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	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
2	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
3	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
4	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
5	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
6	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
7	Vibrational resonant inelastic X-ray scattering in liquid acetic acid: a ruler for molecular chain lengths. Scientific Reports, 2021, 11, 4098.	1.6	7
8	Gator: A Pythonâ€driven program for spectroscopy simulations using correlated wave functions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1528.	6.2	16
9	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
10	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
11	Analytical gradients for core-excited states in the algebraic diagrammatic construction (ADC) framework. Journal of Chemical Physics, 2021, 155, 044106.	1.2	4
12	Naphthodithiophene Diimide Based Chiral Ï€â€Conjugated Nanopillar Molecules. Angewandte Chemie - International Edition, 2021, 60, 24543-24548.	7.2	19
13	Naphthodithiophene Diimide Based Chiral Ï€â€Conjugated Nanopillar Molecules. Angewandte Chemie, 2021, 133, 24748.	1.6	3
14	RÃ¼cktitelbild: Naphthodithiophene Diimide Based Chiral Ï€â€Conjugated Nanopillar Molecules (Angew.) Tj ETQq0 0 0 rgBT /Overlock 10	1.6	
15	Tau Protein Binding Modes in Alzheimerâ€™s Disease for Cationic Luminescent Ligands. Journal of Physical Chemistry B, 2021, 125, 11628-11636.	1.2	14
16	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
17	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
18	Complex excited state polarizabilities in the ADC/ISR framework. Journal of Chemical Physics, 2020, 153, 074112.	1.2	9

#	Article	IF	Citations
19	Nanoscale Organization of a Platinum(II) Acetylide Cholesteric Liquid Crystal Molecular Glass for Photonics Applications. Advanced Functional Materials, 2020, 30, 1910562.	7.8	7
20	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. Journal of Chemical Physics, 2020, 152, 214115.	1.2	45
21	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
22	Probing competing relaxation pathways in malonaldehyde with transient X-ray absorption spectroscopy. Chemical Science, 2020, 11, 4180-4193.	3.7	29
23	Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. Physical Chemistry Chemical Physics, 2019, 21, 17410-17422.	1.3	15
24	Photoelectron Spectroscopy of Molecules Beyond the Electric Dipole Approximation. Journal of Chemical Theory and Computation, 2019, 15, 5483-5494.	2.3	5
25	Elucidating DNA binding of dithienylethenes from molecular dynamics and dichroism spectra. Physical Chemistry Chemical Physics, 2019, 21, 3637-3643.	1.3	12
26	Atomic photoionization cross sections beyond the electric dipole approximation. Journal of Chemical Physics, 2019, 150, 044306.	1.2	5
27	Kinetic Monte Carlo simulations of organic ferroelectrics. Physical Chemistry Chemical Physics, 2019, 21, 1375-1383.	1.3	15
28	Suppressing depolarization by tail substitution in an organic supramolecular ferroelectric. Physical Chemistry Chemical Physics, 2019, 21, 2069-2079.	1.3	25
29	Nuclear dynamics in resonant inelastic X-ray scattering and X-ray absorption of methanol. Journal of Chemical Physics, 2019, 150, 234301.	1.2	26
30	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
31	X-ray absorption spectrum simulations of hexagonal ice. Journal of Chemical Physics, 2019, 150, 034501.	1.2	13
32	Binding sites for luminescent amyloid biomarkers from non-biased molecular dynamics simulations. Chemical Communications, 2018, 54, 3030-3033.	2.2	25
33	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
34	Binding Modes and Selectivity of Ruthenium Complexes to Human Telomeric DNA Gâ€Quadruplexes. Chemistry - A European Journal, 2018, 24, 15577-15588.	1.7	13
35	Simulating X-ray Spectroscopies and Calculating Core-Excited States of Molecules. Chemical Reviews, 2018, 118, 7208-7248.	23.0	214
36	Rotationally averaged linear absorption spectra beyond the electric-dipole approximation. Molecular Physics, 2017, 115, 63-74.	0.8	24

#	Article	IF	Citations
37	Assessing frequency-dependent site polarisabilities in linear response polarisable embedding. Molecular Physics, 2017, 115, 39-47.	0.8	12
38	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
39	Origin of DNA-Induced Circular Dichroism in a Minor-Groove Binder. Journal of the American Chemical Society, 2017, 139, 14947-14953.	6.6	38
40	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
41	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
42	Distinct Electrostatic Interactions Govern the Chiro-Optical Properties and Architectural Arrangement of Peptideâ€“Oligothiophene Hybrid Materials. Macromolecules, 2017, 50, 7102-7110.	2.2	14
43	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
44	A quantum-mechanical perspective on linear response theory within polarizable embedding. Journal of Chemical Physics, 2017, 146, 234101.	1.2	12
45	A complex-polarization-propagator protocol for magneto-chiral axial dichroism and birefringence dispersion. Physical Chemistry Chemical Physics, 2016, 18, 13267-13279.	1.3	13
46	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
47	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
48	Hybrid Complex Polarization Propagator/Molecular Mechanics Method for Heterogeneous Environments. Journal of Chemical Theory and Computation, 2016, 12, 2661-2667.	2.3	10
49	A Polarization Propagator for Nonlinear X-ray Spectroscopies. Journal of Physical Chemistry Letters, 2016, 7, 1991-1995.	2.1	20
50	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
51	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
52	Requirements of first-principles calculations of X-ray absorption spectra of liquid water. Physical Chemistry Chemical Physics, 2016, 18, 566-583.	1.3	30
53	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
54	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

#	Article	IF	Citations
55	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
56	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
57	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
58	A Palette of Fluorescent Thiopheneâ€Based Ligands for the Identification of Protein Aggregates. Chemistry - A European Journal, 2015, 21, 15133-15137.	1.7	74
59	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
60	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
61	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
62	Binding modes of a core-extended metalloporphyrin to human telomeric DNA G-quadruplexes. Organic and Biomolecular Chemistry, 2015, 13, 2453-2463.	1.5	36
63	Nuclear spin circular dichroism. Journal of Chemical Physics, 2014, 140, 134103.	1.2	20
64	A combined MD/QM and experimental exploration of conformational richness in branched oligothiophenes. Physical Chemistry Chemical Physics, 2014, 16, 24841-24852.	1.3	13
65	The <scp>D</scp>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
66	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
67	Spectroscopic signatures of topological and diatom-vacancy defects in single-walled carbon nanotubes. Physical Chemistry Chemical Physics, 2014, 16, 1479-1486.	1.3	13
68	Efficient Calculations of Molecular Linear Response Properties for Spectral Regions. Journal of Chemical Theory and Computation, 2014, 10, 2449-2455.	2.3	51
69	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
70	Computational study of the Rayleigh light scattering properties of atmospheric pre-nucleation clusters. Physical Chemistry Chemical Physics, 2014, 16, 10883-10890.	1.3	37
71	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
72	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

#	Article	IF	Citations
73	Probing single-walled carbon nanotube defect chemistry using resonance Raman spectroscopy. Carbon, 2014, 67, 17-26.	5.4	27
74	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
75	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
76	The magnetic circular dichroism spectrum of the C₆₀ fullerene. Molecular Physics, 2013, 111, 1401-1404.	0.8	17
77	Marine natural products from the deep Pacific as potential non-linear optical chromophores. Physical Chemistry Chemical Physics, 2013, 15, 14814.	1.3	9
78	Photoionization cross section by Stieltjes imaging applied to coupled cluster Lanczos pseudo-spectra. Journal of Chemical Physics, 2013, 139, 094103.	1.2	33
79	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
80	Resonance interaction induced by metal surfaces catalyzes atom-pair breakage. Physical Review A, 2013, 87, .	1.0	2
81	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
82	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
83	Non-additivity of polarizabilities and van der Waals C6 coefficients of fullerenes. Journal of Chemical Physics, 2013, 138, 114107.	1.2	34
84	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
85	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
86	Phenylboronic Ester- and Phenylboronic Acid-Terminated Alkanethiols on Gold Surfaces. Journal of Physical Chemistry C, 2012, 116, 796-806.	1.5	12
87	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
88	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
89	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
90	Atomic C ₆ dispersion coefficients: a four-component relativistic Kohnâ€“Sham study. Molecular Physics, 2012, 110, 2535-2541.	0.8	13

#	Article	IF	Citations
91	Coupled-cluster response theory for near-edge x-ray-absorption fine structure of atoms and molecules. Physical Review A, 2012, 85, .	1.0	137
92	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
93	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
94	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
95	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
96	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
97	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
98	A perspective on nonresonant and resonant electronic response theory for time-dependent molecular properties. Physical Chemistry Chemical Physics, 2011, 13, 20519.	1.3	109
99	Relativistic contributions to single and double core electron ionization energies of noble gases. Journal of Chemical Physics, 2011, 135, 054310.	1.2	19
100	Linear complex polarization propagator in a four-component Kohnâ€“Sham framework. Journal of Chemical Physics, 2010, 133, 064105.	1.2	33
101	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
102	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
103	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
104	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
105	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
106	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
107	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
108	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

#	Article	IF	Citations
109	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
110	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
111	Quadratic response functions in the relativistic four-component Kohn-Sham approximation. Journal of Chemical Physics, 2008, 128, 024105.	1.2	71
112	The A and B Terms of Magnetic Circular Dichroism Revisited. Journal of Physical Chemistry A, 2008, 112, 9615-9618.	1.1	55
113	Cubic Nonlinear Optical Properties of Platinum-Terminated Polyynediyl Chains. Inorganic Chemistry, 2008, 47, 9946-9957.	1.9	66
114	Complex polarization propagator calculations of magnetic circular dichroism spectra. Journal of Chemical Physics, 2008, 128, 094103.	1.2	63
115	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
116	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
117	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
118	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
119	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
120	Electronic circular dichroism spectra from the complex polarization propagator. Journal of Chemical Physics, 2007, 126, 134102.	1.2	61
121	Applications of Response Theory with Relaxation. AIP Conference Proceedings, 2007, , .	0.3	3
122	Self-interaction-corrected time-dependent density-functional-theory calculations of x-ray-absorption spectra. Physical Review A, 2007, 76, .	1.0	52
123	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
124	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
125	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
126	Theoretical Simulations of Clamping Levels in Optical Power Limiting. Journal of Physical Chemistry B, 2006, 110, 20912-20916.	1.2	22

#	Article	IF	Citations
127	Multiphysics modelling of optical materials. , 2006, 6401, 4.		2
128	Multi-functionalized platinum(II) acetylides for optical power limiting. , 2006, , .		3
129	Electric dipole polarizabilities and C6 dipole-dipole dispersion coefficients for sodium clusters and C60. Journal of Chemical Physics, 2006, 125, 124306.	1.2	35
130	Relativistic four-component static-exchange approximation for core-excitation processes in molecules. Physical Review A, 2006, 73, .	1.0	39
131	Microscopic Theory of Nonlinear Optics. Challenges and Advances in Computational Chemistry and Physics, 2006, , 1-49.	0.6	12
132	Evaluation of low-scaling methods for calculation of phosphorescence parameters. Journal of Chemical Physics, 2006, 124, 114106.	1.2	37
133	ResonantLII,IIIx-ray Raman scattering from HCl. Physical Review A, 2006, 74, .	1.0	10
134	X-ray absorption spectra from the resonant-convergent first-order polarization propagator approach. Physical Review A, 2006, 74, .	1.0	75
135	Polarization Propagator for X-Ray Spectra. Physical Review Letters, 2006, 97, 143001.	2.9	111
136	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
137	Two-photon absorption in the relativistic four-component Hartreeâ€“Fock approximation. Journal of Chemical Physics, 2005, 122, 114106.	1.2	15
138	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
139	Nonlinear response theory with relaxation: The first-order hyperpolarizability. Journal of Chemical Physics, 2005, 123, 194103.	1.2	178
140	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
141	C6dipole-dipole dispersion coefficients for then-alkanes: Test of an additivity procedure. Physical Review A, 2004, 69, .	1.0	23
142	Quadratic response functions in the time-dependent four-component Hartree-Fock approximation. Journal of Chemical Physics, 2004, 121, 6145-6154.	1.2	23
143	Few-states models for three-photon absorption. Journal of Chemical Physics, 2004, 121, 2020-2029.	1.2	41
144	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

#	Article	IF	Citations
145	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
146	First-Principle Quantum Modeling of Optical Power Limiting Materials. Journal of Computational and Theoretical Nanoscience, 2004, 1, 343-366.	0.4	9
147	Ab initio calculations of three-photon absorption. Chemical Physics Letters, 2003, 375, 233-239.	1.2	58
148	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
149	Relativistic effects on linear and non-linear polarizabilities of the furan homologues. Computational and Theoretical Chemistry, 2003, 633, 237-246.	1.5	17
150	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
151	Size, Order, and Dimensional Relations for Silicon Cluster Polarizabilities. Journal of Physical Chemistry A, 2002, 106, 395-399.	1.1	20
152	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
153	Optical properties of donor-triad cluster in GaAs and GaN. Applied Physics Letters, 2002, 81, 3158-3160.	1.5	1
154	Theoretical study of linear and nonlinear absorption in platinum-organic compounds. Chemical Physics, 2002, 285, 207-220.	0.9	49
155	Ab initio modeling of excited state absorption of polyenes. Physical Chemistry Chemical Physics, 2001, 3, 2567-2575.	1.3	35
156	Calculations of dynamic hyperpolarizabilities for small and medium-sized molecules. , 2001, , 1-62.		31
157	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
158	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
159	Nonlinear optical susceptibilities of fullerenes in the condensed phase. Physical Review B, 2000, 61, 3060-3066.	1.1	17
160	Modeling of dynamic molecular solvent properties using local and cavity field approaches. Journal of Chemical Physics, 2000, 112, 1868-1875.	1.2	42
161	Solvent-Induced Two-Photon Absorption of a Pushâ^'Pull Moleculeâ€. Journal of Physical Chemistry A, 2000, 104, 4718-4722.	1.1	161
162	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

#	Article	IF	Citations
163	Theoretical calculations of excited state absorption. Physical Chemistry Chemical Physics, 2000, 2, 5357-5363.	1.3	37
164	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
165	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
166	Solvent effects on the polarizabilities and hyperpolarizabilities of conjugated polymers. Journal of Chemical Physics, 1999, 111, 9853-9858.	1.2	30
167	Two-photon absorption in five-membered heteroaromatic oligomers. Optics Communications, 1999, 168, 297-303.	1.0	27
168	Nonlinear optical processes of spiroconjugated dimers. Chemical Physics Letters, 1999, 303, 616-620.	1.2	8
169	Cubic Optical Response of Molecules in a Nonequilibrium and Equilibrium Solvation Model. Journal of Physical Chemistry A, 1999, 103, 8375-8383.	1.1	11
170	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
171	Molecular length dependence of optical properties of hydrocarbon oligomers. Chemical Physics Letters, 1998, 285, 160-163.	1.2	24
172	Calculations of circular intensity differences in electric-field-induced second harmonic generation. Chemical Physics Letters, 1998, 288, 371-376.	1.2	4
173	Structure-to-property relations for two-photon absorption of hydrocarbon oligomers. Chemical Physics Letters, 1998, 296, 8-18.	1.2	54
174	Some recent developments of high-order response theory. International Journal of Quantum Chemistry, 1998, 70, 219-239.	1.0	33
175	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
176	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
177	Electric and magnetic properties of fullerenes. Journal of Chemical Physics, 1998, 109, 572-577.	1.2	70
178	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
179	A semiclassical approximation model for properties of molecules in solution. Journal of Chemical Physics, 1998, 109, 3589-3595.	1.2	37
180	Generalized integral-screening for efficient calculations of nonlinear optical properties of large molecules. Journal of Chemical Physics, 1998, 108, 7973-7979.	1.2	16

#	Article	IF	Citations
181	Dielectric and optical properties of pure liquids by means ofab initioreaction field theory. Physical Review E, 1998, 57, 4778-4785.	0.8	15
182	Nonlinear optical response of molecules in a nonequilibrium solvation model. Journal of Chemical Physics, 1998, 109, 5576-5584.	1.2	58
183	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
184	Vibrational corrections to static and dynamic hyperpolarizabilities of pure liquids: Calculations on methanol. Journal of Chemical Physics, 1998, 109, 3580-3588.	1.2	20
185	Hyperpolarizability depolarization ratios of nitroanilines. Journal of Chemical Physics, 1997, 107, 9063-9066.	1.2	17
186	The hypermagnetizability of molecular oxygen. Journal of Chemical Physics, 1997, 106, 8552-8563.	1.2	18
187	The hyperpolarizability of trans-butadiene: A critical test case for quantum chemical models. Journal of Chemical Physics, 1997, 106, 1827-1835.	1.2	25
188	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
189	Ab initio calculations of the polarizability and the hyperpolarizability of C60. Journal of Chemical Physics, 1997, 106, 8788-8791.	1.2	64
190	Single determinant calculations of excited state polarizabilities. Chemical Physics, 1997, 224, 201-214.	0.9	30
191	Geometry optimization of core electron excited molecules. Computational and Theoretical Chemistry, 1997, 401, 107-115.	1.5	19
192	Excited state properties through cubic response theory: polarizabilities of benzene and naphthalene. Chemical Physics Letters, 1997, 268, 337-344.	1.2	24
193	Cubic response functions in the multiconfiguration selfâ€consistent field approximation. Journal of Chemical Physics, 1996, 105, 6401-6419.	1.2	96
194	Response theory for static and dynamic polarizabilities of excited states. Journal of Chemical Physics, 1996, 105, 581-587.	1.2	46
195	Magnetic hyperpolarizabilities in a cubic response formulation. Theoretica Chimica Acta, 1996, 93, 235-241.	0.9	14
196	Efficient parallel implementation of response theory: Calculations of the second hyperpolarizability of polyacenes. Chemical Physics Letters, 1996, 253, 1-7.	1.2	47
197	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
198	Ground- and excited-state hyperpolarizabilities of cis-, trans- and diphenyl-polyenes. Molecular Physics, 1996, 89, 1409-1421.	0.8	12

#	Article	IF	Citations
199	Cubic response functions in the random phase approximation. Chemical Physics Letters, 1995, 242, 7-16.	1.2	50
200	Response theory calculations of singlet-triplet transitions in molecular nitrogen. Chemical Physics, 1995, 190, 11-29.	0.9	23
201	Character and spectra of triplet states in short polyenes. Chemical Physics, 1995, 194, 19-31.	0.9	25
202	On the vibrational and orientational probing of surface-adsorbates by direct and resonance photoemission. Surface Science, 1994, 311, 375-384.	0.8	0