Laura Gagliardi

List of Publications by Year
in descending order

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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	Nonadiabatic Molecular Dynamics by Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 614-622.	2.3	8
2	Electron transitions in a Ce(iii)-catecholate metalâ€“organic framework. Chemical Communications, 2022, 58, 525-528.	2.2	5
3	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
4	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
5	Multireference Methods are Realistic and Useful Tools for Modeling Catalysis. Israel Journal of Chemistry, 2022, 62, .	1.0	6
6	Zero-Field Splitting Calculations by Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2199-2207.	2.3	6
7	Exact-Two-Component Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 2947-2954.	2.3	7
8	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
9	One-electron bonds in copperâ€“aluminum and copperâ€“gallium complexes. Chemical Science, 2022, 13, 6525-6531.	3.7	6
10	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
11	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
12	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
13	Metal-organic framework supported single-site nickel catalysts for butene dimerization. Journal of Catalysis, 2022, 413, 176-183.	3.1	9
14	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
15	Photocatalytic Biocidal Coatings Featuring Zr₆Ti₄-Based Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2022, 144, 12192-12201.	6.6	35
16	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
17	Tuning the Conductivity of Hexa-Zirconium(IV) Metalâ€“Organic Frameworks by Encapsulating Heterofullerenes. Chemistry of Materials, 2021, 33, 1182-1189.	3.2	17
18	Localized Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2843-2851.	2.3	6

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19	Multiconfiguration Density-Coherence Functional Theory. Journal of Chemical Theory and Computation, 2021, 17, 2775-2782.	2.3	12
20	Role of Triplet States in the Photodynamics of Aniline. Journal of the American Chemical Society, 2021, 143, 5878-5889.	6.6	18
21	Modeling Metal Influence on the Gate Opening in ZIF-8 Materials. Chemistry of Materials, 2021, 33, 4465-4473.	3.2	17
22	Multiconfiguration Pair-Density Functional Theory. Annual Review of Physical Chemistry, 2021, 72, 541-564.	4.8	28
23	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
24	Multiconfiguration Pair-Density Functional Theory for Transition Metal Silicide Bond Dissociation Energies, Bond Lengths, and State Orderings. Molecules, 2021, 26, 2881.	1.7	7
25	Importance of Lattice Constants in QM/MM Calculations on Metalâ€“Organic Frameworks. Journal of Physical Chemistry B, 2021, 125, 5786-5793.	1.2	5
26	Machine learning the quantum-chemical properties of metalâ€“organic frameworks for accelerated materials discovery. Matter, 2021, 4, 1578-1597.	5.0	170
27	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
28	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
29	Cu[Ni(2,3-pyrazinedithiolate)₂] Metalâ€“Organic Framework for Electrocatalytic Hydrogen Evolution. ACS Applied Materials & Interfaces, 2021, 13, 34419-34427.	4.0	23
30	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
31	Machine-Learned Energy Functionals for Multiconfigurational Wave Functions. Journal of Physical Chemistry Letters, 2021, 12, 7761-7767.	2.1	15
32	Using Redox-Active Ligands to Generate Actinide Ligand Radical Species. Inorganic Chemistry, 2021, 60, 15242-15252.	1.9	19
33	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
34	MODELLING METALâ€“ORGANIC FRAMEWORKS AND OTHER FUNCTIONAL MATERIALS WITH ELECTRONIC STRUCTURE THEORIES. , 2021, , .		0
35	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
36	Evolution of water structures in metal-organic frameworks for improved atmospheric water harvesting. Science, 2021, 374, 454-459.	6.0	281

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37	Metalâ€“Metal Bonding in Actinide Dimers: U₂ and U₂^{â€“}. Journal of the American Chemical Society, 2021, 143, 17023-17028.	6.6	11
38	Linker Contribution toward Stability of Metalâ€“Organic Frameworks under Ionizing Radiation. Chemistry of Materials, 2021, 33, 9285-9294.	3.2	16
39	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
40	Excited States of Crystalline Point Defects with Multireference Density Matrix Embedding Theory. Journal of Physical Chemistry Letters, 2021, 12, 11688-11694.	2.1	20
41	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
42	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
43	Quantum-classical hybrid algorithm for the simulation of all-electron correlation. Journal of Chemical Physics, 2021, 155, 244106.	1.2	17
44	Boosting Photoelectric Conductivity in Porphyrin-Based MOFs Incorporating C₆₀. Journal of Physical Chemistry C, 2020, 124, 1878-1887.	1.5	27
45	The role of cations in uranyl nanocluster association: a molecular dynamics study. Physical Chemistry Chemical Physics, 2020, 22, 1847-1854.	1.3	0
46	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
47	Periodic Electronic Structure Calculations with the Density Matrix Embedding Theory. Journal of Chemical Theory and Computation, 2020, 16, 130-140.	2.3	40
48	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
49	Analytic gradients for state-averaged multiconfiguration pair-density functional theory. Journal of Chemical Physics, 2020, 153, 014106.	1.2	16
50	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
51	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
52	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
53	Structure and Reactivity of Single-Site Vanadium Catalysts Supported on Metalâ€“Organic Frameworks. ACS Catalysis, 2020, 10, 10051-10059.	5.5	14
54	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

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55	Using natureâ€™s blueprint to expand catalysis with Earth-abundant metals. Science, 2020, 369, .	6.0	306
56	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
57	Bioinspired Nickel Complexes Supported by an Iron Metalloligand. Inorganic Chemistry, 2020, 59, 14251-14262.	1.9	20
58	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
59	Multi-state pair-density functional theory. Faraday Discussions, 2020, 224, 348-372.	1.6	28
60	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	1.2	425
61	Sulfur Vacancy Clustering and Its Impact on Electronic Properties in Pyrite FeS₂. Chemistry of Materials, 2020, 32, 4820-4831.	3.2	21
62	Variational Localized Active Space Self-Consistent Field Method. Journal of Chemical Theory and Computation, 2020, 16, 4923-4937.	2.3	19
63	Negative cooperativity upon hydrogen bond-stabilized O2 adsorption in a redox-active metalâ€“organic framework. Nature Communications, 2020, 11, 3087.	5.8	36
64	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
65	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
66	Extended separated-pair approximation for transition metal potential energy curves. Journal of Chemical Physics, 2020, 152, 124118.	1.2	13
67	Experimental and Quantum Mechanical Characterization of an Oxygenâ€Bridged Plutonium(IV) Dimer. Chemistry - A European Journal, 2020, 26, 8115-8120.	1.7	9
68	Engineering Electrical Conductivity in Stable Zirconium-Based PCN-222 MOFs with Permanent Mesoporosity. Chemistry of Materials, 2020, 32, 6137-6149.	3.2	34
69	Standard Practices of Reticular Chemistry. ACS Central Science, 2020, 6, 1255-1273.	5.3	142
70	Actinide 2-metallabiphenylenes that satisfy HÃ¼ckelâ€™s rule. Nature, 2020, 578, 563-567.	13.7	43
71	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
72	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

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73	The Role of the Organic Solvent Polarity in Isolating Uranyl Peroxide Capsule Fragments. Inorganic Chemistry, 2020, 59, 1633-1641.	1.9	11
74	Transition Metal Spin-State Energetics by MC-PDFT with High Local Exchange. Journal of Physical Chemistry A, 2020, 124, 1187-1195.	1.1	14
75	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
76	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
77	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
78	Evidence of Alpha Radiolysis in the Formation of a Californium Nitrate Complex. Chemistry - A European Journal, 2020, 26, 8885-8888.	1.7	6
79	Beyond Density Functional Theory: The Multiconfigurational Approach To Model Heterogeneous Catalysis. ACS Catalysis, 2019, 9, 8481-8502.	5.5	75
80	Multiple Bonds in Uraniumâ€“Transition Metal Complexes. Inorganic Chemistry, 2019, 58, 10139-10147.	1.9	16
81	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
82	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
83	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
84	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
85	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
86	Neptunyl Peroxide Chemistry: Synthesis and Spectroscopic Characterization of a Neptunyl Triperoxide Compound, Ca₂[NpO₂(O₂)₃]·9H₂O. Inorganic Chemistry, 2019, 58, 12264-12271.	1.9	6
87	On-Top Ratio for Atoms and Molecules. Journal of Physical Chemistry A, 2019, 123, 8294-8304.	1.1	2
88	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
89	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
90	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	2.3	661

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91	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
92	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
93	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
94	Introduction: Computational Design of Catalysts from Molecules to Materials. Chemical Reviews, 2019, 119, 6507-6508.	23.0	18
95	Lead-free double perovskites Cs₂InCuCl₆ and (CH₃NH₃)₂InCuCl₆: electronic, optical, and electrical properties. Nanoscale, 2019, 11, 11173-11182.	2.8	35
96	Metalâ€“Organic Frameworks with Metalâ€“Catecholates for O₂/N₂ Separation. Journal of Physical Chemistry C, 2019, 123, 12935-12946.	1.5	33
97	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
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	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
100	Enhanced Fe-Centered Redox Flexibility in Feâ€“Ti Heterobimetallic Complexes. Inorganic Chemistry, 2019, 58, 6199-6214.	1.9	29
101	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
102	Weak Interactions in Alkaline Earth Metal Dimers by Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 799-805.	2.1	12
103	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
104	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
105	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
106	A Multireference Ab Initio Study of the Diradical Isomers of Pyrazine. Journal of Physical Chemistry A, 2019, 123, 2049-2057.	1.1	9
107	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
108	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

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109	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
110	Metal doping in cerium metal-organic frameworks for visible-response water splitting photocatalysts. Journal of Chemical Physics, 2019, 150, 041701.	1.2	59
111	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
112	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
113	Valence ÏЄЇ€* Excitations in Benzene Studied by Multiconfiguration Pair-Density Functional Theory. Journal of Physical Chemistry Letters, 2019, 10, 75-81.	2.1	29
114	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
115	Catalytic descriptors and electronic properties of single-site catalysts for ethene dimerization to 1-butene. Catalysis Today, 2018, 312, 149-157.	2.2	16
116	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
117	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
118	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
119	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
120	Resolving Confined ⁷Li Dynamics of Uranyl Peroxide Capsule U₂₄. Inorganic Chemistry, 2018, 57, 5514-5525.	1.9	10
121	Multiconfiguration pair-density functional theory investigation of the electronic spectrum of MnO4â^'. Journal of Chemical Physics, 2018, 148, 124305.	1.2	18
122	Self-Interaction Error in Density Functional Theory: An Appraisal. Journal of Physical Chemistry Letters, 2018, 9, 2353-2358.	2.1	131
123	Rationalizing the Reactivity of Bimetallic Molecular Catalysts for CO₂ Hydrogenation. ACS Catalysis, 2018, 8, 4955-4968.	5.5	39
124	MC-PDFT can calculate singletâ€“triplet splittings of organic diradicals. Journal of Chemical Physics, 2018, 148, 064108.	1.2	30
125	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
126	Excitation spectra of retinal by multiconfiguration pair-density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 7265-7276.	1.3	13

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127	Synthesis and Characterization of Electron-Deficient Asymmetrically Substituted Diarylindenotetracenes. Journal of Organic Chemistry, 2018, 83, 1828-1841.	1.7	10
128	Analytic Gradients for Complete Active Space Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 126-138.	2.3	40
129	Computational Design of Functionalized Metalâ€“Organic Framework Nodes for Catalysis. ACS Central Science, 2018, 4, 5-19.	5.3	148
130	Transition states of spin-forbidden reactions. Physical Chemistry Chemical Physics, 2018, 20, 4129-4136.	1.3	32
131	Active Space Dependence in Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 660-669.	2.3	20
132	Formal Nickelate(â˜I) Complexes Supported by Groupâ€…13 Ions. Angewandte Chemie - International Edition, 2018, 57, 7815-7819.	7.2	37
133	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
134	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
135	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
136	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
137	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
138	Cerium Metalâ€“Organic Framework for Photocatalysis. Journal of the American Chemical Society, 2018, 140, 7904-7912.	6.6	313
139	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
140	Air Separation by Catechol-Ligated Transition Metals: A Quantum Chemical Screening. Journal of Physical Chemistry C, 2018, 122, 22345-22351.	1.5	16
141	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
142	Formal Nickelate(â˜I) Complexes Supported by Groupâ€…13 Ions. Angewandte Chemie, 2018, 130, 7941-7945.	1.6	8
143	Theoretical Investigation of Plutonium-Based Single-Molecule Magnets. Inorganic Chemistry, 2018, 57, 8098-8105.	1.9	29
144	Combining Wave Function Methods with Density Functional Theory for Excited States. Chemical Reviews, 2018, 118, 7249-7292.	23.0	166

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145	Parametrization of Combined Quantum Mechanical and Molecular Mechanical Methods: Bond-Tuned Link Atoms. Molecules, 2018, 23, 1309.	1.7	10
146	State-interaction pair-density functional theory. Journal of Chemical Physics, 2018, 149, 024106.	1.2	27
147	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
148	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
149	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
150	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
151	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
152	Quantum Chemical Characterization of Single Molecule Magnets Based on Uranium. Journal of Physical Chemistry A, 2017, 121, 1726-1733.	1.1	25
153	Computationally-Guided Assignment of Unexpected Signals in the Raman Spectra of Uranyl Triperoxide Complexes. Inorganic Chemistry, 2017, 56, 1574-1580.	1.9	35
154	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
155	Uranyl Peroxide Cage Cluster Solubility in Water and the Role of the Electrical Double Layer. Inorganic Chemistry, 2017, 56, 1333-1339.	1.9	27
156	Elucidating bonding preferences in tetrakis(imido)uranate(VI) dianions. Nature Chemistry, 2017, 9, 850-855.	6.6	54
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