Giovanni Li Manni

List of Publications by Year
in descending order

37 papers	3,951 citations	304701 22 h-index	302107 39 g-index
47 all docs	47 docs citations	47 times ranked	3688 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.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
3	Multiconfiguration Pair-Density Functional Theory. Journal of Chemical Theory and Computation, 2014, 10, 3669-3680.	5.3	334
4	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. Accounts of Chemical Research, 2017, 50, 66-73.	15.6	232
5	The generalized active space concept in multiconfigurational self-consistent field methods. Journal of Chemical Physics, 2011, 135, 044128.	3.0	220
6	Combining the Complete Active Space Self-Consistent Field Method and the Full Configuration Interaction Quantum Monte Carlo within a Super-CI Framework, with Application to Challenging Metal-Porphyrins. Journal of Chemical Theory and Computation, 2016, 12, 1245-1258.	5.3	156
7	SplitGAS Method for Strong Correlation and the Challenging Case of Cr₂. Journal of Chemical Theory and Computation, 2013, 9, 3375-3384.	5.3	97
8	On the Analysis of the Crâ‹¯Cr Multiple Bond in Several Classes of Dichromium Compounds. Inorganic Chemistry, 2010, 49, 5216-5222.	4.0	92
9	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. Journal of Physical Chemistry A, 2018, 122, 4935-4947.	2.5	75
10	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.	13.7	70
11	Multiconfiguration Pair-Density Functional Theory: Barrier Heights and Main Group and Transition Metal Energetics. Journal of Chemical Theory and Computation, 2015, 11, 82-90.	5.3	62
12	Strong correlation treated via effective hamiltonians and perturbation theory. Journal of Chemical Physics, 2011, 134, 034114.	3.0	55
13	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. Journal of Chemical Physics, 2020, 153, 034107.	3.0	55
14	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.	3.3	53
15	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. Journal of Chemical Theory and Computation, 2019, 15, 1492-1497.	5.3	51
16	Systematic Expansion of Active Spaces beyond the CASSCF Limit: A GASSCF/SplitGAS Benchmark Study. Journal of Chemical Theory and Computation, 2015, 11, 3010-3021.	5.3	48
17	Separated-pair approximation and separated-pair pair-density functional theory. Chemical Science, 2016, 7, 2399-2413.	7.4	47
18	Second-Order Perturbation Theory for Generalized Active Space Self-Consistent-Field Wave Functions. Journal of Chemical Theory and Computation, 2016, 12, 3208-3213.	5.3	44

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19	Oxidative Stretching of Metalâ€“Metal Bonds to Their Limits. Inorganic Chemistry, 2014, 53, 4777-4790.	4.0	31
20	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. Journal of Chemical Theory and Computation, 2020, 16, 2202-2215.	5.3	28
21	Computational Insights into Uranium Complexes Supported by Redox-Active Î±-Diimine Ligands. Inorganic Chemistry, 2012, 51, 2058-2064.	4.0	25
22	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Ironâ€“Sulfur Clusters. Journal of Chemical Theory and Computation, 2021, 17, 5684-5703.	5.3	25
23	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.	3.0	22
24	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)₄S₄] Cubanes. Journal of Physical Chemistry A, 2021, 125, 4727-4740.	2.5	22
25	Chemical insights into the electronic structure of Fe(<scp>II</scp>) porphyrin using <scp>FCIQMC</scp>, <scp>DMRG</scp>, and generalized active spaces. International Journal of Quantum Chemistry, 2021, 121, e26454.	2.0	21
26	Stochastic Generalized Active Space Self-Consistent Field: Theory and Application. Journal of Chemical Theory and Computation, 2022, 18, 251-272.	5.3	16
27	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. Topics in Catalysis, 2009, 52, 444-455.	2.8	11
28	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. Nature Physics, 2022, 18, 190-195.	16.7	10
29	Modeling magnetic interactions in high-valent trinuclear [Mn₃^(IV)O₄]⁴⁺ complexes through highly compressed multi-configurational wave functions. Physical Chemistry Chemical Physics, 2021, 23, 19766-19780.	2.8	9
30	Combined unitary and symmetric group approach applied to low-dimensional Heisenberg spin systems. Physical Review B, 2022, 105, .	3.2	9
31	Hydrogenolysis of hydroxymatairesinol on Y derived catalysts: A computational study. Journal of Molecular Catalysis A, 2010, 333, 136-144.	4.8	8
32	Spin Purification in Full-CI Quantum Monte Carlo via a First-Order Penalty Approach. Journal of Physical Chemistry A, 2022, 126, 2050-2060.	2.5	8
33	Quenched Lewis Acidity: Studies on the Medium Dependent Fluorescence of Zinc(II) Complexes. Chemistry - A European Journal, 2021, 27, 15159-15171.	3.3	7
34	Systematic conformational search analysis of the SRR and RRR epimers of 7â€hydroxymatairesinol. Journal of Physical Organic Chemistry, 2010, 23, 141-147.	1.9	6
35	FCIQMC-Tailored Distinguishable Cluster Approach: Open-Shell Systems. Journal of Chemical Theory and Computation, 2022, , .	5.3	4
36	Molecular-Level Characterization of Heterogeneous Catalytic Systems by Algorithmic Time Dependent Monte Carlo. Topics in Catalysis, 2009, 52, 431-443.	2.8	3

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37	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.	3.0	2