Nathan DeYonker

List of Publications by Year
in descending order

84	2,961	218381	168136
papers	citations	26 h-index	53 g-index

87	87	87	2673
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Rovibrational Spectroscopy of Magnesium Tricarbideâ€“Multireference Character Thwarts a Full Analysis of All Isomers. Journal of Physical Chemistry A, 2022, 126, 4132-4146.	1.1	5
2	Automating, Analyzing, and Databasing Quantum Mechanical Enzyme Simulations. Biophysical Journal, 2021, 120, 267a.	0.2	0
3	QM-Cluster Model Study of the Guaiacol Hydrogen Atom Transfer and Oxygen Rebound with Cytochrome P450 Enzyme GcoA. Journal of Physical Chemistry B, 2021, 125, 3296-3306.	1.2	13
4	Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study. Biophysical Journal, 2021, 120, 3577-3587.	0.2	7
5	Rovibrational Quantum Chemical Treatment of Inorganic and Organometallic Astrochemicals. Accounts of Chemical Research, 2021, 54, 271-279.	7.6	8
6	Computational Insight into the Rope-Skipping Isomerization of Diarylether Cyclophanes. Symmetry, 2021, 13, 2127.	1.1	1
7	The structure of ScC2 (Xˆ2A1): A combined Fourier transform microwave/millimeter-wave spectroscopic and computational study. Journal of Chemical Physics, 2020, 153, 034304.	1.2	5
8	Spectroscopic study of magnesium dinitrogen and sodium dinitrogen cation. Monthly Notices of the Royal Astronomical Society, 2020, 498, 5417-5423.	1.6	4
9	Systematic evaluation of the electronic effect of aluminum-containing ligands in iridiumâ€“aluminum and rhodiumâ€“aluminum bimetallic complexes. Dalton Transactions, 2020, 49, 13029-13043.	1.6	0
10	CO₂ Capture by 2â€(Methylamino)pyridine Ligated Aluminum Alkyl Complexes. European Journal of Inorganic Chemistry, 2020, 2020, 2958-2967.	1.0	11
11	Synthesis and Electronic Characterization of Iridiumâ€Aluminum and Rhodiumâ€Aluminum Heterobimetallic Complexes Bridged by 3â€Oxypyridine and 4â€Oxypyridine. European Journal of Inorganic Chemistry, 2020, 2020, 1192-1198.	1.0	3
12	Acylation and deacylation mechanism and kinetics of penicillin G reaction with Streptomyces<scp>R61 DD</scp>â€peptidase. Journal of Computational Chemistry, 2020, 41, 1685-1697.	1.5	4
13	Complex Organic Matter Synthesis on Siloxyl Radicals in the Presence of CO. Frontiers in Chemistry, 2020, 8, 621898.	1.8	4
14	Photodynamics of [FeFe]-Hydrogenase Model Compounds with Bidentate Heterocyclic Ligands. Journal of Physical Chemistry B, 2019, 123, 7137-7148.	1.2	5
15	Theoretical study of the low-lying electronic states of iron hydride cation. Journal of Chemical Physics, 2019, 150, 234304.	1.2	7
16	Hydrogen Activation and Hydrogenolysis Facilitated By Late-Transition-Metalâ€“Aluminum Heterobimetallic Complexes. Inorganic Chemistry, 2019, 58, 12635-12645.	1.9	12
17	On the formation of phosphorous polycyclic aromatics hydrocarbons (PAPHs) in astrophysical environments. Physical Chemistry Chemical Physics, 2019, 21, 8015-8021.	1.3	8
18	Quantifying Inter-Residue Contacts through Interaction Energies. Journal of Chemical Information and Modeling, 2019, 59, 5034-5044.	2.5	10

#	Article	IF	Citations
19	A transition state â€œtrappedâ€? QM-cluster models of engineered threonyl-tRNA synthetase. Organic and Biomolecular Chemistry, 2018, 16, 4090-4100.	1.5	6
20	Synthesis and Characterization of Heterobimetallic Iridiumâ€“Aluminum and Rhodiumâ€“Aluminum Complexes. Inorganic Chemistry, 2018, 57, 1148-1157.	1.9	17
21	Propylene Oxide Formation on a Silica Surface with Peroxo Defects: Implications in Astrochemistry. Journal of Physical Chemistry A, 2018, 122, 9100-9106.	1.1	7
22	Raman and Infrared Studies of Platinum-Based Drugs: Cisplatin, Carboplatin, Oxaliplatin, Nedaplatin, and Heptaplatin. Journal of Physical Chemistry A, 2018, 122, 6934-6952.	1.1	28
23	Prediction of the reduction potential in transitionâ€metal containing complexes: How expensive? For what accuracy?. Journal of Computational Chemistry, 2017, 38, 2430-2438.	1.5	23
24	Gas phase electronic structure of the 3d metal monoacetylides (MCCH, Mâ€‰=â€‰Sc .. Zn). International Journal of Quantum Chemistry, 2017, 117, 104-128.	1.0	6
25	Towards a quantum chemical protocol for the prediction of rovibrational spectroscopic data for transition metal molecules: Exploration of CuCN, CuOH, and CuCCH. Journal of Chemical Physics, 2017, 147, 234303.	1.2	16
26	Enabling Science Support for Better Decisionâ€Making when Responding to Chemical Spills. Journal of Environmental Quality, 2016, 45, 1490-1500.	1.0	20
27	Dipole moments of trans- and cis-(4-methylcyclohexyl)methanol (4-MCHM): obtaining the right conformer for the right reason. Physical Chemistry Chemical Physics, 2016, 18, 17856-17867.	1.3	4
28	Calibrating Reaction Enthalpies: Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials. Journal of Physical Chemistry A, 2016, 120, 9982-9997.	1.1	6
29	H₂ Formation on Cosmic Grain Siliceous Surfaces Grafted with Fe⁺: A Silsesquioxanesâ€Based Computational Model. ChemPhysChem, 2016, 17, 3390-3394.	1.0	7
30	What a Difference a Decade Has Not Made: The Murky Electronic Structure of Iron Monocyanide (FeCN) and Iron Monoisocyanide (FeNC). Journal of Physical Chemistry A, 2015, 119, 215-223.	1.1	17
31	The transâ€“cis isomerization of Ni(Î·2-TEMPO)2: Interconnections and conformational complexity. Inorganica Chimica Acta, 2015, 436, 220-229.	1.2	2
32	A Theoretical Study of Phosphoryl Transfers of Tyrosyl-DNA Phosphodiesterase I (Tdp1) and the Possibility of a â€œDead-Endâ€•Phosphohistidine Intermediate. Biochemistry, 2015, 54, 4236-4247.	1.2	20
33	Partitioning, Aqueous Solubility, and Dipole Moment Data for cis- and trans-(4-Methylcyclohexyl)methanol, Principal Contaminants of the West Virginia Chemical Spill. Environmental Science and Technology Letters, 2015, 2, 123-127.	3.9	24
34	Thermodynamic data of known volatile organic compounds (VOCs) in Rosmarinus officinalis : Implications for forest fire modeling. Computational and Theoretical Chemistry, 2015, 1073, 27-33.	1.1	3
35	Binding energies and interaction origins between nonclassical single-electron hydrogen, sodium and lithium bonds and neutral boron-containing radicals: a theoretical investigation. Science Bulletin, 2014, 59, 2597-2607.	1.7	1
36	The role of coreâ€“valence electron correlation in gallium halides: a comparison of composite methods. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	2

#	Article	IF	Citations
37	Reaction mechanism of oxidative desulfurization of heterocyclic organic sulfides: a computational study. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	10
38	The electronic structure of vanadium monochloride cation (VCl+): Tackling the complexities of transition metal species. Journal of Chemical Physics, 2014, 141, 204302.	1.2	12
39	Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study. Journal of the American Chemical Society, 2013, 135, 13764-13774.	6.6	26
40	Metalâ€“Ligand Synergistic Effects in the Complex Ni(Î·²-TEMPO)₂: Synthesis, Structures, and Reactivity. Inorganic Chemistry, 2013, 52, 13882-13893.	1.9	13
41	Complete basis set limits of local second-order MÃ¸llerâ€“Plesset perturbation theory. Molecular Physics, 2013, 111, 1178-1189.	0.8	0
42	Mechanism and Enantioselectivity of Dirhodium-Catalyzed Intramolecular Câ€“H Amination of Sulfamate. Journal of Organic Chemistry, 2013, 78, 12460-12468.	1.7	37
43	Is near-â€œspectroscopic accuracyâ€•possible for heavy atoms and coupled cluster theory? An investigation of the first ionization potentials of the atoms Gaâ€“Kr. Journal of Chemical Physics, 2013, 138, 164312.	1.2	7
44	Platinum(II)-Catalyzed Cyclization Sequence of Aryl Alkynes via C(sp³)â€“H Activation: A DFT Study. Journal of Organic Chemistry, 2012, 77, 6076-6086.	1.7	13
45	Incorporating a completely renormalized coupled cluster approach into a composite method for thermodynamic properties and reaction paths. Journal of Chemical Physics, 2012, 136, 144109.	1.2	26
46	Photodissociation of a ruthenium(II) arene complex and its subsequent interactions with biomolecules: a density functional theory study. Journal of Molecular Modeling, 2012, 18, 4675-4686.	0.8	6
47	Synthesis, Air Stability, Photobleaching, and DFT Modeling of Blue Light Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes. Organometallics, 2012, 31, 1664-1672.	1.1	104
48	Multireference Character for 3d Transition-Metal-Containing Molecules. Journal of Chemical Theory and Computation, 2012, 8, 460-468.	2.3	237
49	Mechanism of aquation and nucleobase binding of ruthenium (II) and osmium (II) arene complexes: A systematic comparison DFT study. Journal of Organometallic Chemistry, 2012, 704, 17-28.	0.8	11
50	Taming the low-lying electronic states of FeH. Journal of Chemical Physics, 2012, 137, 234303.	1.2	44
51	Prediction of hydrocarbon enthalpies of formation by various thermochemical schemes. Journal of Computational Chemistry, 2012, 33, 2032-2042.	1.5	14
52	Toward Accurate Theoretical Thermochemistry of First Row Transition Metal Complexes. Journal of Physical Chemistry A, 2012, 116, 870-885.	1.1	138
53	Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex. Angewandte Chemie - International Edition, 2012, 51, 5941-5944.	7.2	280
54	Dinuclear Zn(II) Complex Catalyzed Phosphodiester Cleavage Proceeds via a Concerted Mechanism: A Density Functional Theory Study. Journal of the American Chemical Society, 2011, 133, 2904-2915.	6.6	55

#	Article	IF	Citations
55	Ligand Displacement from TpMn(CO)₂L Complexes: A Large Rate Enhancement in Comparison to the CpMn(CO)₂L Analogues. Organometallics, 2011, 30, 3054-3063.	1.1	13
56	Bond Energies, Reaction Volumes, and Kinetics for Ïƒ- and Ï€-Complexes of Mo(CO)5L. Journal of Physical Chemistry A, 2011, 115, 9004-9013.	1.1	6
57	The correlation Consistent composite Approach: The spin contamination effect on an MP2-based composite methodology. Chemical Physics Letters, 2011, 504, 88-94.	1.2	21
58	A pseudopotential-based composite method: The relativistic pseudopotential correlation consistent composite approach for molecules containing 4d transition metals (Yâ€“Cd). Journal of Chemical Physics, 2011, 135, 214103.	1.2	39
59	Three-Coordinate Terminal Imidoiron(III) Complexes: Structure, Spectroscopy, and Mechanism of Formation. Inorganic Chemistry, 2010, 49, 6172-6187.	1.9	95
60	Accurate thermochemistry for transition metal complexes from first-principles calculations. Journal of Chemical Physics, 2009, 131, 024106.	1.2	95
61	Redox Activation of Alkene Ligands in Platinum Complexes with Non-innocent Ligands. Inorganic Chemistry, 2009, 48, 638-645.	1.9	36
62	Enthalpy of Formation of the Cyclohexadienyl Radical and the Câˆ’H Bond Enthalpy of 1,4-Cyclohexadiene: An Experimental and Computational Re-Evaluation. Journal of Physical Chemistry A, 2009, 113, 6955-6963.	1.1	47
63	Towards the intrinsic error of the correlation consistent Composite Approach (ccCA). Molecular Physics, 2009, 107, 1107-1121.	0.8	96
64	A non-classical copper carbonyl on a tri-alkene hydrocarbon support. Dalton Transactions, 2009, , 2085.	1.6	13
65	The Correlation Consistent Composite Approach (ccCA): Efficient and Pan-Periodic Kinetics and Thermodynamics. Progress in Theoretical Chemistry and Physics, 2009, , 197-224.	0.2	13
66	Application of the Correlation Consistent Composite Approach (ccCA) to Third-Row (Gaâˆ’Kr) Molecules. Journal of Chemical Theory and Computation, 2008, 4, 328-334.	2.3	46
67	Hartree-Fock complete basis set limit properties for transition metal diatomics. Journal of Chemical Physics, 2008, 128, 044101.	1.2	34
68	Performance of the correlation consistent composite approach for transition states: A comparison to G3B theory. Journal of Chemical Physics, 2007, 127, 154117.	1.2	34
69	Catalytic Synthesis of Arylisocyanates from Nitroaromatics. A Computational Study. Organometallics, 2007, 26, 910-914.	1.1	10
70	Combined Experimental and Computational Studies on the Nature of Aromatic Câˆ’H Activation by Octahedral Ruthenium(II) Complexes: Evidence for Ïƒ-Bond Metathesis from Hammett Studies. Organometallics, 2007, 26, 6604-6611.	1.1	41
71	Systematically Convergent Correlation Consistent Basis Sets for Molecular Coreâˆ’Valence Correlation Effects:â€‰ The Third-Row Atoms Gallium through Krypton. Journal of Physical Chemistry A, 2007, 111, 11383-11393.	1.1	138
72	Quantitative Computational Thermochemistry of Transition Metal Species. Journal of Physical Chemistry A, 2007, 111, 11269-11277.	1.1	153

#	Article	IF	Citations
73	Computationals-Block Thermochemistry with the Correlation Consistent Composite Approach. Journal of Physical Chemistry A, 2007, 111, 10776-10780.	1.1	46
74	Reactions of a Ru(II) Phenyl Complex with Substrates that Possess Câ^'N or Câ^'O Multiple Bonds:â€‰ Câ^'C Bond Formation, Nâ^'H Bond Cleavage, and Decarbonylation Reactions. Organometallics, 2006, 25, 1500-1510.	1.1	26
75	Accurate Enthalpies of Formation of Alkali and Alkaline Earth Metal Oxides and Hydroxides:Â Assessment of the Correlation Consistent Composite Approach (ccCA). Journal of Physical Chemistry A, 2006, 110, 9767-9770.	1.1	47
76	The correlation consistent composite approach (ccCA): An alternative to the Gaussian-n methods. Journal of Chemical Physics, 2006, 124, 114104.	1.2	269
77	Computation of gas-phase enthalpies of formation with chemical accuracy: The curious case of 3-nitroaniline. Computational and Theoretical Chemistry, 2006, 775, 77-80.	1.5	22
78	The correlation-consistent composite approach: Application to the G3/99 test set. Journal of Chemical Physics, 2006, 125, 104111.	1.2	134
79	The extremely flat torsional potential energy surface of oxalyl chloride. Journal of Chemical Physics, 2005, 122, 234313.	1.2	6
80	Application of equation-of-motion coupled-cluster methods to low-lying singlet and triplet electronic states of HBO and BOH. Journal of Chemical Physics, 2005, 122, 234316.	1.2	7
81	The ground and two lowest-lying singlet excited electronic states of copper hydroxide (CuOH). Journal of Chemical Physics, 2005, 123, 014313.	1.2	10
82	Low-lying electronic states of FeNC and FeCN: A theoretical journey into isomerization and quartet/sextet competition. Journal of Chemical Physics, 2004, 120, 4726-4741.	1.2	39
83	Naphthalenyl, Anthracenyl, Tetracenyl, and Pentacenyl Radicals and Their Anions. Journal of Physical Chemistry A, 2003, 107, 6311-6316.	1.1	16
84	Siloxyl radical initiated HCN polymerization: Computation of N-heterocycles formation and surface passivation. Monthly Notices of the Royal Astronomical Society, 0, , .	1.6	1