics and dichroism spectra. Physical Chemistry Chemical Physics, 2019, 21, 3637-3643.	1.3	12
147	Electronic circular dichroism spectra using the algebraic diagrammatic construction schemes of the polarization propagator up to third order. Journal of Chemical Physics, 2021, 154, 064107.	1.2	12
148	Ground- and excited-state hyperpolarizabilities of cis-, trans- and diphenyl-polyenes. Molecular Physics, 1996, 89, 1409-1421.	0.8	12
149	Cubic Optical Response of Molecules in a Nonequilibrium and Equilibrium Solvation Model. Journal of Physical Chemistry A, 1999, 103, 8375-8383.	1.1	11
150	Excitation and Emission Properties of Platinum(II) Acetylides at High and Low Concentrations. Journal of Physical Chemistry A, 2009, 113, 11242-11249.	1.1	11
151	On the Interplay Between Chirality and Exciton Coupling: A DFT Calculation of the Circular Dichroism in Ï€â€Stacked Ethylene. Chirality, 2014, 26, 483-489.	1.3	11
152	Quantum Mechanics/Molecular Mechanics Density Functional Theory Simulations of the Optical Properties Fingerprinting the Ligand-Binding of Pentameric Formyl Thiophene Acetic Acid in Amyloid-Î²(1â€“42). Journal of Physical Chemistry A, 2020, 124, 875-888.	1.1	11
153	Deciphering the Electronic Transitions of Thiopheneâ€Based Donorâ€Acceptorâ€Donor Pentameric Ligands Utilized for Multimodal Fluorescence Microscopy of Protein Aggregates. ChemPhysChem, 2021, 22, 323-335.	1.0	11
154	Vibrational contributions to solute molecular properties obtained through a semiclassical model employing ellipsoidal cavities. Journal of Chemical Physics, 1999, 110, 7960-7965.	1.2	10
155	ResonantLII,IIIx-ray Raman scattering from HCl. Physical Review A, 2006, 74, .	1.0	10
156	First-order excited state properties in the four-component Hartree-Fock approximation: The excited state electric dipole moments in CsAg and CsAu. Journal of Chemical Physics, 2007, 126, 064313.	1.2	10
157	Platinum(II) and Phosphorus MM3 Force Field Parametrization for Chromophore Absorption Spectra at Room Temperature. Journal of Physical Chemistry A, 2010, 114, 4981-4987.	1.1	10
158	Phosphorescence parameters for platinum (II) organometallic chromophores: A study at the non-collinear four-component Kohnâ€“Sham level of theory. Chemical Physics Letters, 2012, 531, 229-235.	1.2	10
159	Hybrid Complex Polarization Propagator/Molecular Mechanics Method for Heterogeneous Environments. Journal of Chemical Theory and Computation, 2016, 12, 2661-2667.	2.3	10
160	First principle calculations of dipole-dipole dispersion coefficients for the ground and first Ï€ â†' Ï€* excited states of some azabenzenes. Journal of Computational Methods in Sciences and Engineering, 2004, 4, 321-332.	0.1	9
161	First-Principle Quantum Modeling of Optical Power Limiting Materials. Journal of Computational and Theoretical Nanoscience, 2004, 1, 343-366.	0.4	9
162	Characterization of the Chemisorption of Methylsilane on a Au(1,1,1) Surface from the Silicon K- and L-Edge Spectra:â€‰ A Theoretical Study Using the Four-Component Static Exchange Approximation. Journal of Physical Chemistry C, 2007, 111, 13846-13850.	1.5	9

#	Article	IF	Citations
163	Classification of Raman active modes of platinum(II) acetylides: A combined experimental and theoretical study. Chemical Physics Letters, 2009, 481, 209-213.	1.2	9
164	Marine natural products from the deep Pacific as potential non-linear optical chromophores. Physical Chemistry Chemical Physics, 2013, 15, 14814.	1.3	9
165	Four-Component Damped Density Functional Response Theory Study of UV/Vis Absorption Spectra and Phosphorescence Parameters of Group 12 Metal-Substituted Porphyrins. Journal of Chemical Theory and Computation, 2016, 12, 2324-2334.	2.3	9
166	Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112.	1.2	9
167	Nonlinear optical processes of spiroconjugated dimers. Chemical Physics Letters, 1999, 303, 616-620.	1.2	8
168	On the evaluation of quadratic response functions at the four-component Hartree-Fock level: Nonlinear polarization and two-photon absorption in bromo- and iodobenzene. Journal of Chemical Physics, 2006, 124, 214311.	1.2	8
169	Theoretical investigation of thermally and photochemically induced haptotropic rearrangements of chromium ligands on naphthalene systems. Journal of Organometallic Chemistry, 2011, 696, 3861-3866.	0.8	8
170	Ab Initio Excited-State Electronic Circular Dichroism Spectra Exploiting the Third-Order Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator. Journal of Physical Chemistry Letters, 2021, 12, 5132-5137.	2.1	8
171	Relativistic effects on Sternheimer shieldings and the polarizabilities of the electric-field gradient at the nucleus: HX (X=F,Cl,Br,I,At) and Br2. Computational and Theoretical Chemistry, 2003, 633, 163-176.	1.5	7
172	Four-component Hartreeâ€“Fock calculations of magnetic-field induced circular birefringenceâ€”Faraday effectâ€”in noble gases and dihalogens. Journal of Chemical Physics, 2005, 122, 074321.	1.2	7
173	Inter-Excited-State Phosphorescence in the Four-Component Relativistic Kohnâ€“Sham Approximation: A Case Study on Lumiflavin. Journal of Physical Chemistry A, 2015, 119, 11911-11921.	1.1	7
174	Nanoscale Organization of a Platinum(II) Acetylide Cholesteric Liquid Crystal Molecular Glass for Photonics Applications. Advanced Functional Materials, 2020, 30, 1910562.	7.8	7
175	Vibrational resonant inelastic X-ray scattering in liquid acetic acid: a ruler for molecular chain lengths. Scientific Reports, 2021, 11, 4098.	1.6	7
176	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.	1.2	6
177	Resonant-Convergent PCM Response Theory for the Calculation of Second Harmonic Generation in Makaluvamines Aâ€“V: Pyrroloiminoquinone Marine Natural Products from Poriferans of Genus Zyzzya. Journal of Physical Chemistry A, 2015, 119, 5368-5376.	1.1	6
178	Use of two-dimensional photoelectron spectroscopy in the decomposition of an inner-shell excitation spectrum broadened by super-Coster-Kronig decay. Physical Review A, 2013, 88, .	1.0	5
179	Photoelectron Spectroscopy of Molecules Beyond the Electric Dipole Approximation. Journal of Chemical Theory and Computation, 2019, 15, 5483-5494.	2.3	5
180	Atomic photoionization cross sections beyond the electric dipole approximation. Journal of Chemical Physics, 2019, 150, 044306.	1.2	5

#	Article	IF	Citations
181	Size-dependent polarizabilities and van der Waals dispersion coefficients of fullerenes from large-scale complex polarization propagator calculations. Journal of Chemical Physics, 2021, 154, 074304.	1.2	5
182	Calculations of circular intensity differences in electric-field-induced second harmonic generation. Chemical Physics Letters, 1998, 288, 371-376.	1.2	4
183	Polarizabilities and van der WaalsC6coefficients of fullerenes from an atomistic electrodynamics model: Anomalous scaling with number of carbon atoms. Journal of Chemical Physics, 2016, 145, 024311.	1.2	4
184	Resonant-convergent second-order nonlinear response functions at the levels of Hartreeâ€“Fock and Kohnâ€“Sham density functional theory. Journal of Chemical Physics, 2017, 147, 144109.	1.2	4
185	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	1.2	4
186	Multi-functionalized platinum(II) acetylides for optical power limiting. , 2006, , .		3
187	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.	1.1	3
188	Applications of Response Theory with Relaxation. AIP Conference Proceedings, 2007, , .	0.3	3
189	A QM/MM and QM/QM/MM study of Kerr, Cottonâ€“Mouton and Jones linear birefringences in liquid acetonitrile. Physical Chemistry Chemical Physics, 2018, 20, 3831-3840.	1.3	3
190	Efficient implementation of isotropic cubic response functions for two-photon absorption cross sections within the self-consistent field approximation. Journal of Chemical Physics, 2021, 154, 024111.	1.2	3
191	Naphthodithiophene Diimide Based Chiral ï€â€Conjugated Nanopillar Molecules. Angewandte Chemie, 2021, 133, 24748.	1.6	3
192	Multiphysics modelling of optical materials. , 2006, 6401, 4.		2
193	Resonance interaction induced by metal surfaces catalyzes atom-pair breakage. Physical Review A, 2013, 87, .	1.0	2
194	Tyrosine Sideâ€Chain Functionalities at Distinct Positions Determine the Chirooptical Properties and Supramolecular Structures of Pentameric Oligothiophenes. ChemistryOpen, 2020, 9, 1100-1108.	0.9	2
195	Hydrogen bond effects in multimode nuclear dynamics of acetic acid observed via resonant x-ray scattering. Journal of Chemical Physics, 2021, 154, 214304.	1.2	2
196	Optical properties of donor-triad cluster in GaAs and GaN. Applied Physics Letters, 2002, 81, 3158-3160.	1.5	1
197	Electric dipole polarizabilities and C6 dipole-dipole dispersion coefficients for alkali metal clusters and C60. Journal of Computational Methods in Sciences and Engineering, 2008, 7, 475-488.	0.1	1
198	A density functional theory study of magneto-electric Jones birefringence of noble gases, furan homologues, and mono-substituted benzenes. Journal of Chemical Physics, 2013, 139, 194311.	1.2	1

#	Article	IF	Citations
199	Simulations of x-ray absorption spectra for CO desorbing from Ru(0001) with transition-potential and time-dependent density functional theory approaches. Structural Dynamics, 2022, 9, 014101.	0.9	1
200	On the vibrational and orientational probing of surface-adsorbates by direct and resonance photoemission. Surface Science, 1994, 311, 375-384.	0.8	0
201	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
202	RÃ¼cktitelbild: Naphthodithiophene Diimide Based Chiral Ï€â€Conjugated Nanopillar Molecules (Angew.) Tj ETQq0 0 0 rgBT /Overlock 1	1.6	0