Laura Gagliardi

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/108722/publications.pdf

Version: 2024-02-01

422 papers	27,915 citations	5558 82 h-index	9073 144 g-index
450 all docs	450 docs citations	450 times ranked	19802 citing authors

#	Article	IF	Citations
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	1.5	1,317
2	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	13.7	1,026
3	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661
4	On the Mechanism of the cisâ^'trans Isomerization in the Lowest Electronic States of Azobenzene:â€‰ S0, S1, and T1. Journal of the American Chemical Society, 2004, 126, 3234-3243.	6.6	431
5	The restricted active space followed by second-order perturbation theory method: Theory and application to the study of CuO2 and Cu2O2 systems. Journal of Chemical Physics, 2008, 128, 204109.	1.2	430
6	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
7	Oxidation of ethane to ethanol by N2O in a metalâ€“organic framework with coordinatively unsaturated iron(II) sites. Nature Chemistry, 2014, 6, 590-595.	6.6	398
8	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	2.3	334
9	Local properties of quantum chemical systems: The LoProp approach. Journal of Chemical Physics, 2004, 121, 4494-4500.	1.2	320
10	Cerium Metalâ€“Organic Framework for Photocatalysis. Journal of the American Chemical Society, 2018, 140, 7904-7912.	6.6	313
11	A Quantum Chemical Study of the Quintuple Bond between Two Chromium Centers in [PhCrCrPh]:trans-Bent versus Linear Geometry. Angewandte Chemie - International Edition, 2006, 45, 3804-3807.	7.2	312
12	Quantum chemical calculations show that the uranium molecule U2 has a quintuple bond. Nature, 2005, 433, 848-851.	13.7	310
13	Ab initio carbon capture in open-site metalâ€“organic frameworks. Nature Chemistry, 2012, 4, 810-816.	6.6	310
14	Using natureâ€™s blueprint to expand catalysis with Earth-abundant metals. Science, 2020, 369, .	6.0	306
15	Reaching the Maximum Multiplicity of the Covalent Chemical Bond. Angewandte Chemie - International Edition, 2007, 46, 1469-1472.	7.2	289
16	Methane Oxidation to Methanol Catalyzed by Cu-Oxo Clusters Stabilized in NU-1000 Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 10294-10301.	6.6	282
17	Evolution of water structures in metal-organic frameworks for improved atmospheric water harvesting. Science, 2021, 374, 454-459.	6.0	281
18	Are Zr₆-based MOFs water stable? Linker hydrolysis vs. capillary-force-driven channel collapse. Chemical Communications, 2014, 50, 8944.	2.2	277

#	Article	IF	Citations
19	Sintering-Resistant Single-Site Nickel Catalyst Supported by Metalâ€“Organic Framework. Journal of the American Chemical Society, 2016, 138, 1977-1982.	6.6	273
20	The Ruâ”Hbpp Water Oxidation Catalyst. Journal of the American Chemical Society, 2009, 131, 15176-15187.	6.6	253
21	Quantum-Chemical Characterization of the Properties and Reactivities of Metalâ€“Organic Frameworks. Chemical Reviews, 2015, 115, 6051-6111.	23.0	241
22	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. Accounts of Chemical Research, 2017, 50, 66-73.	7.6	232
23	Defining the Proton Topology of the Zr₆-Based Metalâ€“Organic Framework NU-1000. Journal of Physical Chemistry Letters, 2014, 5, 3716-3723.	2.1	228
24	Metalâ€“Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts: NU-1000- and UiO-66-Supported Iridium Complexes. Journal of the American Chemical Society, 2015, 137, 7391-7396.	6.6	228
25	Metalâ€“Organic Framework Supported Cobalt Catalysts for the Oxidative Dehydrogenation of Propane at Low Temperature. ACS Central Science, 2017, 3, 31-38.	5.3	222
26	The generalized active space concept in multiconfigurational self-consistent field methods. Journal of Chemical Physics, 2011, 135, 044128.	1.2	220
27	An Exceptionally Stable Metalâ€“Organic Framework Supported Molybdenum(VI) Oxide Catalyst for Cyclohexene Epoxidation. Journal of the American Chemical Society, 2016, 138, 14720-14726.	6.6	211
28	Reversible CO Binding Enables Tunable CO/H₂ and CO/N₂ Separations in Metalâ€“Organic Frameworks with Exposed Divalent Metal Cations. Journal of the American Chemical Society, 2014, 136, 10752-10761.	6.6	210
29	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 7402-7405.	6.6	208
30	Atomic Cholesky decompositions: A route to unbiased auxiliary basis sets for density fitting approximation with tunable accuracy and efficiency. Journal of Chemical Physics, 2009, 130, 154107.	1.2	185
31	Exploring the Actinideâ”Actinide Bond:Â Theoretical Studies of the Chemical Bond in Ac2, Th2, Pa2, and U2. Journal of the American Chemical Society, 2006, 128, 17000-17006.	6.6	179
32	Theoretical Models on the Cu2O2 Torture Track:â€‰ Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues. Journal of Physical Chemistry A, 2006, 110, 1991-2004.	1.1	179
33	Metalâ€“Alane Adducts with Zero-Valent Nickel, Cobalt, and Iron. Journal of the American Chemical Society, 2011, 133, 20724-20727.	6.6	175
34	Machine learning the quantum-chemical properties of metalâ€“organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	5.0	170
35	The Coordination of Uranyl in Water:Â A Combined Quantum Chemical and Molecular Simulation Study. Journal of the American Chemical Society, 2005, 127, 14250-14256.	6.6	169
36	Combining Wave Function Methods with Density Functional Theory for Excited States. Chemical Reviews, 2018, 118, 7249-7292.	23.0	166

#	Article	IF	Citations
37	Multiconfigurational Second-Order Perturbation Theory Restricted Active Space (RASPT2) Method for Electronic Excited States: A Benchmark Study. Journal of Chemical Theory and Computation, 2011, 7, 153-168.	2.3	164
38	Catalytic Silylation of Dinitrogen with a Dicobalt Complex. Journal of the American Chemical Society, 2015, 137, 4638-4641.	6.6	162
39	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	6.6	157
40	Introduction: Carbon Capture and Separation. Chemical Reviews, 2017, 117, 9521-9523.	23.0	157
41	Mechanism of Oxidation of Ethane to Ethanol at Iron(IV)â€“Oxo Sites in Magnesium-Diluted Fe₂(dobdc). Journal of the American Chemical Society, 2015, 137, 5770-5781.	6.6	156
42	Tuning the Surface Chemistry of Metal Organic Framework Nodes: Proton Topology of the Metal-Oxide-Like Zr₆ Nodes of UiO-66 and NU-1000. Journal of the American Chemical Society, 2016, 138, 15189-15196.	6.6	155
43	Tuning Zr₆ Metalâ€“Organic Framework (MOF) Nodes as Catalyst Supports: Site Densities and Electron-Donor Properties Influence Molecular Iridium Complexes as Ethylene Conversion Catalysts. ACS Catalysis, 2016, 6, 235-247.	5.5	150
44	Structure and Dynamics of Zr₆O₈ Metalâ€“Organic Framework Node Surfaces Probed with Ethanol Dehydration as a Catalytic Test Reaction. Journal of the American Chemical Society, 2018, 140, 3751-3759.	6.6	150
45	Computational Design of Functionalized Metalâ€“Organic Framework Nodes for Catalysis. ACS Central Science, 2018, 4, 5-19.	5.3	148
46	Harnessing redox activity for the formation of uranium tris(imido) compounds. Nature Chemistry, 2014, 6, 919-926.	6.6	145
47	Standard Practices of Reticular Chemistry. ACS Central Science, 2020, 6, 1255-1273.	5.3	142
48	Multiconfigurational quantum chemical methods for molecular systems containing actinides. Chemical Society Reviews, 2007, 36, 893.	18.7	137
49	Self-Interaction Error in Density Functional Theory: An Appraisal. Journal of Physical Chemistry Letters, 2018, 9, 2353-2358.	2.1	131
50	Amidinatoâ€“ and Guanidinatoâ€“Cobalt(I) Complexes: Characterization of Exceptionally Short Coâ€“Co Interactions. Angewandte Chemie - International Edition, 2009, 48, 7406-7410.	7.2	129
51	A Bimetallic Nickelâ€“Gallium Complex Catalyzes CO₂ Hydrogenation via the Intermediacy of an Anionic d¹⁰ Nickel Hydride. Journal of the American Chemical Society, 2017, 139, 14244-14250.	6.6	128
52	Quantum chemical characterization of the mechanism of an iron-based water oxidation catalyst. Chemical Science, 2012, 3, 1293.	3.7	122
53	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 1477-1488.	2.3	121
54	Pushing configuration-interaction to the limit: Towards massively parallel MCSCF calculations. Journal of Chemical Physics, 2017, 147, 184111.	1.2	120

#	Article	IF	Citations
55	Systematic Variation of Metalâ€“Metal Bond Order in Metalâ€“Chromium Complexes. Journal of the American Chemical Society, 2013, 135, 13142-13148.	6.6	119
56	Targeted Single-Site MOF Node Modification: Trivalent Metal Loading via Atomic Layer Deposition. Chemistry of Materials, 2015, 27, 4772-4778.	3.2	116
57	Self-Sorting Chiral Subcomponent Rearrangement During Crystallization. Journal of the American Chemical Society, 2007, 129, 8774-8780.	6.6	114
58	On the Nature of Actinideâ€“ and Lanthanideâ€“Metal Bonds in Heterobimetallic Compounds. Chemistry - A European Journal, 2011, 17, 8424-8433.	1.7	112
59	The Electronic Spectrum of Re2Cl82-:Â A Theoretical Study. Inorganic Chemistry, 2003, 42, 1599-1603.	1.9	111
60	Unusual structure, bonding and properties in a californium borate. Nature Chemistry, 2014, 6, 387-392.	6.6	110
61	Analysing the chromiumâ€“chromium multiple bonds using multiconfigurational quantum chemistry. Chemical Physics Letters, 2009, 471, 1-10.	1.2	109
62	The cisâ€[Ru^{II}(bpy)₂(H₂O)₂]²⁺ Waterâ€Oxidation Catalyst Revisited. Angewandte Chemie - International Edition, 2010, 49, 7745-7747.	7.2	107
63	The Electronic Spectrum of the UO2Molecule. Journal of the American Chemical Society, 2005, 127, 86-91.	6.6	104
64	Single-Site Organozirconium Catalyst Embedded in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2015, 137, 15680-15683.	6.6	103
65	Quantum Chemical Calculations and Experimental Investigations of Molecular Actinide Oxides. Chemical Reviews, 2015, 115, 1725-1759.	23.0	103
66	Selective, Tunable O₂ Binding in Cobalt(II)â€“Triazolate/Pyrazolate Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 7161-7170.	6.6	101
67	Understanding the Structure and Formation of Uranyl Peroxide Nanoclusters by Quantum Chemical Calculations. Journal of the American Chemical Society, 2010, 132, 14503-14508.	6.6	98
68	Pyrene-Edged Fe^{II}₄L₆ Cages Adaptively Reconfigure During Guest Binding. Journal of the American Chemical Society, 2014, 136, 15615-15624.	6.6	98
69	SplitGAS Method for Strong Correlation and the Challenging Case of Cr₂. Journal of Chemical Theory and Computation, 2013, 9, 3375-3384.	2.3	97
70	Tuning the Properties of Zr₆O₈ Nodes in the Metal Organic Framework UiO-66 by Selection of Node-Bound Ligands and Linkers. Chemistry of Materials, 2019, 31, 1655-1663.	3.2	97
71	Experimental and quantum chemical characterization of the water oxidation cycle catalysed by [RuII(damp)(bpy)(H2O)]2+. Chemical Science, 2012, 3, 2576.	3.7	96
72	Differentiating between Trivalent Lanthanides and Actinides. Journal of the American Chemical Society, 2012, 134, 10682-10692.	6.6	96

#	Article	IF	Citations
73	Beyond the Active Site: Tuning the Activity and Selectivity of a Metalâ€“Organic Framework-Supported Ni Catalyst for Ethylene Dimerization. Journal of the American Chemical Society, 2018, 140, 11174-11178.	6.6	94
74	When Does Gold Behave as a Halogen? Predicted Uranium Tetraauride and Other MAu4Tetrahedral Species, (M = Ti, Zr, Hf, Th). Journal of the American Chemical Society, 2003, 125, 7504-7505.	6.6	93
75	Copper(I)â^'Î±-Ketocarboxylate Complexes:â€‰ Characterization and O₂ Reactions That Yield Copperâ^'Oxygen Intermediates Capable of Hydroxylating Arenes. Journal of the American Chemical Society, 2007, 129, 14190-14192.	6.6	93
76	On the Analysis of the Crâ^'Cr Multiple Bond in Several Classes of Dichromium Compounds. Inorganic Chemistry, 2010, 49, 5216-5222.	1.9	92
77	On the Electronic Structure of the UO2 Molecule. Journal of Physical Chemistry A, 2001, 105, 10602-10606.	1.1	91
78	Role of the Metal in the Bonding and Properties of Bimetallic Complexes Involving Manganese, Iron, and Cobalt. Journal of the American Chemical Society, 2014, 136, 1842-1855.	6.6	91
79	Multiconfiguration Pair-Density Functional Theory: A Fully Translated Gradient Approximation and Its Performance for Transition Metal Dimers and the Spectroscopy of Re₂Cl₈^{2â€“}. Journal of Chemical Theory and Computation, 2015, 11, 4077-4085.	2.3	91
80	Dinitrogen Activation at Iron and Cobalt Metallalumatranes. European Journal of Inorganic Chemistry, 2013, 2013, 3898-3906.	1.0	88
81	Well-Defined Rhodiumâ€“Gallium Catalytic Sites in a Metalâ€“Organic Framework: Promoter-Controlled Selectivity in Alkyne Semihydrogenation to E-Alkenes. Journal of the American Chemical Society, 2018, 140, 15309-15318.	6.6	88
82	How Many Hydrogen Atoms Can Be Bound to a Metal? Predicted MH12Species. Journal of the American Chemical Society, 2004, 126, 15014-15015.	6.6	87
83	Synthesis and Properties of a Fifteenâ€Coordinate Complex: The Thorium Aminodiboranate [Th(H₃BNMe₂BH₃)₄]. Angewandte Chemie - International Edition, 2010, 49, 3379-3381.	7.2	87
84	Investigations of the Electronic Structure of Arene-Bridged Diuranium Complexes. Organometallics, 2013, 32, 1341-1352.	1.1	87
85	Large Differences in Secondary Metalâ^'Arene Interactions in the Transition-Metal Dimers ArMMAr (Ar =) Tj ETQq1 1 0.784314 rgBT /Ov Chemical Society, 2008, 130, 5104-5114.	6.6	85
86	Ab Initio Derived Force Fields for Predicting CO₂ Adsorption and Accessibility of Metal Sites in the Metalâ€“Organic Frameworks M-MOF-74 (M = Mn, Co, Ni, Cu). Journal of Physical Chemistry C, 2015, 119, 16058-16071.	1.5	84
87	Lowâ€Coordinate Iron(I) and Manganese(I) Dimers: Kinetic Stabilization of an Exceptionally Short Feï£¿Fe Multiple Bond. Angewandte Chemie - International Edition, 2012, 51, 8294-8298.	7.2	83
88	Thermal Stabilization of Metalâ€“Organic Framework-Derived Single-Site Catalytic Clusters through Nanocasting. Journal of the American Chemical Society, 2016, 138, 2739-2748.	6.6	83
89	Tuning Catalytic Sites on Zr₆O₈ Metalâ€“Organic Framework Nodes via Ligand and Defect Chemistry Probed with tert-Butyl Alcohol Dehydration to Isobutylene. Journal of the American Chemical Society, 2020, 142, 8044-8056.	6.6	83
90	Quantum Chemical Characterization of Structural Single Fe(II) Sites in MIL-Type Metalâ€“Organic Frameworks for the Oxidation of Methane to Methanol and Ethane to Ethanol. ACS Catalysis, 2019, 9, 2870-2879.	5.5	82

#	Article	IF	Citations
91	Theoretical Characterization of End-On and Side-On Peroxide Coordination in Ligated Cu2O2 Models. Journal of Physical Chemistry A, 2006, 110, 11557-11568.	1.1	80
92	From Transition Metals to Lanthanides to Actinides: Metal-Mediated Tuning of Electronic Properties of Isostructural Metalâ€“Organic Frameworks. Inorganic Chemistry, 2018, 57, 13246-13251.	1.9	80
93	Structure, Dynamics, and Reactivity for Light Alkane Oxidation of Fe(II) Sites Situated in the Nodes of a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 18142-18151.	6.6	80
94	A very short uraniumâ€“uranium bond: The predicted metastable U22+. Physical Chemistry Chemical Physics, 2005, 7, 2415.	1.3	79
95	Computationally Guided Discovery of a Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerization. Journal of Physical Chemistry C, 2016, 120, 23576-23583.	1.5	78
96	Î·5-N5-â^'Metalâ^'Î·7-N73-:Â A New Class of Compounds. Journal of Physical Chemistry A, 2002, 106, 4690-4694.	1.1	77
97	Bimetallic Cobaltâ€“Dinitrogen Complexes: Impact of the Supporting Metal on N₂ Activation. Inorganic Chemistry, 2015, 54, 9263-9270.	1.9	77
98	Chemiresistive Detection of Gaseous Hydrocarbons and Interrogation of Charge Transport in Cu[Ni(2,3-pyrazinedithiolate)₂] by Gas Adsorption. Journal of the American Chemical Society, 2019, 141, 5005-5013.	6.6	77
99	Length-Dependent Nanotransport and Charge Hopping Bottlenecks in Long Thiophene-Containing Ï€-Conjugated Molecular Wires. Journal of the American Chemical Society, 2015, 137, 15732-15741.	6.6	76
100	Revised M11 Exchange-Correlation Functional for Electronic Excitation Energies and Ground-State Properties. Journal of Physical Chemistry A, 2019, 123, 2966-2990.	1.1	76
101	Multiconfiguration Pair-Density Functional Theory Is as Accurate as CASPT2 for Electronic Excitation. Journal of Physical Chemistry Letters, 2016, 7, 586-591.	2.1	75
102	Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 8481-8502.	5.5	75
103	Effects of Covalency on Anionic Redox Chemistry in Semiquinoid-Based Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2020, 142, 2653-2664.	6.6	75
104	UO₂²⁺ Uptake by Proteins: Understanding the Binding Features of the Super Uranyl Binding Protein and Design of a Protein with Higher Affinity. Journal of the American Chemical Society, 2014, 136, 17484-17494.	6.6	74
105	Electronic Structure of the [Cu₃(Î¼-O)₃]²⁺ Cluster in Mordenite Zeolite and Its Effects on the Methane to Methanol Oxidation. Journal of Physical Chemistry C, 2017, 121, 22295-22302.	1.5	74
106	Bridging Zirconia Nodes within a Metalâ€“Organic Framework via Catalytic Ni-Hydroxo Clusters to Form Heterobimetallic Nanowires. Journal of the American Chemical Society, 2017, 139, 10410-10418.	6.6	74
107	Quantum Chemistry Predicts Multiply Bonded Diuranium Compounds to Be Stable. Inorganic Chemistry, 2006, 45, 803-807.	1.9	73
108	Is Fullerene C₆₀ Large Enough to Host a Multiply Bonded Dimetal?. Journal of the American Chemical Society, 2008, 130, 7459-7465.	6.6	73

#	Article	IF	Citations
109	Ionization Energies for the Actinide Mono- and Dioxides Series, from Th to Cm: Theory versus Experiment. Journal of Physical Chemistry A, 2010, 114, 6007-6015.	1.1	73
110	Quantum Chemical Calculations Predict the Diphenyl Diuranium Compound [PhUUPh] To Have a Stable1Ag Ground State. Angewandte Chemie - International Edition, 2006, 45, 6210-6213.	7.2	71
111	Generating Cu^{II}â€“Oxyl/Cu^{III}â€“Oxo Species from Cu^Iâ€“Î±â€Ketocarboxylate Complexes and O₂: In Silico Studies on Ligand Effects and Cï¿½Hâ€Activation Reactivity. Chemistry - A European Journal, 2009, 15, 4886-4895.	1.7	70
112	The Ligandâ€Based Quintuple Bondâ€Shortening Concept and Some of Its Limitations. Chemistry - A European Journal, 2013, 19, 9825-9832.	1.7	70
113	A Two-Coordinate Manganese(0) Complex with an Unsupported Mnâ€“Mg Bond: Allowing Access to Low Coordinate Homo- and Heterobimetallic Compounds. Journal of the American Chemical Society, 2014, 136, 5283-5286.	6.6	70
114	Scandium Cycloheptanitride, ScN7:Â A Predicted High-Energy Molecule Containing an [Î·7-N7]3-Ligand. Journal of the American Chemical Society, 2001, 123, 9700-9701.	6.6	69
115	A Theoretical Study of the Structure of Tricarbonatodioxouranate. Inorganic Chemistry, 2001, 40, 2976-2978.	1.9	69
116	Molecular Rhodium Complexes Supported on the Metal-Oxide-Like Nodes of Metal Organic Frameworks and on Zeolite HY: Catalysts for Ethylene Hydrogenation and Dimerization. ACS Applied Materials & Interfaces, 2017, 9, 33511-33520.	4.0	69
117	Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singletâ€“triplet gaps in polyacenes and polyacetylenes. Chemical Science, 2019, 10, 1716-1723.	3.7	69
118	Multiple Metalâ€“Metal Bonds in Ironâ€“Chromium Complexes. Angewandte Chemie - International Edition, 2013, 52, 4449-4452.	7.2	68
119	A theoretical study of the nitrogen clusters formed from the ions N3â^', N5+, and N5â^'. Journal of Chemical Physics, 2001, 114, 10733-10737.	1.2	67
120	A Quantum Chemical and Molecular Dynamics Study of the Coordination of Cm(III) in Water. Journal of the American Chemical Society, 2007, 129, 14136-14137.	6.6	67
121	Infrared Spectroscopy of Extreme Coordination: The Carbonyls of U⁺ and UO₂⁺. Journal of the American Chemical Society, 2010, 132, 15905-15907.	6.6	67
122	How accurate are electronic structure methods for actinoid chemistry?. Theoretical Chemistry Accounts, 2011, 129, 657-666.	0.5	65
123	Molecular integrals by numerical quadrature. I. Radial integration. Theoretical Chemistry Accounts, 2001, 106, 178-187.	0.5	64
124	Bond Length and Bond Order in One of the Shortest Crâ^'Cr Bonds. Inorganic Chemistry, 2008, 47, 11455-11457.	1.9	64
125	Electronic Structure of Oxidized Complexes Derived fromcis-[RuII(bpy)2(H2O)2]2+and Its Photoisomerization Mechanism. Inorganic Chemistry, 2011, 50, 11134-11142.	1.9	64
126	Full configuration interaction calculations on Be2. Chemical Physics, 1994, 185, 47-56.	0.9	63

#	Article	IF	Citations
127	Investigation of the Electronic Ground States for a Reduced Pyridine(diimine) Uranium Series: Evidence for a Ligand Tetraanion Stabilized by a Uranium Dimer. Journal of the American Chemical Society, 2015, 137, 4690-4700.	6.6	62
128	Multiconfiguration Pair-Density Functional Theory: Barrier Heights and Main Group and Transition Metal Energetics. Journal of Chemical Theory and Computation, 2015, 11, 82-90.	2.3	62
129	Computational Study of Structural and Electronic Properties of Lead-Free CsMI₃ Perovskites (M = Ge, Sn, Pb, Mg, Ca, Sr, and Ba). Journal of Physical Chemistry C, 2018, 122, 7838-7848.	1.5	62
130	Actinide Metallocene Hydride Chemistry: Câ€“H Activation in Tetramethylcyclopentadienyl Ligands to Form [Î¼-Î·⁵-C₅Me₃H(CH₂)-ÎºC]^{2â€“} Tuck-over Ligands in a Tetrathorium Octahydride Complex. Organometallics, 2013, 32, 6522-6531.	1.1	61
131	Hydration of Lanthanide Chloride Salts: A Quantum Chemical and Classical Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2010, 114, 15590-15597.	1.2	60
132	Generalized-active-space pair-density functional theory: an efficient method to study large, strongly correlated, conjugated systems. Chemical Science, 2017, 8, 2741-2750.	3.7	60
133	Metal doping in cerium metal-organic frameworks for visible-response water splitting photocatalysts. Journal of Chemical Physics, 2019, 150, 041701.	1.2	59
134	Stereoelectronic Effects on Molecular Geometries and State-Energy Splittings of Ligated Monocopper Dioxygen Complexes. Journal of Physical Chemistry A, 2008, 112, 3754-3767.	1.1	58
135	Diabatization based on the dipole and quadrupole: The DQ method. Journal of Chemical Physics, 2014, 141, 114104.	1.2	58
136	Bulky Guanidinato Nickel(I) Complexes: Synthesis, Characterization, Isomerization, and Reactivity Studies. Chemistry - A European Journal, 2011, 17, 1294-1303.	1.7	57
137	Multiconfiguration Pair-Density Functional Theory Predicts Spin-State Ordering in Iron Complexes with the Same Accuracy as Complete Active Space Second-Order Perturbation Theory at a Significantly Reduced Computational Cost. Journal of Physical Chemistry Letters, 2017, 8, 2026-2030.	2.1	57
138	Charge Transport in 4 nm Molecular Wires with Interrupted Conjugation: Combined Experimental and Computational Evidence for Thermally Assisted Polaron Tunneling. ACS Nano, 2016, 10, 4372-4383.	7.3	56
139	Installing Heterobimetallic Cobaltâ€“Aluminum Single Sites on a Metal Organic Framework Support. Chemistry of Materials, 2016, 28, 6753-6762.	3.2	56
140	Strong correlation treated via effective hamiltonians and perturbation theory. Journal of Chemical Physics, 2011, 134, 034114.	1.2	55
141	Correlated-Participating-Orbitals Pair-Density Functional Method and Application to Multiplet Energy Splittings of Main-Group Divalent Radicals. Journal of Chemical Theory and Computation, 2016, 12, 4274-4283.	2.3	55
142	Multiconfigurational Self-Consistent Field Theory with Density Matrix Embedding: The Localized Active Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2019, 15, 972-986.	2.3	55
143	Elucidating bonding preferences in tetrakis(imido)uranate(VI) dianions. Nature Chemistry, 2017, 9, 850-855.	6.6	54
144	Assessing Metalâ€“Metal Multiple Bonds in Crï£¿Cr, Moï£¿Mo, and Wï£¿W Compounds and a Hypothetical Uï£¿U Compound: A Quantum Chemical Study Comparing DFT and Multireference Methods. Chemistry - A European Journal, 2012, 18, 1737-1749.	1.7	53

#	Article	IF	Citations
145	Theoretical Study of the Lowest1BUStates oftrans-Stilbene. Journal of Physical Chemistry A, 2002, 106, 7355-7361.	1.1	52
146	Cesium and barium as honorary d elements: CsN 7 Ba as an example. Theoretical Chemistry Accounts, 2003, 110, 205-210.	0.5	52
147	Beyond Radical Rebound: Methane Oxidation to Methanol Catalyzed by Iron Species in Metalâ€“Organic Framework Nodes. Journal of the American Chemical Society, 2021, 143, 12165-12174.	6.6	51
148	On the resolution of identity Coulomb energy approximation in density functional theory. Computational and Theoretical Chemistry, 2000, 501-502, 229-239.	1.5	50
149	Systematic truncation of the virtual space in multiconfigurational perturbation theory. Journal of Chemical Physics, 2009, 131, 034113.	1.2	50
150	Structure and Reactivity of X-ray Amorphous Uranyl Peroxide, U₂O₇. Inorganic Chemistry, 2016, 55, 3541-3546.	1.9	50
151	Theoretical Search for Very Short Metalâ€“Actinide Bonds: NUIr and Isoelectronic Systems. Angewandte Chemie - International Edition, 2004, 43, 1573-1576.	7.2	49
152	Unprecedented selectivity in molecular recognition of carbohydrates by a metalâ€“organic framework. Chemical Communications, 2016, 52, 7094-7097.	2.2	49
153	Structural and Spectroscopic Characterization of Reaction Intermediates Involved in a Dinuclear Coâ€“Hbpp Water Oxidation Catalyst. Journal of the American Chemical Society, 2016, 138, 15291-15294.	6.6	49
154	Systematic Expansion of Active Spaces beyond the CASSCF Limit: A GASSCF/SplitGAS Benchmark Study. Journal of Chemical Theory and Computation, 2015, 11, 3010-3021.	2.3	48
155	Separated-pair approximation and separated-pair pair-density functional theory. Chemical Science, 2016, 7, 2399-2413.	3.7	47
156	Predicting Bond Dissociation Energies of Transition-Metal Compounds by Multiconfiguration Pair-Density Functional Theory and Second-Order Perturbation Theory Based on Correlated Participating Orbitals and Separated Pairs. Journal of Chemical Theory and Computation, 2017, 13, 616-626.	2.3	47
157	Coordination of the Neptunyl Ion with Carbonate Ions and Water:Â A Theoretical Study. Inorganic Chemistry, 2002, 41, 1315-1319.	1.9	46
158	Pushing the Limits of Delta Bonding in Metalâ€“Chromium Complexes with Redox Changes and Metal Swapping. Inorganic Chemistry, 2015, 54, 7579-7592.	1.9	46
159	Computational Screening of Bimetal-Functionalized Zr₆O₈ MOF Nodes for Methane Câ€“H Bond Activation. Inorganic Chemistry, 2017, 56, 8739-8743.	1.9	46
160	A Combined Spectroscopic and Computational Study of a High-Spin S = 7/2 Diiron Complex with a Short Ironâ€“Iron Bond. Inorganic Chemistry, 2012, 51, 728-736.	1.9	45
161	CO₂ Adsorption in Fe₂(dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. Journal of Physical Chemistry C, 2014, 118, 12230-12240.	1.5	45
162	Heterobimetallic Complexes That Bond Vanadium to Iron, Cobalt, and Nickel. Inorganic Chemistry, 2015, 54, 11669-11679.	1.9	45

#	Article	IF	Citations
163	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	3.7	45
164	Atomic Layer Deposition in a Metalâ€“Organic Framework: Synthesis, Characterization, and Performance of a Solid Acid. Chemistry of Materials, 2017, 29, 1058-1068.	3.2	45
165	Automatic Selection of an Active Space for Calculating Electronic Excitation Spectra by MS-CASPT2 or MC-PDFT. Journal of Chemical Theory and Computation, 2018, 14, 2017-2025.	2.3	45
166	A Relativistic Density Functional Study on the Uranium Hexafluoride and Plutonium Hexafluoride Monomer and Dimer Species. Journal of the American Chemical Society, 1998, 120, 11727-11731.	6.6	44
167	Cation Templating and Electronic Structure Effects in Uranyl Cage Clusters Probed by the Isolation of Peroxide-Bridged Uranyl Dimers. Inorganic Chemistry, 2015, 54, 4445-4455.	1.9	44
168	Accelerated Computational Analysis of Metalâ€“Organic Frameworks for Oxidation Catalysis. Journal of Physical Chemistry C, 2016, 120, 18707-18712.	1.5	44
169	Second-Order Perturbation Theory for Generalized Active Space Self-Consistent-Field Wave Functions. Journal of Chemical Theory and Computation, 2016, 12, 3208-3213.	2.3	44
170	Single Ni atoms and Ni4 clusters have similar catalytic activity for ethylene dimerization. Journal of Catalysis, 2017, 354, 278-286.	3.1	44
171	Computational screening of MOF-supported transition metal catalysts for activity and selectivity in ethylene dimerization. Journal of Catalysis, 2018, 360, 160-167.	3.1	44
172	Bimetallic nickel-lutetium complexes: tuning the properties and catalytic hydrogenation activity of the Ni site by varying the Lu coordination environment. Chemical Science, 2019, 10, 3375-3384.	3.7	44
173	Combined Triple and Double Bonds to Uranium: The Nâ‰¡Uâ•Nâˆ’H Uranimine Nitride Molecule Prepared in Solid Argon. Inorganic Chemistry, 2011, 50, 3826-3831.	1.9	43
174	Single-Ion Magnetic Anisotropy and Isotropic Magnetic Couplings in the Metalâ€“Organic Framework Fe₂(dobdc). Inorganic Chemistry, 2013, 52, 9379-9389.	1.9	43
175	Uranium(III)-carbon multiple bonding supported by arene Î´-bonding in mixed-valence hexauranium nanometre-scale rings. Nature Communications, 2018, 9, 2097.	5.8	43
176	Actinide 2-metallabiphenylenes that satisfy HÃ¼ckelâ€™s rule. Nature, 2020, 578, 563-567.	13.7	43
177	Understanding, Controlling and Programming Cooperativity in Selfâ€Assembled Polynuclear Complexes in Solution. Chemistry - A European Journal, 2009, 15, 12702-12718.	1.7	42
178	Periodic Trends in Lanthanide and Actinide Phosphonates: Discontinuity between Plutonium and Americium. Inorganic Chemistry, 2012, 51, 6906-6915.	1.9	42
179	The DQ and DQÎ¦ electronic structure diabatization methods: Validation for general applications. Journal of Chemical Physics, 2016, 144, 194101.	1.2	42
180	Mixed-Valent Dicobalt and Ironâ€“Cobalt Complexes with High-Spin Configurations and Short Metalâ€“Metal Bonds. Inorganic Chemistry, 2013, 52, 9216-9228.	1.9	41

#	Article	IF	Citations
181	Synthesis and Characterization of Tris-chelate Complexes for Understanding f-Orbital Bonding in Later Actinides. Journal of the American Chemical Society, 2019, 141, 2356-2366.	6.6	41
182	Multiconfigurational Theoretical Study of the Octamethyldimetalates of Cr(II), Mo(II), W(II), and Re(III):Â Revisiting the Correlation between the Mâ^'M Bond Length and the Î´â†' Î* Transition Energy. Inorganic Chemistry, 2005, 44, 8476-8480.	1.9	40
183	A theoretical study of the ground state and lowest excited states of PuO0/+/+2 and PuO20/+/+2. Physical Chemistry Chemical Physics, 2008, 10, 7278.	1.3	40
184	Second-order perturbation theory with complete and restricted active space reference functions applied to oligomeric unsaturated hydrocarbons. Physical Chemistry Chemical Physics, 2009, 11, 10964.	1.3	40
185	Empirical and Theoretical Insights into the Structural Features and Hostâ€"Guest Chemistry of M₈L₄ Tube Architectures. Journal of the American Chemical Society, 2014, 136, 3972-3980.	6.6	40
186	Multiconfiguration Pair-Density Functional Theory Outperforms Kohnâ€"Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer. Journal of Chemical Theory and Computation, 2015, 11, 3643-3649.	2.3	40
187	Computational Study of First-Row Transition Metals Supported on MOF NU-1000 for Catalytic Acceptorless Alcohol Dehydrogenation. Journal of Physical Chemistry C, 2016, 120, 24697-24705.	1.5	40
188	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 126-138.	2.3	40
189	Periodic Electronic Structure Calculations with the Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 130-140.	2.3	40
190	Insights into the Structureâ€"Activity Relationships in Metalâ€"Organic Framework-Supported Nickel Catalysts for Ethylene Hydrogenation. ACS Catalysis, 2020, 10, 8995-9005.	5.5	40
191	Automation of Active Space Selection for Multireference Methods via Machine Learning on Chemical Bond Dissociation. Journal of Chemical Theory and Computation, 2020, 16, 2389-2399.	2.3	40
192	A Combined Experimental and Theoretical Study of Uranium Polyhydrides with New Evidence for the Large Complex UH4(H2)6. Journal of Physical Chemistry A, 2007, 111, 6383-6387.	1.1	39
193	DFT and CASPT2 Analysis of Polymetallic Uranium Nitride and Oxide Complexes: How Theory Can Help When X-Ray Analysis Is Inadequate. Journal of the American Chemical Society, 2010, 132, 12397-12403.	6.6	39
194	Câ€"H Bond Activation on Bimetallic Two-Atom Co-M Oxide Clusters Deposited on Zr-Based MOF Nodes: Effects of Doping at the Molecular Level. ACS Catalysis, 2018, 8, 2864-2869.	5.5	39
195	Rationalizing the Reactivity of Bimetallic Molecular Catalysts for CO₂ Hydrogenation. ACS Catalysis, 2018, 8, 4955-4968.	5.5	39
196	Can Density Matrix Embedding Theory with the Complete Activate Space Self-Consistent Field Solver Describe Single and Double Bond Breaking in Molecular Systems?. Journal of Chemical Theory and Computation, 2018, 14, 1960-1968.	2.3	39
197	Multiconfiguration Pair-Density Functional Theory for Iron Porphyrin with CAS, RAS, and DMRG Active Spaces. Journal of Physical Chemistry A, 2019, 123, 3389-3394.	1.1	39
198	Advancement of Actinide Metalâ€"Organic Framework Chemistry via Synthesis of Pu-UiO-66. Journal of the American Chemical Society, 2020, 142, 9363-9371.	6.6	38

#	Article	IF	Citations
199	Formal Nickelate(â˜I) Complexes Supported by Groupâ€...13 Ions. Angewandte Chemie - International Edition, 2018, 57, 7815-7819.	7.2	37
200	Infrared spectra and quantum chemical calculations of the uranium-carbon molecules UC, CUC, UCH, and U(CC)2. Journal of Chemical Physics, 2011, 134, 244313.	1.2	36
201	In Situ Formation of Unprecedented Neptunium-Oxide Wheel Clusters Stabilized in a Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 11842-11846.	6.6	36
202	Negative cooperativity upon hydrogen bond-stabilized O2 adsorption in a redox-active metalâ€“organic framework. Nature Communications, 2020, 11, 3087.	5.8	36
203	Microwave Spectra of Benzotriazole and Pyrimidinotriazole. Journal of Molecular Spectroscopy, 1993, 161, 136-148.	0.4	35
204	Predicted Group 4 Tetra-azides M(N3)4(M = Tiâ˜Hf, Th):Â The First Examples of Linear Mâ˜NNN Coordination. Inorganic Chemistry, 2003, 42, 3074-3078.	1.9	35
205	Experimental and Computational Study of a New Wheel-Shaped {[W₅O₂₁]₃[(U^{VI}O₂)₂(Î¼-O₂)] Polyoxometalate. Inorganic Chemistry, 2012, 51, 8784-8790.	4.9	35
206	Computationally-Guided Assignment of Unexpected Signals in the Raman Spectra of Uranyl Triperoxide Complexes. Inorganic Chemistry, 2017, 56, 1574-1580.	1.9	35
207	Lead-free double perovskites Cs₂InCuCl₆ and (CH₃NH₃)₂InCuCl₆: electronic, optical, and electrical properties. Nanoscale, 2019, 11, 11173-11182.	2.8	35
208	Influence of First and Second Coordination Environment on Structural Fe(II) Sites in MIL-101 for Câ€“H Bond Activation in Methane. ACS Catalysis, 2021, 11, 579-589.	5.5	35
209	Photocatalytic Biocidal Coatings Featuring Zr₆Ti₄-Based Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2022, 144, 12192-12201.	6.6	35
210	Spinâ€“orbit coupling within a two-component density functional theory approach: theory, implementation and first applications. Chemical Physics Letters, 2001, 344, 207-212.	1.2	34
211	Engineering Electrical Conductivity in Stable Zirconium-Based PCN-222 MOFs with Permanent Mesoporosity. Chemistry of Materials, 2020, 32, 6137-6149.	3.2	34
212	Quantum Chemical Characterization of the Bonding of N-Heterocyclic Carbenes to Cp2MI Compounds [M = Ce(III), U(III)]. Inorganic Chemistry, 2006, 45, 9442-9447.	1.9	33
213	Prediction of new inorganic molecules with quantum chemical methods. Theoretical Chemistry Accounts, 2006, 116, 307-315.	0.5	33
214	A Dichromium(II) Bis(Î·⁸-pentalene) Double-Sandwich Complex with a Spin Equilibrium: Synthetic, Structural, Magnetic, and Theoretical Studies. Organometallics, 2008, 27, 2013-2020.	1.1	33
215	Metalâ€“Organic Frameworks with Metalâ€“Catecholates for O₂/N₂ Separation. Journal of Physical Chemistry C, 2019, 123, 12935-12946.	1.5	33
216	Helicate Extension as a Route to Molecular Wires. Chemistry - A European Journal, 2008, 14, 7180-7185.	1.7	32

#	Article	IF	Citations
217	What Active Space Adequately Describes Oxygen Activation by a Late Transition Metal? CASPT2 and RASPT2 Applied to Intermediates from the Reaction of O2 with a Cu(I)-Î±-Ketocarboxylate. Journal of Chemical Theory and Computation, 2009, 5, 2967-2976.	2.3	32
218	Hopping Transport and Rectifying Behavior in Long Donorâ€“Acceptor Molecular Wires. Journal of Physical Chemistry C, 2014, 118, 26485-26497.	1.5	32
219	Predicting paramagnetic ¹H NMR chemical shifts and state-energy separations in spin-crossover hostâ€“guest systems. Physical Chemistry Chemical Physics, 2014, 16, 10620-10628.	1.3	32
220	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
221	Transition states of spin-forbidden reactions. Physical Chemistry Chemical Physics, 2018, 20, 4129-4136.	1.3	32
222	Infrared Spectra of the WH4(H2)4Complex in Solid Hydrogen. Journal of the American Chemical Society, 2008, 130, 1972-1978.	6.6	31
223	Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Nickel Atoms with Halomethanes. Organometallics, 2009, 28, 5623-5632.	1.1	31
224	Crystal structure of octabromoditechnetate(iii) and a multi-configurational quantum chemical study of the Î´â†'Î´* transition in quadruply bonded [M2X8]2â^' dimers (M = Tc, Re; X = Cl, Br). Dalton Transactions, 2009, , 5954.	1.6	31
225	Stretch Effects Induced by Molecular Strain on Weakening Ïƒ-Bonds: Molecular Design of Long-Lived Diradicals (Biradicals). Journal of Organic Chemistry, 2012, 77, 7612-7619.	1.7	31
226	Uranium and Thorium Hydride Complexes as Multielectron Reductants: A Combined Neutron Diffraction and Quantum Chemical Study. Inorganic Chemistry, 2012, 51, 3613-3624.	1.9	31
227	Ab Initio Extension of the AMOEBA Polarizable Force Field to Fe²⁺. Journal of Chemical Theory and Computation, 2013, 9, 3062-3071.	2.3	31
228	Oxidative Stretching of Metalâ€“Metal Bonds to Their Limits. Inorganic Chemistry, 2014, 53, 4777-4790.	1.9	31
229	Multiconfiguration Pair-Density Functional Theory Is Free From Delocalization Error. Journal of Physical Chemistry Letters, 2017, 8, 5616-5620.	2.1	31
230	Tuning the properties of metalâ€“organic framework nodes as supports of single-site iridium catalysts: node modification by atomic layer deposition of aluminium. Faraday Discussions, 2017, 201, 195-206.	1.6	30
231	MC-PDFT can calculate singletâ€“triplet splittings of organic diradicals. Journal of Chemical Physics, 2018, 148, 064108.	1.2	30
232	X-ray Absorption Spectroscopic and Computational Investigation of a Possible SÂ·Â·Â·S Interaction in the [Cu₃S₂]³⁺ Core. Journal of the American Chemical Society, 2011, 133, 17180-17191.	6.6	29
233	Efficient algorithm for multiconfiguration pair-density functional theory with application to the heterolytic dissociation energy of ferrocene. Journal of Chemical Physics, 2017, 146, 034101.	1.2	29
234	Theoretical Investigation of Plutonium-Based Single-Molecule Magnets. Inorganic Chemistry, 2018, 57, 8098-8105.	1.9	29

#	Article	IF	Citations
235	Enhanced Fe-Centered Redox Flexibility in Feâ€“Ti Heterobimetallic Complexes. Inorganic Chemistry, 2019, 58, 6199-6214.	1.9	29
236	Valence Ï€Ï€* Excitations in Benzene Studied by Multiconfiguration Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 75-81.	2.1	29
237	Experimental and Theoretical Evidence for U(C₆H₆) and Th(C₆H₆) Complexes. Journal of Physical Chemistry A, 2007, 111, 11996-12000.	1.1	28
238	Ab initio DFT study of Zâ€“E isomerization pathways of Nâ€“benzylideneaniline. Theoretical Chemistry Accounts, 2007, 118, 271-279.	0.5	28
239	Binding Motifs for Lanthanide Hydrides: A Combined Experimental and Theoretical Study of the MHx(H2)y Species (M = Laâ†’Gd; x = 1â†’4; y = 0â†’6). Journal of Physical Chemistry A, 2009, 113, 2446-2455.	1.1	28
240	Unravelling the Hydration Structure of ThX₄ (X = Br, Cl) Water Solutions by Molecular Dynamics Simulations and X-ray Absorption Spectroscopy. Journal of Physical Chemistry B, 2012, 116, 6465-6475.	1.2	28
241	Multi-state pair-density functional theory. Faraday Discussions, 2020, 224, 348-372.	1.6	28
242	Multiconfiguration Pair-Density Functional Theory. Annual Review of Physical Chemistry, 2021, 72, 541-564.	4.8	28
243	A theoretical study of the gas-phase chemi-ionization reaction between uranium and oxygen atoms. Journal of Chemical Physics, 2005, 122, 144317.	1.2	27
244	Early Excited State Dynamics of 6-Styryl-Substituted Pyrylium Salts Exhibiting Dual Fluorescence. Journal of Physical Chemistry A, 2006, 110, 9988-9994.	1.1	27
245	Uranium Oxo and Superoxo Cations Revealed Using Infrared Spectroscopy in the Gas Phase. Journal of Physical Chemistry Letters, 2011, 2, 1662-1666.	2.1	27
246	Uranyl Peroxide Cage Cluster Solubility in Water and the Role of the Electrical Double Layer. Inorganic Chemistry, 2017, 56, 1333-1339.	1.9	27
247	Multiconfiguration Pair-Density Functional Theory and Complete Active Space Second Order Perturbation Theory. Bond Dissociation Energies of FeC, NiC, FeS, NiS, FeSe, and NiSe. Journal of Physical Chemistry A, 2017, 121, 9392-9400.	1.1	27
248	State-interaction pair-density functional theory. Journal of Chemical Physics, 2018, 149, 024106.	1.2	27
249	Boosting Photoelectric Conductivity in Porphyrin-Based MOFs Incorporating C₆₀. Journal of Physical Chemistry C, 2020, 124, 1878-1887.	1.5	27
250	How useful are vibrational frequencies of isotopomeric O2 fragments for assessing local symmetry? Some simple systems and the vexing case of a galactose oxidase model. Journal of Biological Inorganic Chemistry, 2005, 10, 778-789.	1.1	26
251	Magnetic Coupling in a Tris-hydroxo-Bridged Chromium Dimer Occurs through Ligand Mediated Superexchange in Conjunction with Through-Space Coupling. Journal of the American Chemical Society, 2020, 142, 16644-16650.	6.6	26
252	Study of the MAu6(Mâ€‰=â€‰Cr, Mo, W) molecular species: A transition from halogenlike to hydrogenlike chemical behavior for gold. Physical Chemistry Chemical Physics, 2004, 6, 2904-2906.	1.3	25

#	Article	IF	Citations
253	Noble Gas Matrices May Change the Electronic Structure of Trapped Molecules: The UO₂(Ng)₄ [Ng=Ne, Ar] Case. Chemistry - A European Journal, 2010, 16, 12804-12807.	1.7	25
254	Computational Insights into Uranium Complexes Supported by Redox-Active Î±-Diimine Ligands. Inorganic Chemistry, 2012, 51, 2058-2064.	1.9	25
255	Infrared Spectra and Electronic Structure Calculations for NN Complexes with U, UN, and NUN in Solid Argon, Neon, and Nitrogen. Journal of Physical Chemistry A, 2014, 118, 5289-5303.	1.1	25
256	Quantum Chemical Characterization of Single Molecule Magnets Based on Uranium. Journal of Physical Chemistry A, 2017, 121, 1726-1733.	1.1	25
257	Hydrogen Atom or Proton Coupled Electron Transfer? Câ€“H Bond Activation by Transition-Metal Oxides. Journal of the American Chemical Society, 2019, 141, 14603-14611.	6.6	25
258	Infrared Spectra of ThH₂, ThH₄, and the Hydride Bridging ThH₄(H₂)_x (x = 1â^’4) Complexes in Solid Neon and Hydrogen. Journal of Physical Chemistry A, 2008, 112, 1754-1761.	1.1	24
259	Structure and bonding of group 4-nickel heterobimetallics supported by 2-(diphenylphosphino)pyrrolide ligands. Dalton Transactions, 2016, 45, 9892-9901.	1.6	24
260	Partial Fluorination as a Strategy for Crystal Engineering of Rubrene Derivatives. Crystal Growth and Design, 2017, 17, 643-658.	1.4	24
261	Origin of the Failure of Density Functional Theories in Predicting Inverted Singletâ€“Triplet Gaps. Journal of Physical Chemistry A, 2022, 126, 1378-1385.	1.1	24
262	Computational study of the cooperative effects of nitrogen and silicon atoms on the singletâ€“triplet energy spacing in 1,3â€diradicals and the reactivity of their singlet states. Journal of Physical Organic Chemistry, 2010, 23, 300-307.	0.9	23
263	Carbon dioxide reduction by mononuclear ruthenium polypyridyl complexes. Physical Chemistry Chemical Physics, 2011, 13, 19480.	1.3	23
264	Calculation of Heats of Formation for Zn Complexes: Comparison of Density Functional Theory, Second Order Perturbation Theory, Coupled-Cluster and Complete Active Space Methods. Journal of Chemical Theory and Computation, 2013, 9, 5277-5285.	2.3	23
265	Origin of the Strong Interaction between Polar Molecules and Copper(II) Paddle-Wheels in Metal Organic Frameworks. Journal of Physical Chemistry C, 2017, 121, 15135-15144.	1.5	23
266	Synthesis and characterization of tetrairidium clusters in the metal organic framework UiO-67: Catalyst for ethylene hydrogenation. Journal of Catalysis, 2020, 382, 165-172.	3.1	23
267	Cu[Ni(2,3-pyrazinedithiolate)₂] Metalâ€“Organic Framework for Electrocatalytic Hydrogen Evolution. ACS Applied Materials & Interfaces, 2021, 13, 34419-34427.	4.0	23
268	Torsional potential energy surfaces and vibrational levels in trans Stilbene. Journal of Molecular Structure, 2002, 612, 383-391.	1.8	22
269	Synthesis of a Uranyl Persulfide Complex and Quantum Chemical Studies of Formation and Topologies of Hypothetical Uranyl Persulfide Cage Clusters. Inorganic Chemistry, 2012, 51, 7801-7809.	1.9	22
270	Controversial electronic structures and energies of Fe2, ${m Fe}_2^ +$ Fe 2+, and ${m Fe}_2^ -$ Fe 2â^’ resolved by RASPT2 calculations. Journal of Chemical Physics, 2014, 141, 204309.	1.2	22

#	Article	IF	Citations
271	Uranylâ€“Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. Journal of Physical Chemistry C, 2014, 118, 24730-24740.	1.5	22
272	Multiconfiguration Pair-Density Functional Theory Spectral Calculations Are Stable to Adding Diffuse Basis Functions. Journal of Physical Chemistry Letters, 2015, 6, 4184-4188.	2.1	22
273	Pocket and antipocket conformations for the CH4@C84 endohedral fullerene. International Journal of Quantum Chemistry, 2007, 107, 1162-1169.	1.0	21
274	The chemiionization reactions Ce + O and Ce + O₂: Assignment of the observed chemielectron bands. International Journal of Quantum Chemistry, 2009, 109, 2068-2079.	1.0	21
275	Synthesis and Characterization of the First 2â€‰D Neptunyl Structure Stabilized by Sideâ€on Cationâ€“Cation Interactions. Chemistry - A European Journal, 2013, 19, 2937-2941.	1.7	21
276	Infrared Spectra and Electronic Structure Calculations for the NUN(NN)_{1â€“5} and NU(NN)_{1â€“6} Complexes in Solid Argon. Inorganic Chemistry, 2013, 52, 9989-9993.	1.9	21
277	Hydration properties of Cm(iii) and Th(iv) combining coordination free energy profiles with electronic structure analysis. Physical Chemistry Chemical Physics, 2014, 16, 5824.	1.3	21
278	CO₂ Adsorption in M-IRMOF-10 (M = Mg, Ca, Fe, Cu, Zn, Ge, Sr, Cd, Sn, Ba). Journal of Physical Chemistry C, 2016, 120, 12819-12830.	1.5	21
279	A New Mixing of Nonlocal Exchange and Nonlocal Correlation with Multiconfiguration Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2020, 11, 10158-10163.	2.1	21
280	Correlating Electronic Structure and Magnetic Anisotropy in Actinide Complexes [An(COT)₂], An^{III/IV} = U, Np, and Pu. Inorganic Chemistry, 2020, 59, 6815-6825.	1.9	21
281	Sulfur Vacancy Clustering and Its Impact on Electronic Properties in Pyrite FeS₂. Chemistry of Materials, 2020, 32, 4820-4831.	3.2	21
282	Precise Control of Cu Nanoparticle Size and Catalytic Activity through Pore Templating in Zr Metalâ€“Organic Frameworks. Chemistry of Materials, 2020, 32, 3078-3086.	3.2	21
283	Site Densities, Rates, and Mechanism of Stable Ni/UiO-66 Ethylene Oligomerization Catalysts. Journal of the American Chemical Society, 2021, 143, 20274-20280.	6.6	21
284	The gas-phase chemiionization reaction between samarium and oxygen atoms: A theoretical study. Journal of Chemical Physics, 2004, 120, 9998-10001.	1.2	20
285	Can Multiconfigurational Self-Consistent Field Theory and Density Functional Theory Correctly Predict the Ground State of Metalâ€“Metal-Bonded Complexes?. Journal of Chemical Theory and Computation, 2015, 11, 4093-4101.	2.3	20
286	Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. Journal of Physical Chemistry C, 2017, 121, 10463-10469.	1.5	20
287	Systematic design of active spaces for multi-reference calculations of singletâ€“triplet gaps of organic diradicals, with benchmarks against doubly electron-attached coupled-cluster data. Journal of Chemical Physics, 2017, 147, 164120.	1.2	20
288	Active Space Dependence in Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 660-669.	2.3	20

#	Article	IF	Citations
289	Bioinspired Nickel Complexes Supported by an Iron Metalloligand. Inorganic Chemistry, 2020, 59, 14251-14262.	1.9	20
290	Excited States of Crystalline Point Defects with Multireference Density Matrix Embedding Theory. Journal of Physical Chemistry Letters, 2021, 12, 11688-11694.	2.1	20
291	Theoretical Study of the Gas-Phase Chemiionization Reactions La + O and La + O₂. Journal of Physical Chemistry A, 2008, 112, 7825-7830.	1.1	19
292	Infrared Spectra of Small Insertion and Methylidene Complexes in Reactions of Laser-Ablated Palladium Atoms with Halomethanes. Organometallics, 2009, 28, 6871-6879.	1.1	19
293	Structural, Spectroscopic, and Multiconfigurational Quantum Chemical Investigations of the Electron-Rich Metalâ^'Metal Triple-Bonded Tc₂X₄(PMe₃)₄ (X = Cl, Br) Complexes. Inorganic Chemistry, 2010, 49, 6646-6654.	1.9	19
294	Volatilities of Actinide and Lanthanide N,N-Dimethylaminodiboranate Chemical Vapor Deposition Precursors: A DFT Study. Journal of Physical Chemistry C, 2012, 116, 23194-23200.	1.5	19
295	Variational Localized Active Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2020, 16, 4923-4937.	2.3	19
296	A Ranked-Orbital Approach to Select Active Spaces for High-Throughput Multireference Computation. Journal of Chemical Theory and Computation, 2021, 17, 2817-2831.	2.3	19
297	Using Redox-Active Ligands to Generate Actinide Ligand Radical Species. Inorganic Chemistry, 2021, 60, 15242-15252.	1.9	19
298	Quantum Monte Carlo study of the ground state and low-lying excited states of the scandium dimer. Journal of Chemical Physics, 2008, 128, 194315.	1.2	18
299	Multiconfiguration pair-density functional theory investigation of the electronic spectrum of MnO4â^'. Journal of Chemical Physics, 2018, 148, 124305.	1.2	18
300	Introduction: Computational Design of Catalysts from Molecules to Materials. Chemical Reviews, 2019, 119, 6507-6508.	23.0	18
301	Role of Triplet States in the Photodynamics of Aniline. Journal of the American Chemical Society, 2021, 143, 5878-5889.	6.6	18
302	Electronic structure of strongly correlated systems: recent developments in multiconfiguration pair-density functional theory and multiconfiguration nonclassical-energy functional theory. Chemical Science, 2022, 13, 7685-7706.	3.7	18
303	A theoretical study of AmO_nand CmO_n(n = 1, 2). Physical Chemistry Chemical Physics, 2008, 10, 1114-1117.	1.3	17
304	Preferential Location of Germanium in the UTL and IPC-2a Zeolites. Journal of Physical Chemistry C, 2014, 118, 26939-26946.	1.5	17
305	Tuning the Conductivity of Hexa-Zirconium(IV) Metalâ€"Organic Frameworks by Encapsulating Heterofullerenes. Chemistry of Materials, 2021, 33, 1182-1189.	3.2	17
306	Modeling Metal Influence on the Gate Opening in ZIF-8 Materials. Chemistry of Materials, 2021, 33, 4465-4473.	3.2	17

#	Article	IF	Citations
307	Quantum-classical hybrid algorithm for the simulation of all-electron correlation. Journal of Chemical Physics, 2021, 155, 244106.	1.2	17
308	MAGIC: An integrated computational environment for the modelling of heavy-atom chemistry. International Reviews in Physical Chemistry, 2000, 19, 327-362.	0.9	16
309	U and P4Reaction Products: A Quantum Chemical and Matrix Isolation Spectroscopic Investigation. Inorganic Chemistry, 2010, 49, 9230-9235.	1.9	16
310	Thorium and Uranium Carbide Cluster Cations in the Gas Phase: Similarities and Differences between Thorium and Uranium. Inorganic Chemistry, 2013, 52, 10968-10975.	1.9	16
311	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
312	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. Catalysis Today, 2018, 312, 149-157.	2.2	16
313	Combined quantum mechanical and molecular mechanical method for metalâ€“organic frameworks: proton topologies of NU-1000. Physical Chemistry Chemical Physics, 2018, 20, 1778-1786.	1.3	16
314	Air Separation by Catechol-Ligated Transition Metals: A Quantum Chemical Screening. Journal of Physical Chemistry C, 2018, 122, 22345-22351.	1.5	16
315	Intramolecular Charge Transfer and Local Excitation in Organic Fluorescent Photoredox Catalysts Explained by RASCI-PDFT. Journal of Physical Chemistry C, 2018, 122, 12061-12070.	1.5	16
316	Multiple Bonds in Uraniumâ€“Transition Metal Complexes. Inorganic Chemistry, 2019, 58, 10139-10147.	1.9	16
317	Full Correlation in a Multiconfigurational Study of Bimetallic Clusters: Restricted Active Space Pair-Density Functional Theory Study of [2Feâ€“2S] Systems. Journal of Physical Chemistry C, 2019, 123, 11899-11907.	1.5	16
318	Assessment of MC-PDFT Excitation Energies for a Set of QM/MM Models of Rhodopsins. Journal of Chemical Theory and Computation, 2019, 15, 1915-1923.	2.3	16
319	Analytic gradients for state-averaged multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2020, 153, 014106.	1.2	16
320	Linker Contribution toward Stability of Metalâ€“Organic Frameworks under Ionizing Radiation. Chemistry of Materials, 2021, 33, 9285-9294.	3.2	16
321	Full configuration interaction study of the ground state of closed-shell cyclicPPP polyenes. International Journal of Quantum Chemistry, 1994, 51, 13-25.	1.0	15
322	Structural and Electronic Effects on the Properties of Fe₂(dobdc) upon Oxidation with N₂O. Inorganic Chemistry, 2016, 55, 4924-4934.	1.9	15
323	Nature of the 1¹B_u and 2¹A_g Excited States of Butadiene and the Goldilocks Principle of Basis Set Diffuseness. Journal of Chemical Theory and Computation, 2019, 15, 4591-4601.	2.3	15
324	Isomerization and Selective Hydrogenation of Propyne: Screening of Metalâ€“Organic Frameworks Modified by Atomic Layer Deposition. Journal of the American Chemical Society, 2020, 142, 20380-20389.	6.6	15

#	Article	IF	Citations
325	Machine-Learned Energy Functionals for Multiconfigurational Wave Functions. Journal of Physical Chemistry Letters, 2021, 12, 7761-7767.	2.1	15
326	Metalâ^'Polyhydride Molecules Are Compact Inside a Fullerene Cage. Journal of Chemical Theory and Computation, 2005, 1, 1172-1175.	2.3	14
327	Quantum Chemical Characterization of Low-Energy States of Calicene in the Gas Phase and in Solution. Journal of Organic Chemistry, 2007, 72, 2823-2831.	1.7	14
328	Matrix Infrared Spectroscopic and Computational Investigation of Late Lanthanide Metal Hydride Species MH_x(H₂)_y (M = Tbâ^'Lu, x = 1â^'4, y) Tj ET Q q 0 0 0 rg BT /Ove	1.4	14
329	Catalysis in MOFs: general discussion. Faraday Discussions, 2017, 201, 369-394.	1.6	14
330	Multilink F* Method for Combined Quantum Mechanical and Molecular Mechanical Calculations of Complex Systems. Journal of Chemical Theory and Computation, 2019, 15, 4208-4217.	2.3	14
331	Valence and Structure Isomerism of Al2FeO4+: Synergy of Spectroscopy and Quantum Chemistry. Journal of the American Chemical Society, 2020, 142, 18050-18059.	6.6	14
332	Structure and Reactivity of Single-Site Vanadium Catalysts Supported on Metalâ€“Organic Frameworks. ACS Catalysis, 2020, 10, 10051-10059.	5.5	14
333	Transition Metal Spin-State Energetics by MC-PDFT with High Local Exchange. Journal of Physical Chemistry A, 2020, 124, 1187-1195.	1.1	14
334	Leveraging Nitrogen Linkages in the Formation of a Porous Thoriumâ€“Organic Nanotube Suitable for Iodine Capture. Inorganic Chemistry, 2022, 61, 9480-9492.	1.9	14
335	New Group 2 Chemistry:â€‰ A Multiple Bariumâ^'Nitrogen Bond in the CsNBa Molecule. Journal of the American Chemical Society, 2002, 124, 8757-8761.	6.6	13
336	The study of actinide chemistry with multiconfigurational quantum chemical methods. International Journal of Quantum Chemistry, 2011, 111, 3302-3306.	1.0	13
337	What Is the Preferred Conformation of Phosphatidylserineâ€“Copper(II) Complexes? A Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry B, 2016, 120, 12883-12889.	1.2	13
338	Redox Pairs of Diiron and Ironâ€“Cobalt Complexes with High-Spin Ground States. Inorganic Chemistry, 2016, 55, 9725-9735.	1.9	13
339	On-Top Pair Density as a Measure of Leftâ€“Right Correlation in Bond Breaking. Journal of Physical Chemistry A, 2017, 121, 5540-5547.	1.1	13
340	Excitation spectra of retinal by multiconfiguration pair-density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 7265-7276.	1.3	13
341	Extended separated-pair approximation for transition metal potential energy curves. Journal of Chemical Physics, 2020, 152, 124118.	1.2	13
342	First emission studies of Tc2X82â^' systems (X = Cl, Br). Dalton Transactions, 2010, 39, 11322.	1.6	12

#	Article	IF	Citations
343	Elucidation of Tetraboric Acid with a New Borate Fundamental Building Block in a Chiral Uranyl Fluoroborate. Inorganic Chemistry, 2012, 51, 11211-11213.	1.9	12
344	Multi-configurational quantum chemical studies of the Tc2X8nâ^' (X = Cl, Br; n = 2, 3) anions. Crystallographic structure of octabromoditechnetate(3â^'). Dalton Transactions, 2012, 41, 2869.	1.6	12
345	Reactivity of lanthanoid mono-cations with ammonia: A combined inductively coupled plasma mass spectrometry and computational investigation. International Journal of Mass Spectrometry, 2013, 334, 27-37.	0.7	12
346	Influence of Copper Oxidation State on the Bonding and Electronic Structure of Cobaltâ€"Copper Complexes. Inorganic Chemistry, 2015, 54, 11330-11338.	1.9	12
347	Methane functionalization by an Ir(III) catalyst supported on a metalâ€"organic framework: an alternative explanation of steric confinement effects. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	12
348	State-interaction pair density functional theory for locally avoided crossings of potential energy surfaces in methylamine. Physical Chemistry Chemical Physics, 2019, 21, 13486-13493.	1.3	12
349	State-Interaction Pair-Density Functional Theory Can Accurately Describe a Spiro Mixed Valence Compound. Journal of Physical Chemistry A, 2019, 123, 2100-2106.	1.1	12
350	Weak Interactions in Alkaline Earth Metal Dimers by Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 799-805.	2.1	12
351	Multiconfiguration Density-Coherence Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2775-2782.	2.3	12
352	Active Learning Configuration Interaction for Excited-State Calculations of Polycyclic Aromatic Hydrocarbons. Journal of Chemical Theory and Computation, 2021, 17, 7518-7530.	2.3	12
353	The Characterisation of Molecular Alkali-Metal Azides. Chemistry - A European Journal, 2006, 12, 3580-3586.	1.7	11
354	Carbon Dioxide Reduction Catalyzed by Dinuclear Ruthenium Polypyridyl Complexes. ChemCatChem, 2013, 5, 3897-3903.	1.8	11
355	Calculation of Chemical Reaction Barrier Heights by Multiconfiguration Pair-Density Functional Theory with Correlated Participating Orbitals. Journal of Physical Chemistry A, 2019, 123, 9809-9817.	1.1	11
356	Spin-State Ordering in Metal-Based Compounds Using the Localized Active Space Self-Consistent Field Method. Journal of Physical Chemistry Letters, 2019, 10, 5507-5513.	2.1	11
357	The Role of the Organic Solvent Polarity in Isolating Uranyl Peroxide Capsule Fragments. Inorganic Chemistry, 2020, 59, 1633-1641.	1.9	11
358	Thermal Treatment Effect on CO and NO Adsorption on Fe(II) and Fe(III) Species in Fe₃O-Based MIL-Type Metalâ€"Organic Frameworks: A Density Functional Theory Study. Inorganic Chemistry, 2021, 60, 11813-11824.	1.9	11
359	Metalâ€"Metal Bonding in Actinide Dimers: U₂ and U₂^{â€"}. Journal of the American Chemical Society, 2021, 143, 17023-17028.	6.6	11
360	Multiconfiguration pair-density functional theory for doublet excitation energies and excited state geometries: the excited states of CN. Physical Chemistry Chemical Physics, 2017, 19, 30089-30096.	1.3	10

#	Article	IF	Citations
361	Resolving Confined ⁷Li Dynamics of Uranyl Peroxide Capsule U₂₄. Inorganic Chemistry, 2018, 57, 5514-5525.	1.9	10
362	Synthesis and Characterization of Electron-Deficient Asymmetrically Substituted Diarylindenotetracenes. Journal of Organic Chemistry, 2018, 83, 1828-1841.	1.7	10
363	Parametrization of Combined Quantum Mechanical and Molecular Mechanical Methods: Bond-Tuned Link Atoms. Molecules, 2018, 23, 1309.	1.7	10
364	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
365	Multiconfiguration Pair-Density Functional Theory Calculations of Iron(II) Porphyrin: Effects of Hybrid Pair-Density Functionals and Expanded RAS and DMRG Active Spaces on Spin-State Orderings. Journal of Physical Chemistry A, 2022, 126, 3957-3963.	1.1	10
366	A theoretical study of plutonium diketone complexes for solvent extraction. Chemical Physics, 2000, 252, 47-55.	0.9	9
367	A Trigonal-Prismatic Hexanuclear Technetium(II) Bromide Cluster: Solid-State Synthesis and Crystallographic and Electronic Structure. Inorganic Chemistry, 2013, 52, 5660-5662.	1.9	9
368	AMOEBA force field parameterization of the azabenzenes. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	9
369	Pushing Single-Oxygen-Atom-Bridged Bimetallic Systems to the Right: A Cryptand-Encapsulated Coâ€“Oâ€“Co Unit. Journal of the American Chemical Society, 2015, 137, 15354-15357.	6.6	9
370	Electronic, magnetic and photophysical properties of MOFs and COFs: general discussion. Faraday Discussions, 2017, 201, 87-99.	1.6	9
371	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057.	1.1	9
372	Experimental and Quantum Mechanical Characterization of an Oxygenâ€Bridged Plutonium(IV) Dimer. Chemistry - A European Journal, 2020, 26, 8115-8120.	1.7	9
373	Metal-organic framework supported single-site nickel catalysts for butene dimerization. Journal of Catalysis, 2022, 413, 176-183.	3.1	9
374	Theoretic study of the electronic spectra of neutral and cationic PaO and PaO2. Structural Chemistry, 2013, 24, 917-925.	1.0	8
375	Formal Nickelate(â˜I) Complexes Supported by Groupâ€…13 Ions. Angewandte Chemie, 2018, 130, 7941-7945.	1.6	8
376	Multireference Methods for Calculating the Dissociation Enthalpy of Tetrahedral P4 to Two P2. Journal of Physical Chemistry A, 2018, 122, 5742-5749.	1.1	8
377	Analytic gradients for multiconfiguration pair-density functional theory with density fitting: Development and application to geometry optimization in the ground and excited states. Journal of Chemical Physics, 2021, 154, 074108.	1.2	8
378	Nonadiabatic Molecular Dynamics by Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 614-622.	2.3	8

#	Article	IF	Citations
379	DFT Study on the Catalytic Activity of ALD-Grown Diiron Oxide Nanoclusters for Partial Oxidation of Methane to Methanol. Journal of Physical Chemistry A, 2020, 124, 1580-1592.	1.1	7
380	Multiconfiguration Pair-Density Functional Theory for Transition Metal Silicide Bond Dissociation Energies, Bond Lengths, and State Orderings. Molecules, 2021, 26, 2881.	1.7	7
381	Calculation of the Zeeman Effect for Transition-Metal Complexes by Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 5050-5063.	2.3	7
382	Dipole Moment Calculations Using Multiconfiguration Pair-Density Functional Theory and Hybrid Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 7586-7601.	2.3	7
383	Exact-Two-Component Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2947-2954.	2.3	7
384	Complete active-space configuration interaction with optimized orbitals: Application to Li2. International Journal of Quantum Chemistry, 1995, 55, 277-280.	1.0	6
385	New directions in gas sorption and separation with MOFs: general discussion. Faraday Discussions, 2017, 201, 175-194.	1.6	6
386	Neptunyl Peroxide Chemistry: Synthesis and Spectroscopic Characterization of a Neptunyl Triperoxide Compound, Ca₂[NpO₂(O₂)₃]Â·9H₂O. Inorganic Chemistry, 2019, 58, 12264-12271.	1.9	6
387	Evidence of Alpha Radiolysis in the Formation of a Californium Nitrate Complex. Chemistry - A European Journal, 2020, 26, 8885-8888.	1.7	6
388	Localized Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2843-2851.	2.3	6
389	Multireference Methods are Realistic and Useful Tools for Modeling Catalysis. Israel Journal of Chemistry, 2022, 62, .	1.0	6
390	Zero-Field Splitting Calculations by Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2199-2207.	2.3	6
391	One-electron bonds in copperâ€“aluminum and copperâ€“gallium complexes. Chemical Science, 2022, 13, 6525-6531.	3.7	6
392	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
393	A theoretical study of the 21Agâ†•11Agtwo-photon transition and its vibronic band intrans-stilbene. Molecular Physics, 2002, 100, 1791-1796.	0.8	5
394	The electronic spectra of 2-(2â€²-hydroxybenzoyl)pyrrole and 2-(2â€²-methoxybenzoyl)pyrrole: a theoretical study. Journal of Physical Organic Chemistry, 2005, 18, 1099-1106.	0.9	5
395	Theoretical prediction of linear free energy relationships using proton nucleomers. Journal of Physical Organic Chemistry, 2008, 21, 136-145.	0.9	5
396	Molecular and electronic structure of Tc2(O2CCH3)2Cl4 studied by multiconfigurational quantum chemical methods. Polyhedron, 2014, 70, 144-147.	1.0	5

#	Article	IF	Citations
397	A Decade of Dinuclear Technetium Complexes with Multiple Metal-Metal Bonds. European Journal of Inorganic Chemistry, 2014, 2014, 4484-4495.	1.0	5
398	A Precise and Scalable Post-Modification of Mesoporous Metal-Organic Framework NU-1000 Via Atomic Layer Deposition. ECS Transactions, 2016, 75, 93-99.	0.3	5
399	The effects of active site and support on hydrogen elimination over transition-metal-functionalized yttria-decorated metalâ€“organic frameworks. Catalysis Science and Technology, 2019, 9, 7003-7015.	2.1	5
400	Importance of Lattice Constants in QM/MM Calculations on Metalâ€“Organic Frameworks. Journal of Physical Chemistry B, 2021, 125, 5786-5793.	1.2	5
401	Singlet-to-Triplet Spin Transitions Facilitate Selective 1-Butene Formation during Ethylene Dimerization in Ni(II)-MFU-4l. Journal of Physical Chemistry C, 2021, 125, 22036-22043.	1.5	5
402	Electron transitions in a Ce(iii)-catecholate metalâ€“organic framework. Chemical Communications, 2022, 58, 525-528.	2.2	5
403	Investigating the effect of metal nuclearity on activity for ethylene hydrogenation by metal-organic-framework-supported oxy-Ni(II) catalysts. Journal of Catalysis, 2022, 407, 162-173.	3.1	5
404	Synthesis and redox reactivity of a phosphine-ligated dichromium paddlewheel. Inorganica Chimica Acta, 2015, 424, 336-344.	1.2	4
405	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	1.6	4
406	Correction to â€œTuning Zr₆ Metal-Organic Framework (MOF) Nodes as Catalyst Supports: Site Densities and Electron-Donor Properties Influence Molecular Iridium Complexes as Ethylene Conversion Catalystsâ€• ACS Catalysis, 2018, 8, 2364-2364.	5.5	3
407	Scaling exchange and correlation in the on-top density functional of multiconfiguration pair-density functional theory: effect on electronic excitation energies and bond energies. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	3
408	Comment on â€œFe2: As simple as a Herculean labour. Neutral (Fe2), cationic (Fe2+), and anionic (Fe2â˜) speciesâ€•[J. Chem. Phys. 142, 244304 (2015)]. Journal of Chemical Physics, 2016, 144, 027101.	1.2	2
409	Correction to â€œComputationally Guided Discovery of Catalytic Cobalt-Decorated Metalâ€“Organic Framework for Ethylene Dimerizationâ€• Journal of Physical Chemistry C, 2017, 121, 11975-11975.	1.5	2
410	On-Top Ratio for Atoms and Molecules. Journal of Physical Chemistry A, 2019, 123, 8294-8304.	1.1	2
411	Intrastrand Photolesion Formation in Thio-Substituted DNA: A Case Study Including Single-Reference and Multireference Methods. Journal of Physical Chemistry A, 2020, 124, 10422-10433.	1.1	2
412	Correction to â€œCatechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separationâ€• Journal of Physical Chemistry C, 2017, 121, 20553-20553.	1.5	1
413	Unsaturated Sulfur Crown Ethers Can Extract Mercury(II) and Show Promise for Future Copernicium(II) Studies: A Combined Experimental and Computational Study. Inorganic Chemistry, 2022, 61, 807-817.	1.9	1
414	Quantum Chemical Calculations Show that the Uranium Molecule U2 Has a Quintuple Bond.. ChemInform, 2005, 36, no.	0.1	0

#	Article	IF	Citations
415	Physical Chemistry at the University of Geneva. Chimia, 2009, 63, 807.	0.3	0
416	Preface for the Forum on Insights into Spectroscopy and Reactivity from Electronic Structure Theory. Inorganic Chemistry, 2014, 53, 6357-6360.	1.9	0
417	MOF. , 2016, , .		0
418	The role of cations in uranyl nanocluster association: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 1847-1854.	1.3	0
419	MODELLING METALâ€“ORGANIC FRAMEWORKS AND OTHER FUNCTIONAL MATERIALS WITH ELECTRONIC STRUCTURE THEORIES. , 2021, , .		0
420	BjÃ¶rn O. Roos. , 2006, , 1272-1278.		0
421	Multiple bonds in diactinide compounds. , 2006, , 890-890.		0
422	On the nature of the metal-metal multiple bond. , 2006, , 6-22.		0