Niranjan Govind

List of Publications by Year
in descending order

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162 papers	12,716 citations	50244 46 h-index	29127 104 g-index
172 all docs	172 docs citations	172 times ranked	16463 citing authors

#	Article	IF	Citations
1	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740
2	A generalized synchronous transit method for transition state location. Computational Materials Science, 2003, 28, 250-258.	1.4	1,050
3	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
4	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	2.9	236
5	Modeling Fast Electron Dynamics with Real-Time Time-Dependent Density Functional Theory: Application to Small Molecules and Chromophores. Journal of Chemical Theory and Computation, 2011, 7, 1344-1355.	2.3	217
6	Electronic-structure calculations by first-principles density-based embedding of explicitly correlated systems. Journal of Chemical Physics, 1999, 110, 7677-7688.	1.2	216
7	Orbital-free kinetic-energy density functionals with a density-dependent kernel. Physical Review B, 1999, 60, 16350-16358.	1.1	212
8	Molecular structure and stability of dissolved lithium polysulfide species. Physical Chemistry Chemical Physics, 2014, 16, 10923-10932.	1.3	210
9	Quantitatively Probing the Al Distribution in Zeolites. Journal of the American Chemical Society, 2014, 136, 8296-8306.	6.6	199
10	Linear-Response and Real-Time Time-Dependent Density Functional Theory Studies of Core-Level Near-Edge X-Ray Absorption. Journal of Chemical Theory and Computation, 2012, 8, 3284-3292.	2.3	192
11	Accurate ab initio energetics of extended systems via explicit correlation embedded in a density functional environment. Chemical Physics Letters, 1998, 295, 129-134.	1.2	189
12	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	2.1	145
13	Periodic density functional embedding theory for complete active space self-consistent field and configuration interaction calculations: Ground and excited states. Journal of Chemical Physics, 2002, 116, 42.	1.2	142
14	Real-Time Time-Dependent Electronic Structure Theory. Chemical Reviews, 2020, 120, 9951-9993.	23.0	141
15	Orbital-free kinetic-energy functionals for the nearly free electron gas. Physical Review B, 1998, 58, 13465-13471.	1.1	139
16	Nanotube-based gas sensors â€“ Role of structural defects. Chemical Physics Letters, 2006, 421, 58-62.	1.2	137
17	Supersaturated calcium carbonate solutions are classical. Science Advances, 2018, 4, eaao6283.	4.7	116
18	Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles. Physical Review Letters, 2001, 86, 5954-5957.	2.9	111

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19	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. Journal of Physical Chemistry A, 2011, 115, 10930-10949.	1.1	110
20	Comparison of Real-Time and Linear-Response Time-Dependent Density Functional Theories for Molecular Chromophores Ranging from Sparse to High Densities of States. Journal of Chemical Theory and Computation, 2015, 11, 1102-1109.	2.3	98
21	Toward Understanding the Nature of Internal Rotation Barriers with a New Energy Partition Scheme: Ethane andn-Butane. Journal of Physical Chemistry A, 2008, 112, 6690-6699.	1.1	90
22	Revisiting the hydration structure of aqueous Na+. Journal of Chemical Physics, 2017, 146, 084504.	1.2	90
23	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
24	Excited-State Studies of Polyacenes: A Comparative Picture Using EOMCCSD, CR-EOMCCSD(T), Range-Separated (LR/RT)-TDDFT, TD-PM3, and TD-ZINDO. Journal of Chemical Theory and Computation, 2011, 7, 3686-3693.	2.3	84
25	Long Live Vinylidene! A New View of the H2CC:â€‰â†’ HCâ‹®CH Rearrangement from ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2001, 123, 641-657.	6.6	83
26	Accurate dipole polarizabilities for water clusters n=2â€“12 at the coupled-cluster level of theory and benchmarking of various density functionals. Journal of Chemical Physics, 2009, 131, 214103.	1.2	83
27	Core and valence excitations in resonant X-ray spectroscopy using restricted excitation window time-dependent density functional theory. Journal of Chemical Physics, 2012, 137, 194306.	1.2	83
28	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. Journal of Chemical Theory and Computation, 2015, 11, 3305-3320.	2.3	75
29	ISiCLE: A Quantum Chemistry Pipeline for Establishing in Silico Collision Cross Section Libraries. Analytical Chemistry, 2019, 91, 4346-4356.	3.2	74
30	Tracking the Chemical Transformations at the BrÃ¸nsted Acid Site upon Water-Induced Deprotonation in a Zeolite Pore. Chemistry of Materials, 2017, 29, 9030-9042.	3.2	71
31	Excited State Absorption from Real-Time Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4294-4303.	2.3	70
32	Magnetic Ordering in Gold Nanoclusters. ACS Omega, 2017, 2, 2607-2617.	1.6	69
33	Gaussian Basis Set and Planewave Relativistic Spinâ¨Orbit Methods in NWChem. Journal of Chemical Theory and Computation, 2009, 5, 491-499.	2.3	66
34	Excited States of DNA Base Pairs Using Long-Range Corrected Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 9761-9765.	1.1	64
35	Excitation Energies of Zinc Porphyrin in Aqueous Solution Using Long-Range Corrected Time-Dependent Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 6041-6043.	1.1	60
36	Exploring the origin of the internal rotational barrier for molecules with one rotatable dihedral angle. Journal of Chemical Physics, 2008, 129, 094104.	1.2	59

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37	Active-space completely-renormalized equation-of-motion coupled-cluster formalism: Excited-state studies of green fluorescent protein, free-base porphyrin, and oligoporphyrin dimer. Journal of Chemical Physics, 2010, 132, 154103.	1.2	59
38	Simulating Ru L₃-Edge X-ray Absorption Spectroscopy with Time-Dependent Density Functional Theory: Model Complexes and Electron Localization in Mixed-Valence Metal Dimers. Journal of Physical Chemistry A, 2013, 117, 4444-4454.	1.1	59
39	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. Nature Chemistry, 2021, 13, 343-349.	6.6	59
40	Performance of DFT Methods in the Calculation of Optical Spectra of TCF-Chromophores. Journal of Chemical Theory and Computation, 2009, 5, 2835-2846.	2.3	54
41	Structure and Dynamics of Polysulfide Clusters in a Nonaqueous Solvent Mixture of 1,3-Dioxolane and 1,2-Dimethoxyethane. Chemistry of Materials, 2019, 31, 2308-2319.	3.2	54
42	Zeolite-Catalyzed Hydrocarbon Formation from Methanol: Density Functional Simulations. International Journal of Molecular Sciences, 2002, 3, 423-434.	1.8	51
43	Simulating One-Photon Absorption and Resonance Raman Scattering Spectra Using Analytical Excited State Energy Gradients within Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 5490-5503.	2.3	49
44	Simulating Valence-to-Core X-ray Emission Spectroscopy of Transition Metal Complexes with Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 5804-5809.	2.3	49
45	Carbon-supported Pt during aqueous phenol hydrogenation with and without applied electrical potential: X-ray absorption and theoretical studies of structure and adsorbates. Journal of Catalysis, 2018, 368, 8-19.	3.1	49
46	Near and Above Ionization Electronic Excitations with Non-Hermitian Real-Time Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 4939-4946.	2.3	48
47	Electric Field Gradients Calculated from Two-Component Hybrid Density Functional Theory Including Spinâ^'Orbit Coupling. Journal of Chemical Theory and Computation, 2010, 6, 2669-2686.	2.3	47
48	DFT study of methanol conversion to hydrocarbons in a zeolite catalyst. International Journal of Quantum Chemistry, 2003, 91, 467-473.	1.0	46
49	Structural Elucidation of cis/trans Dicaffeoylquinic Acid Photoisomerization Using Ion Mobility Spectrometry-Mass Spectrometry. Journal of Physical Chemistry Letters, 2017, 8, 1381-1388.	2.1	45
50	Optical Properties of Nanocrystal Interfaces in Compressed MgO Nanopowders. ACS Nano, 2011, 5, 3003-3009.	7.3	43
51	Optical Absorption and Band Gap Reduction in (Fe1â€“xCrx)2O3 Solid Solutions: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 25504-25512.	1.5	43
52	Infrared and Raman Spectroscopy from Ab Initio Molecular Dynamics and Static Normal Mode Analysis: The Câ€“H Region of DMSO as a Case Study. Journal of Physical Chemistry B, 2016, 120, 1429-1436.	1.2	43
53	Benchmark results and theoretical treatments for valence-to-core x-ray emission spectroscopy in transition metal compounds. Physical Review B, 2017, 96, .	1.1	43
54	Scalar Relativistic Computations of Nuclear Magnetic Shielding and g-Shifts with the Zeroth-Order Regular Approximation and Range-Separated Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 3278-3292.	2.3	42

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55	Communication: Application of state-specific multireference coupled cluster methods to core-level excitations. Journal of Chemical Physics, 2012, 137, 171101.	1.2	42
56	Comprehensive Experimental and Computational Spectroscopic Study of Hexacyanoferrate Complexes in Water: From Infrared to X-ray Wavelengths. Journal of Physical Chemistry B, 2018, 122, 5075-5086.	1.2	40
57	Highly Selective Colorimetric and Luminescence Response of a Square-Planar Platinum(II) Terpyridyl Complex to Aqueous TcO₄^{â€“}. Inorganic Chemistry, 2015, 54, 9914-9923.	1.9	39
58	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
59	Reliable modeling of the electronic spectra of realistic uranium complexes. Journal of Chemical Physics, 2013, 139, 034301.	1.2	37
60	An automated framework for NMR chemical shift calculations of small organic molecules. Journal of Cheminformatics, 2018, 10, 52.	2.8	37
61	Efficient Algorithms for Estimating the Absorption Spectrum within Linear Response TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 5197-5208.	2.3	35
62	Optical absorption and spectral photoconductivity in Î±-(Fe_{1â^'x}Cr_x)₂O₃ solid-solution thin films. Journal of Physics Condensed Matter, 2013, 25, 392002.	0.7	33
63	Influence of Coherent Tunneling and Incoherent Hopping on the Charge Transfer Mechanism in Linear Donorâ€“Bridgeâ€“Acceptor Systems. Journal of Physical Chemistry Letters, 2015, 6, 4889-4897.	2.1	32
64	Excited-state absorption in tetrapyridyl porphyrins: comparing real-time and quadratic-response time-dependent density functional theory. Physical Chemistry Chemical Physics, 2017, 19, 27452-27462.	1.3	32
65	Total-energy calculations using a gradient-expanded kinetic-energy functional. Physical Review B, 1994, 50, 11175-11178.	1.1	31
66	Equilibrium structure and bonding of small silicon clusters studied using an orbital-free kinetic-energy functional. Physical Review B, 1995, 51, 7101-7103.	1.1	31
67	Excited-State Absorption from Real-Time Time-Dependent Density Functional Theory: Optical Limiting in Zinc Phthalocyanine. Journal of Physical Chemistry Letters, 2016, 7, 1387-1391.	2.1	31
68	Probing Sulfur Chemical and Electronic Structure with Experimental Observation and Quantitative Theoretical Prediction of KÎ± and Valence-to-Core KÎ² X-ray Emission Spectroscopy. Journal of Physical Chemistry A, 2020, 124, 5415-5434.	1.1	30
69	Photochemical Properties, Composition, and Structure in Molecular Beam Epitaxy Grown Fe â€œDopedâ€• and (Fe,N) Codoped Rutile TiO₂(110). Journal of Physical Chemistry C, 2011, 115, 15416-15424.	1.5	28
70	Excitons in potassium bromide: A study using embedded time-dependent density functional theory and equation-of-motion coupled cluster methods. Chemical Physics Letters, 2009, 470, 353-357.	1.2	27
71	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	6.2	27
72	X-ray circular dichroism signals: a unique probe of local molecular chirality. Chemical Science, 2017, 8, 5969-5978.	3.7	27

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73	Visible Light Absorption of N-Doped TiO₂ Rutile Using (LR/RT)-TDDFT and Active Space EOMCCSD Calculations. Journal of Physical Chemistry Letters, 2011, 2, 2696-2701.	2.1	26
74	KlÃ¼neret al.Reply:. Physical Review Letters, 2002, 88, .	2.9	25
75	Entangled Valence Electronâ€“Hole Dynamics Revealed by Stimulated Attosecond X-ray Raman Scattering. Journal of Physical Chemistry Letters, 2012, 3, 2326-2331.	2.1	25
76	Elucidation of the photoaquation reaction mechanism in ferrous hexacyanide using synchrotron x-rays with sub-pulse-duration sensitivity. Journal of Chemical Physics, 2019, 151, 144306.	1.2	24
77	Unsupervised machine learning for unbiased chemical classification in X-ray absorption spectroscopy and X-ray emission spectroscopy. Physical Chemistry Chemical Physics, 2021, 23, 23586-23601.	1.3	23
78	Formation, stability, and mobility of self-trapped excitations in NaI and NaI<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Tl<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>from first principles. Physical Review B, 2013, 87, .	1.1	22
79	Lithium Insertion Mechanism in Iron Fluoride Nanoparticles Prepared by Catalytic Decomposition of Fluoropolymer. ACS Applied Energy Materials, 2019, 2, 1832-1843.	2.5	21
80	Surface Functionalization of Black Phosphorus with Nitrenes: Identification of P=N Bonds by Using Isotopic Labeling. Angewandte Chemie - International Edition, 2021, 60, 9127-9134.	7.2	21
81	Activity of Cuâ€“Alâ€“Oxo Extra-Framework Clusters for Selective Methane Oxidation on Cu-Exchanged Zeolites. Jacs Au, 2021, 1, 1412-1421.	3.6	21
82	EOMCC, MRPT, and TDDFT Studies of Charge Transfer Processes in Mixed-Valence Compounds: Application to the Spiro Molecule^{â€}. Journal of Physical Chemistry A, 2010, 114, 8764-8771.	1.1	20
83	A Redundant Communication Approach to Scalable Fault Tolerance in PGAS Programming Models. , 2011, , .		20
84	Electronic and Chemical State of Aluminum from the Single- (K) and Double-Electron Excitation (KL_{II&III}, KL_I) X-ray Absorption Near-Edge Spectra of Î±-Alumina, Sodium Aluminate, Aqueous Al³⁺Â·(H₂O)₆, and Aqueous Al(OH)₄^{â€“}. Journal of Physical Chemistry B, 2015, 119, 8380-8388.	1.2	20
85	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2020, 16, 6418-6427.	2.3	20
86	Comparison of Cluster, Slab, and Analytic Potential Models for the Dimethyl Methylphosphonate (DMMP)/TiO₂(110) Intermolecular Interaction. Journal of Physical Chemistry C, 2013, 117, 17613-17622.	1.5	18
87	Monitoring Long-Range Electron Transfer Pathways in Proteins by Stimulated Attosecond Broadband X-ray Raman Spectroscopy. Journal of Physical Chemistry Letters, 2014, 5, 3656-3661.	2.1	18
88	Emerging investigator series: methylmercury speciation and dimethylmercury production in sulfidic solutions. Environmental Sciences: Processes and Impacts, 2018, 20, 584-594.	1.7	17
89	Revealing the bonding of solvated Ru complexes with valence-to-core resonant inelastic X-ray scattering. Chemical Science, 2021, 12, 3713-3725.	3.7	17
90	Scalable Molecular GW Calculations: Valence and Core Spectra. Journal of Chemical Theory and Computation, 2021, 17, 7504-7517.	2.3	17

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91	Direct Dynamics Simulation of Dissociation of the [CH₃--I--OH]^{â^'} Ionâ€“Molecule Complex. Journal of Physical Chemistry A, 2015, 119, 817-825.	1.1	16
92	Precursor Ionâ€“Ion Aggregation in the Brustâ€“Schiffrin Synthesis of Alkanethiol Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 19837-19847.	1.5	16
93	Modeling Optical Spectra of Large Organic Systems Using Real-Time Propagation of Semiempirical Effective Hamiltonians. Journal of Chemical Theory and Computation, 2017, 13, 4410-4420.	2.3	16
94	Resonant Inelastic X-ray Scattering Calculations of Transition Metal Complexes Within a Simplified Time-Dependent Density Functional Theory Framework. Journal of Chemical Theory and Computation, 2021, 17, 3031-3038.	2.3	16
95	Dissociation Chemistry of Gas Molecules on Carbon Nanotubesâ€”Applications to Chemical Sensing. IEEE Sensors Journal, 2008, 8, 837-841.	2.4	15
96	An Ab Initio Multiple Cloning Method for Non-Adiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2021, 17, 3629-3643.	2.3	15
97	Effect of surface phosphorus on the oxidative dehydrogenation of ethane: A first-principles investigation. Journal of Chemical Physics, 2002, 117, 8080-8088.	1.2	14
98	Self-learning kinetic Monte Carlo simulations of Al diffusion in Mg. Journal of Physics Condensed Matter, 2016, 28, 155001.	0.7	14
99	<scp>iSPECTRON</scp>: A simulation interface for linear and nonlinear spectra with abâ€initio quantum chemistry software. Journal of Computational Chemistry, 2021, 42, 644-659.	1.5	14
100	Theoretical study of the mechanism behind the para-selective nitration of toluene in zeolite H-Beta. Molecular Simulation, 2008, 34, 1025-1039.	0.9	13
101	Photoelectron spectroscopy of higher bromine and iodine oxide anions: Electron affinities and electronic structures of BrO2,3 and IO2â€“4 radicals. Journal of Chemical Physics, 2011, 135, 184309.	1.2	13
102	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	1.2	13
103	Nonequilibrium Chemical Effects in Single-Molecule SERS Revealed by Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2017, 121, 1344-1350.	1.1	13
104	Influence of Interligand Interactions and Core-Charge Distribution on Gold Cluster Stability: Enthalpy Versus Entropy. Journal of Physical Chemistry C, 2019, 123, 24899-24911.	1.5	13
105	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na+. Journal of Chemical Physics, 2018, 149, 124503.	1.2	12
106	10. Computational Materials Science with Materials Studio$^{lap{LARGE(circ)},hskip.5ptaise3pthbox{inym R}},$: Applications in Catalysis. Lecture Notes in Physics, 0, , 207-221.	0.3	11
107	Electron transfer beyond the static picture: A TDDFT/TD-ZINDO study of a pentacene dimer. Journal of Chemical Physics, 2012, 137, 22A502.	1.2	11
108	A Combined Gasâ€Phase Photoelectron Spectroscopic and Theoretical Study of Zeiseâ€™s Anion and Its Bromine and Iodine Analogues. Angewandte Chemie - International Edition, 2012, 51, 6356-6360.	7.2	11

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109	Simulating Cl K-edge X-ray absorption spectroscopy in MCl6 2â^' (MÂ=ÂU, Np, Pu) complexes and UOCl5 â^' using time-dependent density functional theory. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	11
110	Toward Enabling Large-Scale Open-Shell Equation-of-Motion Coupled Cluster Calculations: Triplet States of Î²-Carotene. Journal of Physical Chemistry A, 2014, 118, 9087-9093.	1.1	11
111	Efficient block preconditioned eigensolvers for linear response time-dependent density functional theory. Computer Physics Communications, 2017, 221, 42-52.	3.0	11
112	Double core hole valence-to-core x-ray emission spectroscopy: A theoretical exploration using time-dependent density functional theory. Journal of Chemical Physics, 2019, 151, 144114.	1.2	11
113	Near-Edge X-ray Absorption Fine Structure Spectroscopy of Heteroatomic Core-Hole States as a Probe for Nearly Indistinguishable Chemical Environments. Journal of Physical Chemistry Letters, 2020, 11, 556-561.	2.1	11
114	Ion Mobility Spectrometry Characterization of the Intermediate Hydrogen-Containing Gold Cluster Au₇(PPh₃)₇H₅²⁺. Journal of Physical Chemistry Letters, 2021, 12, 2502-2508.	2.1	11
115	Spectral Signatures of Ultrafast Excited-State Intramolecular Proton Transfer from Computational Multi-edge Transient X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2021, 12, 9840-9847.	2.1	11
116	Time Domain Simulations of Single Molecule Raman Scattering. Journal of Physical Chemistry A, 2018, 122, 7437-7442.	1.1	10
117	A semiempirical effective Hamiltonian based approach for analyzing excited state wave functions and computing excited state absorption spectra using real-time dynamics. Journal of Chemical Physics, 2019, 150, 104103.	1.2	10
118	Valence-to-core X-ray emission spectroscopy of vanadium oxide and lithiated vanadyl phosphate materials. Journal of Materials Chemistry A, 2020, 8, 16332-16344.	5.2	10
119	Computational approaches for XANES, VtC-XES, and RIXS using linear-response time-dependent density functional theory based methods. Physical Chemistry Chemical Physics, 2022, 24, 14680-14691.	1.3	10
120	Density-functional study of the stabilization of the Si(001) dimer vacancy by Ni. Physical Review B, 2002, 66, .	1.1	9
121	The role of cytosine methylation on charge transport through a DNA strand. Journal of Chemical Physics, 2015, 143, 094306.	1.2	9
122	Coupled Cluster Studies of Ionization Potentials and Electron Affinities of Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2017, 121, 1328-1335.	1.1	9
123	Projector-Based Quantum Embedding for Molecular Systems: An Investigation of Three Partitioning Approaches. Journal of Physical Chemistry A, 2021, 125, 6384-6393.	1.1	9
124	Manipulating valence and core electronic excitations of a transition-metal complex using UV/Vis and X-ray cavities. Chemical Science, 2021, 12, 8088-8095.	3.7	9
125	Femtosecond X-ray Spectroscopy Directly Quantifies Transient Excited-State Mixed Valency. Journal of Physical Chemistry Letters, 2022, 13, 378-386.	2.1	9
126	Basis Set Selection for Molecular Core-Level GW Calculations. Journal of Chemical Theory and Computation, 2022, 18, 4919-4926.	2.3	9

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127	Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177.	0.9	8
128	Cationâ€“Cation Interactions in [(UO₂)₂(OH)_n]^{4â€“n} Complexes. Inorganic Chemistry, 2013, 52, 11269-11279.	1.9	8
129	Quantum time dynamics employing the Yang-Baxter equationÂfor circuit compression. Physical Review A, 2022, 106, .	1.0	8
130	Aqua-Vanadyl Ion Interaction with NafionÃ‚Â® Membranes. Frontiers in Energy Research, 2015, 3, .	1.2	7
131	Simplified Ab Initio Molecular Dynamics-Based Raman Spectral Simulations. Applied Spectroscopy, 2020, 74, 1350-1357.	1.2	7
132	Resonant Stimulated X-ray Raman Spectroscopy of Mixed-Valence Manganese Complexes. Journal of Physical Chemistry Letters, 2021, 12, 5925-5931.	2.1	7
133	Informed Chemical Classification of Organophosphorus Compounds via Unsupervised Machine Learning of X-ray Absorption Spectroscopy and X-ray Emission Spectroscopy. Journal of Physical Chemistry A, 2022, 126, 4862-4872.	1.1	7
134	Electron Ionization Mass Spectrum of Tellurium Hexafluoride. Inorganic Chemistry, 2015, 54, 4821-4826.	1.9	6
135	In Silico Ultrafast Nonlinear Spectroscopy Meets Experiments: The Case of Perylene Bisimide Dye. Journal of Chemical Theory and Computation, 2021, 17, 7134-7145.	2.3	6
136	Proton Affinity Values of Fentanyl and Fentanyl Analogues Pertinent to Ambient Ionization and Detection. Journal of the American Society for Mass Spectrometry, 2022, 33, 482-490.	1.2	6
137	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals. Journal of Chemical Theory and Computation, 2022, 18, 2331-2340.	2.3	6
138	Near-Quantitative Predictions of the First-Shell Coordination Structure of Hydrated First-Row Transition Metal Ions Using K-Edge X-ray Absorption Near-Edge Spectroscopy. Journal of Physical Chemistry Letters, 2022, 13, 6323-6330.	2.1	6
139	Substituent effects on the geometric and electronic properties of tetracyano-p-quinodimethane (TCNQ): a theoretical study. Molecular Simulation, 2013, 39, 350-356.	0.9	5
140	Resonant X-ray Sum-Frequency-Generation Spectroscopy of K-Edges in Acetyl Fluoride. Journal of Chemical Theory and Computation, 2019, 15, 6832-6839.	2.3	5
141	Ultrafast x-ray pump x-ray probe transient absorption spectroscopy: A computational study and proposed experiment probing core-valence electronic correlations in solvated complexes. Journal of Chemical Physics, 2021, 154, 214107.	1.2	5
142	Quantum technology in catalysis. Applied Catalysis A: General, 2005, 280, 105-113.	2.2	4
143	Effect of doping and chemical ordering on the optoelectronic properties of complex oxides: Fe₂O₃â€“V₂O₃ solid solutions and hetero-structures. Physical Chemistry Chemical Physics, 2017, 19, 1097-1107.	1.3	4
144	Deviation from the trans-Effect in Ligand-Exchange Reactions of Zeiseâ€™s Ions PtCl₃(C₂H₄)^{â^’} with Heavier Halides (Br^{â€“},) Tj ET1		

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145	Application-Specific Fault Tolerance via Data Access Characterization. Lecture Notes in Computer Science, 2011, , 340-352.	1.0	4
146	Chapter 4. Embedding Methods in Materials Discovery. , 2018, , 87-116.		4
147	X-ray absorption spectroscopy of trivalent Eu, Gd, Tb, and Dy chlorides and oxychlorides. Journal of Alloys and Compounds, 2022, 897, 162629.	2.8	4
148	Reply to â€œComment on â€˜Excited States of DNA Base Pairs Using Long-Range Corrected Time-Dependent Density Functional Theoryâ€™â€• Journal of Physical Chemistry A, 2009, 113, 11095-11095.	1.1	3
149	Magnetic-Bottle and velocity-map imaging photoelectron spectroscopy of APSâ^' (A=C14H10 or) Tj ETQq1 1 0.784314 rgBT /Overloc Journal of Chemical Physics, 2018, 31, 463-470.	0.6	3
150	Evidence of Skewness and Sub-Gaussian Character in Temperature-Dependent Distributions of One Million Electronic Excitation Energies in PbS Quantum Dots. Journal of Physical Chemistry Letters, 2020, 11, 986-992.	2.1	3
151	Mechanistic Investigation of Dimethylmercury Formation Mediated by a Sulfide Mineral Surface. Journal of Physical Chemistry A, 2021, 125, 5397-5405.	1.1	3
152	Simulating Cl K-edge X-ray absorption spectroscopy in MCl6 2- (M = U, Np, Pu) complexes and UOCl5 - using time-dependent density functional theory. Highlights in Theoretical Chemistry, 2015, , 247-253.	0.0	2
153	Ab initio calculations of the rate of carrier trapping and release at dopant sites in NaI: Tl beyond the harmonic approximation. Physical Review B, 2020, 101, .	1.1	2
154	Numerical study of a model for driven interface dynamics. Journal of Physics A, 1992, 25, 5485-5492.	1.6	1
155	Performance of DFT Methods in the Calculation of Optical Spectra of Chromophores. , 2008, , .		1
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