Niranjan Govind

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/8916560/publications.pdf

Version: 2024-02-01

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	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
2	Iron redox analysis of silicate-based minerals and glasses using synchrotron X-ray absorption and laboratory X-ray emission spectroscopy. Journal of Non-Crystalline Solids, 2022, 577, 121326.	1.5	0
3	Femtosecond X-ray Spectroscopy Directly Quantifies Transient Excited-State Mixed Valency. Journal of Physical Chemistry Letters, 2022, 13, 378-386.	2.1	9
4	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
5	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals. Journal of Chemical Theory and Computation, 2022, 18, 2331-2340.	2.3	6
6	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
7	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
8	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
9	Quantum time dynamics employing the Yang-Baxter equationÂfor circuit compression. Physical Review A, 2022, 106, .	1.0	8
10	Basis Set Selection for Molecular Core-Level GW Calculations. Journal of Chemical Theory and Computation, 2022, 18, 4919-4926.	2.3	9
11	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
12	Surface Functionalization of Black Phosphorus with Nitrenes: Identification of P=N Bonds by Using Isotopic Labeling. Angewandte Chemie, 2021, 133, 9209-9216.	1.6	0
13	<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
14	Direct observation of coherent femtosecond solvent reorganization coupled to intramolecular electron transfer. Nature Chemistry, 2021, 13, 343-349.	6.6	59
15	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
16	From NWChem to NWChemEx: Evolving with the Computational Chemistry Landscape. Chemical Reviews, 2021, 121, 4962-4998.	23.0	39
17	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
18	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

#	Article	IF	Citations
19	Resonant Stimulated X-ray Raman Spectroscopy of Mixed-Valence Manganese Complexes. Journal of Physical Chemistry Letters, 2021, 12, 5925-5931.	2.1	7
20	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
21	Mechanistic Investigation of Dimethylmercury Formation Mediated by a Sulfide Mineral Surface. Journal of Physical Chemistry A, 2021, 125, 5397-5405.	1.1	3
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	Scalable Molecular GW Calculations: Valence and Core Spectra. Journal of Chemical Theory and Computation, 2021, 17, 7504-7517.	2.3	17
30	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
31	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
32	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
33	Real-Time Time-Dependent Electronic Structure Theory. Chemical Reviews, 2020, 120, 9951-9993.	23.0	141
34	First Principles Nonadiabatic Excited-State Molecular Dynamics in NWChem. Journal of Chemical Theory and Computation, 2020, 16, 6418-6427.	2.3	20
35	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
36	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425

#	Article	IF	Citations
37	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
38	Simplified Ab Initio Molecular Dynamics-Based Raman Spectral Simulations. Applied Spectroscopy, 2020, 74, 1350-1357.	1.2	7
39	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
40	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
41	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
42	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
43	Lithium Insertion Mechanism in Iron Fluoride Nanoparticles Prepared by Catalytic Decomposition of Fluoropolymer. ACS Applied Energy Materials, 2019, 2, 1832-1843.	2.5	21
44	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
45	ISiCLE: A Quantum Chemistry Pipeline for Establishing in Silico Collision Cross Section Libraries. Analytical Chemistry, 2019, 91, 4346-4356.	3.2	74
46	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
47	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
48	Supersaturated calcium carbonate solutions are classical. Science Advances, 2018, 4, eaao6283.	4.7	116
49	Deviation from the trans-Effect in Ligand-Exchange Reactions of Zeiseâ€™s Ions PtCl₃(C₂H₄)^{â^’} with Heavier Halides (Br^{â€“},) Tj ETQq1 1 0.784314	1.2	7
50	Emerging investigator series: methylmercury speciation and dimethylmercury production in sulfidic solutions. Environmental Sciences: Processes and Impacts, 2018, 20, 584-594.	1.7	17
51	Magnetic-Bottle and velocity-map imaging photoelectron spectroscopy of APSâ^’ (A=C14H10 or) Tj ETQq1 1 0.784314 rgBT /Overlock Journal of Chemical Physics, 2018, 31, 463-470.	0.6	3
52	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
53	Unraveling the spectral signatures of solvent ordering in K-edge XANES of aqueous Na+. Journal of Chemical Physics, 2018, 149, 124503.	1.2	12
54	An automated framework for NMR chemical shift calculations of small organic molecules. Journal of Cheminformatics, 2018, 10, 52.	2.8	37

#	Article	IF	Citations
55	Time Domain Simulations of Single Molecule Raman Scattering. Journal of Physical Chemistry A, 2018, 122, 7437-7442.	1.1	10
56	Chapter 4. Embedding Methods in Materials Discovery. , 2018, , 87-116.		4
57	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
58	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
59	Revisiting the hydration structure of aqueous Na+. Journal of Chemical Physics, 2017, 146, 084504.	1.2	90
60	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
61	Magnetic Ordering in Gold Nanoclusters. ACS Omega, 2017, 2, 2607-2617.	1.6	69
62	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
63	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
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	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
66	Efficient block preconditioned eigensolvers for linear response time-dependent density functional theory. Computer Physics Communications, 2017, 221, 42-52.	3.0	11
67	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
68	X-ray circular dichroism signals: a unique probe of local molecular chirality. Chemical Science, 2017, 8, 5969-5978.	3.7	27
69	Monitoring Excited State Charge Transfer of Transition Metal Mixed-Valence Complexes with Femtosecond X-ray Absorption and Emission Spectroscopy. , 2016, , .		1
70	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
71	Precursor Ionâ€“Ion Aggregation in the Brustâ€“Schiffrin Synthesis of Alkanethiol Nanoparticles. Journal of Physical Chemistry C, 2016, 120, 19837-19847.	1.5	16
72	Theoretical studies of the global minima and polarizabilities of small lithium clusters. Chemical Physics Letters, 2016, 644, 235-242.	1.2	13

#	Article	IF	Citations
73	Self-learning kinetic Monte Carlo simulations of Al diffusion in Mg. Journal of Physics Condensed Matter, 2016, 28, 155001.	0.7	14
74	Time-Domain Simulations of Transient Species in Experimentally Relevant Environments. Journal of Physical Chemistry A, 2016, 120, 556-561.	1.1	1
75	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
76	The role of cytosine methylation on charge transport through a DNA strand. Journal of Chemical Physics, 2015, 143, 094306.	1.2	9
77	Aqua-Vanadyl Ion Interaction with NafionÃ‚Â® Membranes. Frontiers in Energy Research, 2015, 3, .	1.2	7
78	Charge-Transfer Versus Charge-Transfer-Like Excitations Revisited. Journal of Chemical Theory and Computation, 2015, 11, 3305-3320.	2.3	75
79	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
80	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
81	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
82	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
83	Electron Ionization Mass Spectrum of Tellurium Hexafluoride. Inorganic Chemistry, 2015, 54, 4821-4826.	1.9	6
84	Excited State Absorption from Real-Time Time-Dependent Density Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4294-4303.	2.3	70
85	Efficient Algorithms for Estimating the Absorption Spectrum within Linear Response TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 5197-5208.	2.3	35
86	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
87	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
88	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
89	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
90	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

#	Article	IF	Citations
91	Quantitatively Probing the Al Distribution in Zeolites. Journal of the American Chemical Society, 2014, 136, 8296-8306.	6.6	199
92	Molecular structure and stability of dissolved lithium polysulfide species. Physical Chemistry Chemical Physics, 2014, 16, 10923-10932.	1.3	210
93	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
94	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
95	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
96	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
97	Cationâ€“Cation Interactions in [(UO₂)₂(OH)_n]^{4â€“n} Complexes. Inorganic Chemistry, 2013, 52, 11269-11279.	1.9	8
98	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
99	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	21
100	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
101	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
102	Reliable modeling of the electronic spectra of realistic uranium complexes. Journal of Chemical Physics, 2013, 139, 034301.	1.2	37
103	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
104	Dissecting X-Ray Raman Resonances Using Four-Wave Mixing. EPJ Web of Conferences, 2013, 41, 05040.	0.1	0
105	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
106	Communication: Application of state-specific multireference coupled cluster methods to core-level excitations. Journal of Chemical Physics, 2012, 137, 171101.	1.2	42
107	Curvature and Frontier Orbital Energies in Density Functional Theory. Journal of Physical Chemistry Letters, 2012, 3, 3740-3744.	2.1	145
108	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

#	Article	IF	Citations
109	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
110	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	2.9	236
111	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
112	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
113	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
114	Optical Properties of Nanocrystal Interfaces in Compressed MgO Nanopowders. ACS Nano, 2011, 5, 3003-3009.	7.3	43
115	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
116	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
117	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
118	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
119	Theoretical Study of the Mechanism behind the Para-Selective Nitration of Toluene in Zeolite H-Beta. , 2011, , 1-22.		0
120	Optical Rotation Calculated with Time-Dependent Density Functional Theory: The OR45 Benchmark. Journal of Physical Chemistry A, 2011, 115, 10930-10949.	1.1	110
121	A Redundant Communication Approach to Scalable Fault Tolerance in PGAS Programming Models. , 2011, , .		20
122	NWChem: scalable parallel computational chemistry. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 888-894.	6.2	27
123	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
124	Advances in Scalable Computational Chemistry. Annual Reports in Computational Chemistry, 2011, 7, 151-177.	0.9	8
125	Application-Specific Fault Tolerance via Data Access Characterization. Lecture Notes in Computer Science, 2011, , 340-352.	1.0	4
126	NWChem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 2010, 181, 1477-1489.	3.0	4,740

#	Article	IF	Citations
127	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
128	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
129	Utilizing high performance computing for chemistry: parallel computational chemistry. Physical Chemistry Chemical Physics, 2010, 12, 6896.	1.3	84
130	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
131	Computational Nanoscience with NWChem. Journal of Computational and Theoretical Nanoscience, 2009, 6, 1297-1304.	0.4	1
132	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
133	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
134	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
135	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
136	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
137	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
138	Gaussian Basis Set and Planewave Relativistic Spinâ˜Orbit Methods in NWChem. Journal of Chemical Theory and Computation, 2009, 5, 491-499.	2.3	66
139	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
140	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
141	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
142	Performance of DFT Methods in the Calculation of Optical Spectra of Chromophores. , 2008, , .		1
143	Dissociation Chemistry of Gas Molecules on Carbon Nanotubesâ€”Applications to Chemical Sensing. IEEE Sensors Journal, 2008, 8, 837-841.	2.4	15
144	Nanotube-based gas sensors â€“ Role of structural defects. Chemical Physics Letters, 2006, 421, 58-62.	1.2	137

#	Article	IF	Citations
145	Quantum technology in catalysis. Applied Catalysis A: General, 2005, 280, 105-113.	2.2	4
146	DFT study of methanol conversion to hydrocarbons in a zeolite catalyst. International Journal of Quantum Chemistry, 2003, 91, 467-473.	1.0	46
147	A generalized synchronous transit method for transition state location. Computational Materials Science, 2003, 28, 250-258.	1.4	1,050
148	KlÃ¼neret al.Reply:. Physical Review Letters, 2002, 88, .	2.9	25
149	Density-functional study of the stabilization of the Si(001) dimer vacancy by Ni. Physical Review B, 2002, 66, .	1.1	9
150	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
151	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
152	Zeolite-Catalyzed Hydrocarbon Formation from Methanol: Density Functional Simulations. International Journal of Molecular Sciences, 2002, 3, 423-434.	1.8	51
153	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
154	Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles. Physical Review Letters, 2001, 86, 5954-5957.	2.9	111
155	Orbital-free kinetic-energy density functionals with a density-dependent kernel. Physical Review B, 1999, 60, 16350-16358.	1.1	212
156	Electronic-structure calculations by first-principles density-based embedding of explicitly correlated systems. Journal of Chemical Physics, 1999, 110, 7677-7688.	1.2	216
157	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
158	Orbital-free kinetic-energy functionals for the nearly free electron gas. Physical Review B, 1998, 58, 13465-13471.	1.1	139
159	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
160	Total-energy calculations using a gradient-expanded kinetic-energy functional. Physical Review B, 1994, 50, 11175-11178.	1.1	31
161	Numerical study of a model for driven interface dynamics. Journal of Physics A, 1992, 25, 5485-5492.	1.6	1
162	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