

# Kenneth Ruud

## List of Publications by Year in descending order

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335  
papers

16,495  
citations

14614

66  
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23472

111  
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364  
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364  
docs citations

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times ranked

8299  
citing authors

#	ARTICLE	IF	CITATIONS
1	Choosing Bad versus Worse: Predictions of Two-Photon-Absorption Strengths Based on Popular Density Functional Approximations. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1046-1060.	2.3	26
2	Accurate X-ray Absorption Spectra near L- and M-Edges from Relativistic Four-Component Damped Response Time-Dependent Density Functional Theory. <i>Inorganic Chemistry</i> , 2022, 61, 830-846.	1.9	12
3	Behind the scenes of spin-forbidden decay pathways in transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 59-81.	1.3	14
4	Harmonic Infrared and Raman Spectra in Molecular Environments Using the Polarizable Embedding Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3599-3617.	2.3	6
5	FAIR and transparent research data. <i>Open Science Talk</i> , 2021, , .	0.1	0
6	Demystifying the Origin of Vibrational Coherence Transfer Between the S <sub>1</sub> and T <sub>1</sub> States of the Pt-pop Complex. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9768-9773.	2.1	6
7	DORA in practice. <i>Septentrio Conference Series</i> , 2021, , .	0.0	0
8	Relativistic Four-Component DFT Calculations of Vibrational Frequencies. <i>Journal of Physical Chemistry A</i> , 2021, 125, 10315-10320.	1.1	2
9	A generalized few-state model for the first hyperpolarizability. <i>Journal of Chemical Physics</i> , 2020, 152, 244106.	1.2	7
10	Two-photon absorption in host-guest complexes. <i>Molecular Physics</i> , 2020, 118, e1777335.	0.8	3
11	Computational Investigation on the Photophysical Properties of Halogenated Tetraphenyl BODIPY. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11100-11109.	1.5	5
12	ReSpect: Relativistic spectroscopy DFT program package. <i>Journal of Chemical Physics</i> , 2020, 152, 184101.	1.2	90
13	Dalton Project: A Python platform for molecular- and electronic-structure simulations of complex systems. <i>Journal of Chemical Physics</i> , 2020, 152, 214115.	1.2	45
14	Arctic Advanced Education and Research. , 2020, , 133-141.		0
15	Opening speech for the 15th Munin Conference on Scholarly Publishing 2020. <i>Septentrio Conference Series</i> , 2020, , .	0.0	0
16	Implementing DORA. <i>Open Science Talk</i> , 2020, , .	0.1	0
17	Photo-Transformation Trajectories of Nitro-Spiropyran in Hybrid Compounds with [60]Fullerene. <i>Journal of Physical Chemistry C</i> , 2019, 123, 18215-18221.	1.5	3
18	All-electron fully relativistic Kohn-Sham theory for solids based on the Dirac-Coulomb Hamiltonian and Gaussian-type functions. <i>Physical Review B</i> , 2019, 99, .	1.1	24

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19	Relativistic four-component linear damped response TDDFT for electronic absorption and circular dichroism calculations. <i>Journal of Chemical Physics</i> , 2019, 151, 194112.	1.2	17
20	Strong Duschinsky Mixing Induced Breakdown of Kasha's Rule in an Organic Phosphor. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 369-374.	2.1	28
21	Electron-Spin Structure and Metal-Ligand Bonding in Open-Shell Systems from Relativistic EPR and NMR: A Case Study of Square-Planar Iridium Catalysts. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 201-214.	2.3	17
22	Geometric Energy Derivatives at the Complete Basis Set Limit: Application to the Equilibrium Structure and Molecular Force Field of Formaldehyde. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1333-1350.	2.3	41
23	Darmstadtium, roentgenium, and copernicium form strong bonds with cyanide. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25393.	1.0	9
24	Insight into the fluorescence quenching of Trp214 at HSA by the Dimetridazole ligand from simulation. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2018, 354, 86-100.	2.0	7
25	Resolution-of-identity accelerated relativistic two- and four-component electron dynamics approach to chiroptical spectroscopies. <i>Journal of Chemical Physics</i> , 2018, 149, 204104.	1.2	23
26	An efficient pseudo-spectral method for the description of atomic electronic wave functions "Application to the hydrogen atom in a uniform magnetic field. <i>Chemical Physics</i> , 2018, 515, 299-314.	0.9	1
27	Rare and Nonexistent Nitrosyls: Periodic Trends and Relativistic Effects in Ruthenium and Osmium Porphyrin-Based {MNO} Complexes. <i>ACS Omega</i> , 2018, 3, 10513-10516.	1.6	10
28	Benchmarking the Performance of Exchange-Correlation Functionals for Predicting Two-Photon Absorption Strengths. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3677-3685.	2.3	56
29	Unraveling the Microscopic Origin of Triplet Lasing from Organic Solids. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4314-4318.	2.1	9
30	Implementing DORA at UiT The Arctic University of Norway. <i>Septentrio Conference Series</i> , 2018, , .	0.0	0
31	Molecular Electric, Magnetic, and Optical Properties. , 2017, , 497-592.		5
32	Origin of Dual-Peak Phosphorescence and Ultralong Lifetime of 4,6-Diethoxy-2-carbazolyl-1,3,5-triazine. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1253-1258.	2.1	22
33	Interplay of twist angle and solvents with two-photon optical channel interference in aryl-substituted BODIPY dyes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 29461-29471.	1.3	11
34	Anomalous Phosphorescence from an Organometallic White-Light Phosphor. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4893-4897.	2.1	17
35	Cryptophanes for Methane and Xenon Encapsulation: A Comparative Density Functional Theory Study of Binding Properties and NMR Chemical Shifts. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9669-9677.	1.1	8
36	Channel interference in multiphoton absorption. <i>Journal of Chemical Physics</i> , 2017, 146, 244116.	1.2	16

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37	Gauge-origin independent calculations of electric-field-induced second-harmonic generation circular intensity difference using London atomic orbitals. <i>Molecular Physics</i> , 2017, 115, 241-251.	0.8	5
38	Open-ended formulation of self-consistent field response theory with the polarizable continuum model for solvation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 366-379.	1.3	5
39	Four-component relativistic density functional theory with the polarisable continuum model: application to EPR parameters and paramagnetic NMR shifts. <i>Molecular Physics</i> , 2017, 115, 214-227.	0.8	21
40	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2017, , 693-723.		2
41	Institutional transformation towards Open Science: Experiences from UiT The Arctic University of Norway. <i>Septentrio Conference Series</i> , 2017, , .	0.0	0
42	NMR absolute shielding scale and nuclear magnetic dipole moment of $^{207}\text{Pb}$ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16483-16490.	1.3	23
43	Indirect NMR spin-spin coupling constants in diatomic alkali halides. <i>Journal of Chemical Physics</i> , 2016, 145, 244308.	1.2	7
44	Magnetic properties with multiwavelets and DFT: the complete basis set limit achieved. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21145-21161.	1.3	40
45	Mercury Methylation by Cobalt Corrinoids: Relativistic Effects Dictate the Reaction Mechanism. <i>Angewandte Chemie</i> , 2016, 128, 11675-11678.	1.6	4
46	Open-ended response theory with polarizable embedding: multiphoton absorption in biomolecular systems. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28339-28352.	1.3	23
47	Mercury Methylation by Cobalt Corrinoids: Relativistic Effects Dictate the Reaction Mechanism. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 11503-11506.	7.2	33
48	Chiral recognition by fullerenes: CHFClBr enantiomers in the C <sub>82</sub> cage. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 26057-26068.	1.3	12
49	Complete analytic anharmonic hyper-Raman scattering spectra. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22331-22342.	1.3	5
50	Acceleration of Relativistic Electron Dynamics by Means of X2C Transformation: Application to the Calculation of Nonlinear Optical Properties. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5823-5833.	2.3	48
51	Structure, NMR and Electronic Spectra of [ <i>m,n</i> ]Paracyclophanes with Varying Bridges Lengths ( <i>m, n</i> = 4). <i>Journal of Physical Chemistry A</i> , 2016, 120, 724-736.	1.1	10
52	Three-photon circular dichroism: towards a generalization of chiroptical non-linear light absorption. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4174-4184.	1.3	10
53	Analytic calculations of anharmonic infrared and Raman vibrational spectra. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 4201-4215.	1.3	27
54	Absolute NMR shielding scales and nuclear spin-rotation constants in $^{175}\text{LuX}$ and $^{197}\text{AuX}$ (X = 19F,) <i>J. Chem. Phys.</i> 142, 184101 (2015)	1.2	18

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55	Experimental and four-component relativistic DFT studies of tungsten carbonyl complexes. <i>Journal of Physical Organic Chemistry</i> , 2015, 28, 723-731.	0.9	17
56	Pyrrolo[3,2- <i>b</i> ]pyrroles—From Unprecedented Solvatochromism to Two-Photon Absorption. <i>Chemistry - A European Journal</i> , 2015, 21, 18364-18374.	1.7	93
57	FemEx—female excellence in theoretical and computational chemistry. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 1195-1196.	1.0	3
58	The origin dependence of the material constants: the permittivity and the inverse permeability. <i>Molecular Physics</i> , 2015, 113, 1899-1913.	0.8	7
59	NMR shielding and spin-rotation constants in XCO (X = Ni, Pd, Pt) molecules. <i>Molecular Physics</i> , 2015, 113, 1576-1584.	0.8	19
60	Open-Ended Recursive Calculation of Single Residues of Response Functions for Perturbation-Dependent Basis Sets. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4814-4824.	2.3	5
61	Four-Component Relativistic Density Functional Theory Calculations of EPR- and Hyperfine-Coupling Tensors Using Hybrid Functionals: Validation on Transition-Metal Complexes with Large Tensor Anisotropies and Higher-Order Spin-Orbit Effects. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12892-12905.	1.1	49
62	Polarizable Density Embedding: A New QM/QM/MM-Based Computational Strategy. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5344-5355.	1.1	78
63	Excitation Energies from Real-Time Propagation of the Four-Component Dirac-Kohn-Sham Equation. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 980-991.	2.3	72
64	Open-Ended Recursive Approach for the Calculation of Multiphoton Absorption Matrix Elements. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1129-1144.	2.3	35
65	Molecular quantum mechanical gradients within the polarizable embedding approach—Application to the internal vibrational Stark shift of acetophenone. <i>Journal of Chemical Physics</i> , 2015, 142, 034119.	1.2	17
66	Benchmarking two-photon absorption cross sections: performance of CC2 and CAM-B3LYP. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 19306-19314.	1.3	160
67	Four-Component Relativistic Density-Functional Theory Calculations of Nuclear Spin-Rotation Constants: Relativistic Effects in <i>p</i> -Block Hydrides. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3729-3739.	2.3	32
68	Five-Photon Absorption and Selective Enhancement of Multiphoton Absorption Processes. <i>ACS Photonics</i> , 2015, 2, 572-577.	3.2	16
69	X-ray absorption resonances near L <sub>2,3</sub> -edges from real-time propagation of the Dirac-Kohn-Sham density matrix. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22566-22570.	1.3	58
70	Structure, solvent, and relativistic effects on the NMR chemical shifts in square-planar transition-metal complexes: assessment of DFT approaches. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24944-24955.	1.3	82
71	DFT as a Powerful Predictive Tool in Photoredox Catalysis: Redox Potentials and Mechanistic Analysis. <i>Organometallics</i> , 2015, 34, 4218-4228.	1.1	57
72	Communication: The absolute shielding scales of oxygen and sulfur revisited. <i>Journal of Chemical Physics</i> , 2015, 142, 091102.	1.2	27

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73	Molecular Electric, Magnetic, and Optical Properties. , 2015, , 1-97.		2
74	Relativistic Theory of Nuclear Spin-Rotation Tensor. , 2015, , 1-31.		0
75	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	1.5	22
76	Analytic calculations of hyper-Raman spectra from density functional theory hyperpolarizability gradients. Journal of Chemical Physics, 2014, 141, 134107.	1.2	12
77	The <sc>D</sc>alton quantum chemistry program system. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 269-284.	6.2	1,166
78	Intermolecular charge transfer enhances two-photon absorption in yellow fluorescent protein. Physical Chemistry Chemical Physics, 2014, 16, 5958.	1.3	46
79	Spin-Rotation and NMR Shielding Constants in XF Molecules (X = B, Al, Ga, In, and Tl). Journal of Physical Chemistry A, 2014, 118, 9588-9595.	1.1	15
80	A general, recursive, and open-ended response code. Journal of Computational Chemistry, 2014, 35, 622-633.	1.5	34
81	Analytic cubic and quartic force fields using density-functional theory. Journal of Chemical Physics, 2014, 140, 034103.	1.2	38
82	Analytic Density Functional Theory Calculations of Pure Vibrational Hyperpolarizabilities: The First Dipole Hyperpolarizability of Retinal and Related Molecules. Journal of Physical Chemistry A, 2014, 118, 748-756.	1.1	6
83	Cob(II)alamin: Relativistic DFT Analysis of the EPR Parameters. Journal of Chemical Theory and Computation, 2014, 10, 2125-2136.	2.3	12
84	Chemical Control of Channel Interference in Two-Photon Absorption Processes. Accounts of Chemical Research, 2014, 47, 1604-1612.	7.6	59
85	Ab initio and relativistic DFT study of spin-rotation and NMR shielding constants in XF <sub>6</sub> molecules, X = S, Se, Te, Mo, and W. Journal of Chemical Physics, 2014, 140, 194308.	1.2	35
86	Theoretical investigation of two model systems for molecular photoswitch functionality. I. 2-(4-nitropyrimidin-2-yl)ethanol. Molecular Physics, 2014, 112, 818-835.	0.8	1
87	Convergence of environment polarization effects in multiscale modeling of excitation energies. Computational and Theoretical Chemistry, 2014, 1040-1041, 304-311.	1.1	36
88	Shape-Dependent Electronic Excitations in Metallic Chains. Journal of Physical Chemistry C, 2014, 118, 13059-13069.	1.5	10
89	Rotational averaging of multiphoton absorption cross sections. Journal of Chemical Physics, 2014, 141, 204103.	1.2	30
90	Effect of donor-acceptor orientation on solvent-dependent three-photon activity in through-space charge-transfer systems - case study of [2,2]-paracyclophane derivatives. Physical Chemistry Chemical Physics, 2013, 15, 17570.	1.3	7

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91	Four-Component Relativistic Density Functional Theory Calculations of NMR Shielding Tensors for Paramagnetic Systems. <i>Journal of Physical Chemistry A</i> , 2013, 117, 14209-14219.	1.1	60
92	All-Metal Aromaticity: Revisiting the Ring Current Model among Transition Metal Clusters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4789-4796.	2.3	90
93	The Absolute Shielding Constants of Heavy Nuclei: Resolving the Enigma of the $^{119}\text{Sn}$ Absolute Shielding. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 459-463.	2.1	64
94	Cob(II)alamin: Insight Into the Nature of Electronically Excited States Elucidated via Quantum Chemical Computations and Analysis of Absorption, CD and MCD Data. <i>Journal of Physical Chemistry A</i> , 2013, 117, 863-876.	1.1	24
95	A polarizable embedding DFT study of one-photon absorption in fluorescent proteins. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4735.	1.3	44
96	Determination of Absolute Configuration and Conformation of a Cyclic Dipeptide by NMR and Chiral Spectroscopic Methods. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1721-1736.	1.1	59
97	Multiconfigurational Self-Consistent Field Calculations of the Magnetically Induced Current Density Using Gauge-Including Atomic Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2189-2198.	2.3	34
98	Fully adaptive algorithms for multivariate integral equations using the non-standard form and multiwavelets with applications to the Poisson and bound-state Helmholtz kernels in three dimensions. <i>Molecular Physics</i> , 2013, 111, 1143-1160.	0.8	37
99	Four-component relativistic chemical shift calculations of halogenated organic compounds. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 679-687.	0.9	19
100	First Principles Studies of the Vibrationally Resolved Magnetic Circular Dichroism Spectra of Biphenylene. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1557-1567.	2.3	19
101	Effective time-independent studies on resonance Raman spectroscopy of trans-stilbene including the Duschinsky effect. <i>Molecular Physics</i> , 2013, 111, 1511-1525.	0.8	4
102	Role of zero-point vibrational corrections to carbon hyperfine coupling constants in organic $\dot{\text{C}}$ radicals. <i>Journal of Chemical Physics</i> , 2013, 138, 054310.	1.2	6
103	Analytic evaluation of the dipole Hessian matrix in coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2013, 139, 154106.	1.2	6
104	Spin-rotation and NMR shielding constants in HCl. <i>Journal of Chemical Physics</i> , 2013, 139, 234302.	1.2	25
105	Plasmon resonances in linear noble-metal chains. <i>Journal of Chemical Physics</i> , 2012, 137, 194307.	1.2	35
106	Hyper Raman spectra calculated in a time-dependent Hartree-Fock method. <i>Molecular Physics</i> , 2012, 110, 2315-2320.	0.8	5
107	A general toolbox for the calculation of higher-order molecular properties using SCF wave functions at the one-, two- and four-component levels of theory. , 2012, , .		0
108	Porphyrim Protonation Studied by Magnetic Circular Dichroism. <i>Journal of Physical Chemistry A</i> , 2012, 116, 778-783.	1.1	32

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109	Transferability of Various Molecular Property Tensors in Vibrational Spectroscopy. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 977-985.	2.3	60
110	A Combined Atomic Force Microscopy and Computational Approach for the Structural Elucidation of Breitfussin A and B: Highly Modified Halogenated Dipeptides from <i>Thuiaria breitfussi</i> . <i>Angewandte Chemie - International Edition</i> , 2012, 51, 12238-12241.	7.2	92
111	Calculation of two-photon absorption strengths with the approximate coupled cluster singles and doubles model CC2 using the resolution-of-identity approximation. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 1175-1184.	1.3	76
112	Charge-Transfer Excitations in Uranyl Tetrachloride ( $[\text{UO}_2\text{Cl}_4]^{2-}$ ): How Reliable are Electronic Spectra from Relativistic Time-Dependent Density Functional Theory?. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7397-7404.	1.1	47
113	A combined quantum mechanics/molecular mechanics study of the one- and two-photon absorption in the green fluorescent protein. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5440.	1.3	76
114	Vibrationally resolved circular dichroism spectra of a molecule with isotopically engendered chirality. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3669.	1.3	10
115	Absolute Configuration of a Cyclic Dipeptide Reflected in Vibrational Optical Activity: Ab Initio and Experimental Investigation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2554-2563.	1.1	30
116	High-Polarity Solvents Decreasing the Two-Photon Transition Probability of Through-Space Charge-Transfer Systems – A Surprising In Silico Observation. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 961-966.	2.1	38
117	Efficient Calculation of ROA Tensors with Analytical Gradients and Fragmentation. <i>Chirality</i> , 2012, 24, 1018-1030.	1.3	15
118	Parallelization of the polarizable embedding scheme for higher-order response functions. <i>Molecular Physics</i> , 2012, 110, 2579-2586.	0.8	2
119	Determining the Absolute Configuration of Two Marine Compounds Using Vibrational Chiroptical Spectroscopy. <i>Journal of Organic Chemistry</i> , 2012, 77, 858-869.	1.7	71
120	<i>Ab initio</i> calculation of magnetic circular dichroism. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 443-455.	6.2	27
121	Recent Advances in Wave Function-Based Methods of Molecular-Property Calculations. <i>Chemical Reviews</i> , 2012, 112, 543-631.	23.0	549
122	Structure and NMR spectra of cyclophanes with unsaturated bridges (cyclophenes). <i>Magnetic Resonance in Chemistry</i> , 2012, 50, 449-457.	1.1	4
123	Molecular Electric, Magnetic, and Optical Properties. , 2012, , 361-441.		13
124	Zero-point vibrational corrections to isotropic hyperfine coupling constants in polyatomic molecules. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 696-707.	1.3	14
125	The optical activity of $\hat{I}^2, \hat{I}^3$ -enones in ground and excited states using circular dichroism and circularly polarized luminescence. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 643-650.	1.3	45
126	Electronically Excited States of Vitamin B <sub>12</sub> and Methylcobalamin: Theoretical Analysis of Absorption, CD, and MCD Data. <i>Journal of Physical Chemistry B</i> , 2011, 115, 737-748.	1.2	43



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127	Electronically Excited States of Vitamin B <sub>12</sub> : Benchmark Calculations Including Time-Dependent Density Functional Theory and Correlated ab Initio Methods. <i>Journal of Physical Chemistry A</i> , 2011, 115, 1280-1292.	1.1	94
128	Excitation Energies in Solution: The Fully Polarizable QM/MM/PCM Method. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3027-3037.	1.2	118
129	Explicit versus Implicit Solvent Modeling of Raman Optical Activity Spectra. <i>Journal of Physical Chemistry B</i> , 2011, 115, 4128-4137.	1.2	92
130	The ab initio calculation of molecular electric, magnetic and geometric properties. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2627-2651.	1.3	58
131	Structure and NMR Spectra of Some [2.2]Paracyclophanes. The Dilemma of [2.2]Paracyclophane Symmetry. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10638-10649.	1.1	30
132	The First and Second Static Electronic Hyperpolarizabilities of Zigzag Boron Nitride Nanotubes. An ab Initio Approach through the Coupled Perturbed Kohn-Sham Scheme. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12631-12637.	1.1	31
133	Relativistic four-component calculations of Buckingham birefringence using London atomic orbitals. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 685-699.	0.5	4
134	GEN1INT: A unified procedure for the evaluation of one-electron integrals over Gaussian basis functions and their geometric derivatives. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 858-872.	1.0	43
135	Differences in Two-Photon and One-Photon Absorption Profiles Induced by Vibronic Coupling: The Case of Dioxaborine Heterocyclic Dye. <i>ChemPhysChem</i> , 2011, 12, 3392-3403.	1.0	22
136	Coupled-Cluster Calculations of Vibrational Raman Optical Activity Spectra. <i>ChemPhysChem</i> , 2011, 12, 3442-3448.	1.0	34
137	Gauge-origin independent calculations of Jones birefringence. <i>Journal of Chemical Physics</i> , 2011, 135, 134114.	1.2	8
138	Calculation of the first static hyperpolarizability tensor of three-dimensional periodic compounds with a local basis set: A comparison of LDA, PBE, PBE0, B3LYP, and HF results. <i>Journal of Chemical Physics</i> , 2010, 132, 244106.	1.2	68
139	Arbitrary-Order Density Functional Response Theory from Automatic Differentiation. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1971-1980.	2.3	174
140	Ab initio study of coherent anti-Stokes Raman scattering (CARS) of the 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) explosive. <i>Chemical Physics Letters</i> , 2010, 485, 320-325.	1.2	6
141	The aqueous Raman optical activity spectra of 4-hydroxyproline: theory and experiment. <i>Journal of Raman Spectroscopy</i> , 2010, 41, 1200-1210.	1.2	16
142	Excited-state polarizabilities of solvated molecules using cubic response theory and the polarizable continuum model. <i>Journal of Chemical Physics</i> , 2010, 132, 024107.	1.2	8
143	Solvatochromic shift of phenol blue in water from a combined Car-Parrinello molecular dynamics hybrid quantum mechanics-molecular mechanics and ZINDO approach. <i>Journal of Chemical Physics</i> , 2010, 132, 234508.	1.2	25
144	Computational Study of the One- and Two-Photon Absorption and Circular Dichroism of L-Tryptophan. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6500-6512.	1.2	45

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145	An Atomic-Orbital-Based Lagrangian Approach for Calculating Geometric Gradients of Linear Response Properties. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1028-1047.	2.3	28
146	Benchmarking density-functional-theory calculations of rotational g tensors and magnetizabilities using accurate coupled-cluster calculations. <i>Journal of Chemical Physics</i> , 2009, 131, 144104.	1.2	60
147	Theoretical approaches to the calculation of Raman optical activity spectra. <i>Chirality</i> , 2009, 21, E54-67.	1.3	97
148	Spatial structure and NMR spectra of strained [2.2.2]cyclophanes. <i>Magnetic Resonance in Chemistry</i> , 2009, 47, 407-414.	1.1	5
149	Atomic orbital-based cubic response theory for one-, two-, and four-component relativistic self-consistent field models. <i>Chemical Physics</i> , 2009, 356, 177-186.	0.9	18
150	Synthesis, characterization and assignment of the absolute configuration of 4,4-dimethyl-5-oxo-tetrahydrofuran-3-carboxylic acid and its esters: a combined experimental and theoretical investigation. <i>Tetrahedron: Asymmetry</i> , 2009, 20, 1459-1467.	1.8	7
151	Jones and magnetoelectric birefringence of pure substances "A computational study. <i>Canadian Journal of Chemistry</i> , 2009, 87, 1352-1361.	0.6	5
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