Nicholas A Besley

List of Publications by Year
in descending order

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136	11,288	87401 40	33145 104
papers	citations	h-index	g-index

136	136	136	12059
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	1.5	617
4	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
5	Self-Consistent Field Calculations of Excited States Using the Maximum Overlap Method (MOM). Journal of Physical Chemistry A, 2008, 112, 13164-13171.	1.1	435
6	Direct transformation of graphene to fullerene. Nature Chemistry, 2010, 2, 450-453.	6.6	361
7	Self-consistent-field calculations of core excited states. Journal of Chemical Physics, 2009, 130, 124308.	1.2	254
8	Time-dependent density functional theory calculations of the spectroscopy of core electrons. Physical Chemistry Chemical Physics, 2010, 12, 12024.	1.3	202
9	Time-dependent density functional theory calculations of near-edge X-ray absorption fine structure with short-range corrected functionals. Physical Chemistry Chemical Physics, 2009, 11, 10350.	1.3	168
10	Theoretical Studies toward Quantitative Protein Circular Dichroism Calculations. Journal of the American Chemical Society, 1999, 121, 9636-9644.	6.6	151
11	X-ray and Electron Spectroscopy of Water. Chemical Reviews, 2016, 116, 7551-7569.	23.0	143
12	Probing the Reactivity of Photoinitiators for Free Radical Polymerization:Â Time-Resolved Infrared Spectroscopic Study of Benzoyl Radicals. Journal of the American Chemical Society, 2002, 124, 14952-14958.	6.6	128
13	Ab Initio Study of the Electronic Spectrum of Formamide with Explicit Solvent. Journal of the American Chemical Society, 1999, 121, 8559-8566.	6.6	87
14	Reactions of the inner surface of carbon nanotubes and nanoprotrusion processes imaged at the atomic scale. Nature Chemistry, 2011, 3, 732-737.	6.6	83
15	Time-Dependent Density Functional Theory Study of the X-ray Absorption Spectroscopy of Acetylene, Ethylene, and Benzene on Si(100). Journal of Physical Chemistry C, 2007, 111, 3333-3340.	1.5	76
16	Ab Initio Study of the Effect of Solvation on the Electronic Spectra of Formamide andN-Methylacetamide. Journal of Physical Chemistry A, 1998, 102, 10791-10797.	1.1	69
17	A Sequential Molecular Mechanics/Quantum Mechanics Study of the Electronic Spectra of Amides. Journal of the American Chemical Society, 2004, 126, 13502-13511.	6.6	68
18	Assessment of time-dependent density functional theory with the restricted excitation space approximation for excited state calculations of large systems. Molecular Physics, 2018, 116, 1452-1459.	0.8	64

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19	A family of intracules, a conjecture and the electron correlation problem. Physical Chemistry Chemical Physics, 2006, 8, 15-25.	1.3	61
20	Equation of motion coupled cluster theory calculations of the X-ray emission spectroscopy of water. Chemical Physics Letters, 2012, 542, 42-46.	1.2	60
21	Modeling of the spectroscopy of core electrons with density functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1527.	6.2	60
22	Density Functional Theory Based Methods for the Calculation of X-ray Spectroscopy. Accounts of Chemical Research, 2020, 53, 1306-1315.	7.6	59
23	Unusual spectroscopic and photophysical properties of meso-tert-butylBODIPY in comparison to related alkylated BODIPY dyes. RSC Advances, 2015, 5, 89375-89388.	1.7	58
24	Calculation of near-edge X-ray absorption fine structure with the CIS(D) method. Chemical Physics Letters, 2008, 463, 267-271.	1.2	55
25	Calculation of the electronic spectra of molecules in solution and on surfaces. Chemical Physics Letters, 2004, 390, 124-129.	1.2	53
26	Ab Initio Modeling of Amide Vibrational Bands in Solution. Journal of Physical Chemistry A, 2004, 108, 10794-10800.	1.1	52
27	Coupled ab initio potential energy surfaces for the reaction Cl(2P)+HClâ†'ClH+Cl(2P). Physical Chemistry Chemical Physics, 1999, 1, 957-966.	1.3	50
28	Di-8-ANEPPS Emission Spectra in Phospholipid/Cholesterol Membranes: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 4160-4167.	1.2	50
29	Assessment of basis sets for density functional theory-based calculations of core-electron spectroscopies. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	50
30	Computation of the amide I band of polypeptides and proteins using a partial Hessian approach. Journal of Chemical Physics, 2007, 126, 035101.	1.2	47
31	Calculating excited state properties using Kohn-Sham density functional theory. Journal of Chemical Physics, 2013, 138, 064101.	1.2	47
32	Modeling the Absorption Spectrum of Tryptophan in Proteins. Journal of Physical Chemistry B, 2005, 109, 23061-23069.	1.2	46
33	QM/MM Excited State Molecular Dynamics and Fluorescence Spectroscopy of BODIPY. Journal of Physical Chemistry A, 2013, 117, 2644-2650.	1.1	46
34	Two-electron distribution functions and intracules. Theoretical Chemistry Accounts, 2003, 109, 241-250.	0.5	45
35	Structural optimization of molecular clusters with density functional theory combined with basin hopping. Journal of Chemical Physics, 2012, 137, 134106.	1.2	45
36	The role of Hartreeâ€"Fock exchange in the simulation of X-ray absorption spectra: A study of photoexcited. Chemical Physics Letters, 2013, 580, 179-184.	1.2	43

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37	Quantum Chemical Calculations of X-ray Emission Spectroscopy. Journal of Chemical Theory and Computation, 2014, 10, 4557-4564.	2.3	43
38	Photoaquation Mechanism of Hexacyanoferrate(II) Ions: Ultrafast 2D UV and Transient Visible and IR Spectroscopies. Journal of the American Chemical Society, 2017, 139, 7335-7347.	6.6	43
39	Investigating the Calculation of Anharmonic Vibrational Frequencies Using Force Fields Derived from Density Functional Theory. Journal of Physical Chemistry A, 2012, 116, 4417-4425.	1.1	42
40	Structure and Bonding in Ionized Water Clusters. Journal of Physical Chemistry A, 2013, 117, 5385-5391.	1.1	41
41	van der Waals-Induced Chromatic Shifts in Hydrogen-Bonded Two-Dimensional Porphyrin Arrays on Boron Nitride. ACS Nano, 2015, 9, 10347-10355.	7.3	40
42	Theoretical study of the structures and stabilities of iron clusters. Computational and Theoretical Chemistry, 1995, 341, 75-90.	1.5	39
43	Proton transfer or hemibonding? The structure and stability of radical cation clusters. Physical Chemistry Chemical Physics, 2013, 15, 16214.	1.3	39
44	Cyclometallated platinum(<scp>ii</scp>) complexes containing NHC ligands: synthesis, characterization, photophysics and their application as emitters in OLEDs. Dalton Transactions, 2015, 44, 7152-7162.	1.6	37
45	Relationship between x-ray emission and absorption spectroscopy and the local H-bond environment in water. Journal of Chemical Physics, 2018, 148, 144507.	1.2	37
46	N-doping enabled defect-engineering of MoS2 for enhanced and selective adsorption of CO2: A DFT approach. Applied Surface Science, 2021, 542, 148556.	3.1	37
47	Theoretical Study of the 13C NMR Spectroscopy of Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2005, 127, 17948-17953.	6.6	36
48	Modelling the spectroscopy and dynamics of plastocyanin. Physical Chemistry Chemical Physics, 2010, 12, 9667.	1.3	35
49	Ultrafast nonadiabatic dynamics probed by nitrogen K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 2667-2676.	1.3	34
50	NMR chemical shifts of molecules encapsulated in single walled carbon nanotubes. Journal of Chemical Physics, 2008, 128, 101102.	1.2	33
51	Electronic Structure of 5-Hydroxyindole: From Gas Phase to Explicit Solvation. Journal of Physical Chemistry B, 2009, 113, 2535-2541.	1.2	33
52	Basis sets for the calculation of core-electron binding energies. Chemical Physics Letters, 2018, 699, 279-285.	1.2	32
53	Density Functional Theory Based Analysis of Photoinduced Electron Transfer in a Triazacryptand Based K⁺ Sensor. Journal of Physical Chemistry A, 2015, 119, 2902-2907.	1.1	31
54	Kohn-Sham density functional theory calculations of non-resonant and resonant x-ray emission spectroscopy. Journal of Chemical Physics, 2017, 146, .	1.2	29

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55	Synthesis and characterisation of rylene diimide dimers using molecular handcuffs. Chemical Science, 2019, 10, 3723-3732.	3.7	28
56	Partial Hessian Vibrational Analysis of Organic Molecules Adsorbed on Si(100). Journal of Physical Chemistry C, 2008, 112, 4308-4314.	1.5	27
57	Time dependent density functional theory study of the near-edge x-ray absorption fine structure of benzene in gas phase and on metal surfaces. Journal of Chemical Physics, 2008, 129, 064705.	1.2	26
58	Photochemical Dihydrogen Production Using an Analogue of the Active Site of [NiFe] Hydrogenase. Inorganic Chemistry, 2014, 53, 4430-4439.	1.9	26
59	The effect of basis set and exchange-correlation functional on time-dependent density functional theory calculations within the Tamm-Dancoff approximation of the x-ray emission spectroscopy of transition metal complexes. Journal of Chemical Physics, 2016, 144, 114104.	1.2	26
60	Fast Time-Dependent Density Functional Theory Calculations of the X-ray Absorption Spectroscopy of Large Systems. Journal of Chemical Theory and Computation, 2016, 12, 5018-5025.	2.3	26
61	Electronic Excited States of Si(100) and Organic Molecules Adsorbed on Si(100). Journal of Physical Chemistry B, 2006, 110, 1701-1710.	1.2	25
62	Monitoring the Formation and Reactivity of Organometallic Alkane and Fluoroalkane Complexes with Silanes and Xe Using Time-Resolved X-ray Absorption Fine Structure Spectroscopy. Journal of the American Chemical Society, 2019, 141, 11471-11480.	6.6	25
63	Electronic Structure of a Rigid Cyclic Diamide. Journal of Physical Chemistry B, 2000, 104, 12371-12377.	1.2	23
64	Theoretical calculations of the excited state potential energy surfaces of nitric oxide. Chemical Physics Letters, 2011, 513, 179-183.	1.2	23
65	Dimers of acetic acid in helium nanodroplets. Physical Chemistry Chemical Physics, 2019, 21, 13950-13958.	1.3	23
66	Quantized momentum mechanics of inelastic and reactive collisions: the role of energy and angular momentum constraints. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 4267-4282.	0.6	22
67	Substrate-induced shifts and screening in the fluorescence spectra of supramolecular adsorbed organic monolayers. Journal of Chemical Physics, 2018, 149, 054701.	1.2	22
68	Response to â€œComment on â€˜Improving protein circular dichroism calculations in the far-ultraviolet through reparameterizing the amide chromophoreâ€™â€‰â€•[J. Chem. Phys. 111, 2844 (1999)]. Journal of Chemical Physics, 1999, 111, 2846-2847.	1.2	21
69	Computation of molecular Hartreeâ€“Fock Wigner intracules. Journal of Chemical Physics, 2003, 118, 2033-2038.	1.2	21
70	Modelling excited states of weakly bound complexes with density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 14455-14462.	1.3	21
71	Probing Elusive Cations: Infrared Spectroscopy of Protonated Acetic Acid. Journal of Physical Chemistry Letters, 2019, 10, 2108-2112.	2.1	21
72	Computation and analysis of molecular Hartreeâ€”Fock momentum intracules. Molecular Physics, 2002, 100, 1763-1770.	0.8	20

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73	A theoretical study of the near edge X-ray absorption fine structure of amino acids and proteins. Chemical Physics Letters, 2011, 501, 540-546.	1.2	20
74	Rapid anharmonic vibrational corrections derived from partial Hessian analysis. Journal of Chemical Physics, 2012, 136, 224102.	1.2	20
75	Simulation of Two-Dimensional Infrared Spectroscopy of Peptides Using Localized Normal Modes. Journal of Chemical Theory and Computation, 2016, 12, 1905-1918.	2.3	20
76	Atomic and molecular intracules for excited states. Journal of Chemical Physics, 2004, 120, 7290-7297.	1.2	19
77	Theoretical study of the electronic spectroscopy of CO adsorbed on Pt(111). Journal of Chemical Physics, 2005, 122, 184706.	1.2	19
78	Empirical density functional and the adsorption of organic molecules on Si(100). Physical Review B, 2003, 67, .	1.1	18
79	Zinc 1s Valence-to-Core X-ray Emission Spectroscopy of Halozincate Complexes. Journal of Physical Chemistry A, 2019, 123, 9552-9559.	1.1	18
80	Dynamical angular momentum models for rotational transfer in polyatomic molecules. Journal of Chemical Physics, 1995, 102, 7945-7952.	1.2	17
81	Calculating the Fluorescence of 5-Hydroxytryptophan in Proteins. Journal of Physical Chemistry B, 2009, 113, 14521-14528.	1.2	17
82	Infrared Spectroscopy of NaCl(CH₃OH)_n Complexes in Helium Nanodroplets. Journal of Physical Chemistry A, 2016, 120, 8085-8092.	1.1	17
83	Modeling the Infrared and Circular Dichroism Spectroscopy of a Bridged Cyclic Diamide. Journal of Physical Chemistry B, 2011, 115, 5526-5535.	1.2	16
84	Water order profiles on phospholipid/cholesterol membrane bilayer surfaces. Journal of Computational Chemistry, 2011, 32, 2613-2618.	1.5	16
85	Quantum chemical calculations of tryptophan â†' heme electron and excitation energy transfer rates in myoglobin. Journal of Computational Chemistry, 2017, 38, 1495-1502.	1.5	16
86	A QM/MM study of the nature of the entatic state in plastocyanin. Journal of Computational Chemistry, 2017, 38, 1431-1437.	1.5	16
87	NEXAFS spectroscopy of ionic liquids: experiments versus calculations. Physical Chemistry Chemical Physics, 2017, 19, 31156-31167.	1.3	16
88	Improving the predictive quality of timeâ€dependent density functional theory calculations of the Xâ€ray emission spectroscopy of organic molecules. Journal of Computational Chemistry, 2020, 41, 1081-1090.	1.5	16
89	Theoretical simulation of the spectroscopy and dynamics of a red copper protein. Faraday Discussions, 2011, 148, 55-70.	1.6	15
90	Can density functional theory describe the NO(X2Î)-Ar and NO(A2Î£+)-Ar van der Waals complexes?. Journal of Chemical Physics, 2012, 136, 244313.	1.2	15

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91	Computing protein infrared spectroscopy with quantum chemistry. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2007, 365, 2799-2812.	1.6	14
92	Calculating singlet excited states: Comparison with fast time-resolved infrared spectroscopy of coumarins. Journal of Chemical Physics, 2015, 142, 154119.	1.2	14
93	Simulation of Ultra-Fast Dynamics Effects in Resonant Inelastic X-ray Scattering of Gas-Phase Water. Journal of Chemical Theory and Computation, 2018, 14, 2586-2595.	2.3	14
94	Infrared spectroscopy of a small ion solvated by helium: OH stretching region of HeNâ^'HOCO+. Journal of Chemical Physics, 2019, 151, 194307.	1.2	14
95	A systematic shift in the electronic spectra of substituted benzene molecules trapped in helium nanodroplets. Journal of Chemical Physics, 2005, 123, 021102.	1.2	13
96	Photoionization of the iodine 3d, 4s, and 4p orbitals in methyl iodide. Journal of Chemical Physics, 2018, 149, 144302.	1.2	13
97	Hydrogen bonding in protein circular dichroism calculations. Computational and Theoretical Chemistry, 2000, 506, 161-167.	1.5	12
98	Calculation of the vibrational frequencies of carbon clusters and fullerenes with empirical potentials. Physical Chemistry Chemical Physics, 2015, 17, 3898-3908.	1.3	12
99	An empirical force field for the simulation of the vibrational spectroscopy of carbon nanomaterials. Carbon, 2017, 113, 299-308.	5.4	12
100	The growth and fluorescence of phthalocyanine monolayers, thin films and multilayers on hexagonal boron nitride. Chemical Communications, 2018, 54, 12021-12024.	2.2	12
101	Density functional theory study of the near edge X-ray absorption fine structure and infrared spectroscopy of acetylene and benzene on group IV semiconductor surfaces. Surface Science, 2009, 603, 158-164.	0.8	11
102	Auger electron angular distributions following excitation or ionization of the I 3d level in methyl iodide. Journal of Chemical Physics, 2018, 149, 094304.	1.2	11
103	Quantum Chemical Characterization and Design of Quantum Dots for Sensing Applications. Journal of Physical Chemistry A, 2022, 126, 2899-2908.	1.1	11
104	Wigner intracule for the Kellner helium-like ions. International Journal of Quantum Chemistry, 2004, 100, 166-171.	1.0	10
105	Application of Wigner and Husimi intracule based electron correlation models to excited states. Journal of Chemical Physics, 2006, 125, 074104.	1.2	10
106	Accurate time-dependent density functional theory calculations of the near edge X-ray absorption fine structure of large systems. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	10
107	Density functional theory calculations of the non-resonant and resonant X-ray emission spectroscopy of carbon fullerenes and nanotubes. Chemical Physics Letters, 2018, 696, 119-124.	1.2	10
108	A scaled CIS(D) based method for the calculation of valence and core electron ionization energies. Journal of Chemical Physics, 2019, 151, 034104.	1.2	10

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109	Observation of Double Excitations in the Resonant Inelastic X-ray Scattering of Nitric Oxide. Journal of Physical Chemistry Letters, 2020, 11, 7476-7482.	2.1	10
110	Ab Initio Finite-Temperature Electronic Absorption Spectrum of Formamide. Journal of Chemical Theory and Computation, 2006, 2, 1598-1604.	2.3	9
111	Computational Study of the Structure and Electronic Circular Dichroism Spectroscopy of Blue Copper Proteins. Journal of Physical Chemistry B, 2013, 117, 8105-8112.	1.2	9
112	The structure and bonding of mixed component radical cation clusters. Chemical Physics Letters, 2014, 601, 110-115.	1.2	9
113	Reactivity of the O₂⁺Â·(H₂O)_n and NO⁺Â·(H₂O)_n cluster ions in the D-region of the ionosphere. Physical Chemistry Chemical Physics, 2018, 20, 25931-25938.	1.3	9
114	A combined time-resolved infrared and density functional theory study of the lowest excited states of 9-fluorenone and 2-naphthaldehyde. Chemical Physics, 2018, 512, 44-52.	0.9	9
115	Spectroscopic and structural analysis of mixed carbon dioxide and fluorinated methane clusters. Chemical Physics Letters, 2015, 638, 191-195.	1.2	8
116	Simulation of the Raman spectroscopy of multi-layered carbon nanomaterials. Physical Chemistry Chemical Physics, 2018, 20, 28001-28010.	1.3	8
117	AIRBED: A Simplified Density Functional Theory Model for Physisorption on Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 5628-5634.	2.3	8
118	Photoionization of the I 4d and valence orbitals of methyl iodide. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 155101.	0.6	8
119	Density Functional Theory Calculations of Coreâ€“Electron Binding Energies at the K-Edge of Heavier Elements. Journal of Chemical Theory and Computation, 2021, 17, 3644-3651.	2.3	8
120	Computation of Husimi intracules. Chemical Physics Letters, 2005, 409, 63-69.	1.2	7
121	Theoretical Study of the Electronic Spectra of Small Molecules That Incorporate Analogues of the Copperâ€“Cysteine Bond. Journal of Physical Chemistry A, 2012, 116, 8507-8514.	1.1	7
122	Time-dependent density functional theory study of the X-ray emission spectroscopy of amino acids and proteins. Chemical Physics Letters, 2020, 757, 137860.	1.2	7
123	Photoabsorption, photoionization, and Auger processes at the carbon K edge in CH3I. Physical Review A, 2020, 101, .	1.0	7
124	Metastable Aluminum Atoms Floating on the Surface of Helium Nanodroplets. Physical Review Letters, 2015, 114, 233401.	2.9	6
125	Quantum chemical study of the structure, spectroscopy and reactivity of NO + .(H 2 O) n =1â^'5 clusters. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170152.	1.6	6
126	The impact of sulfur functionalisation on nitrogen-based ionic liquid cations. Chemical Communications, 2018, 54, 11403-11406.	2.2	6

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127	Probing the electronic structure of ether functionalised ionic liquids using X-ray photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 1624-1631.	1.3	5
128	Vibrational Analysis of Carbon Nanotube-Based Nanomechanical Resonators. Journal of Physical Chemistry C, 2020, 124, 16714-16721.	1.5	4
129	Simulation of vibrationally resolved absorption spectra of neutral and cationic polyaromatic hydrocarbons. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	4
130	Interaction of the NO 3pÏ€ Rydberg state with Ar: Potential energy surfaces and spectroscopy. Journal of Chemical Physics, 2013, 138, 214313.	1.2	3
131	Interaction of the NO 3pÏ€ (Câ€‰2Î) Rydberg state with RG (RG = Ne, Kr, and Xe): Potential energy surfaces and spectroscopy. Journal of Chemical Physics, 2015, 142, 034311.	1.2	3
132	Electronically excited state geometries and vibrational frequencies calculated using the algebraic diagrammatic construction scheme for the polarization propagator. Chemical Physics Letters, 2019, 726, 62-68.	1.2	3
133	Influence of molecular design on radical spin multiplicity: characterisation of BODIPY dyad and triad radical anions. Physical Chemistry Chemical Physics, 2020, 22, 4429-4438.	1.3	2
134	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
135	Theoretical studies of electronically excited states. , 2014, , .		1
136	Quantitative protein circular dichroism calculations. Special Publication - Royal Society of Chemistry, 0, , 20-30.	0.0	0