Giovanni Li Manni

List of Publications by Citations

34 papers	2,850 citations	20 h-index	47 g-index
47 ext. papers	3,424 ext. citations	5.8 avg, IF	5.05 L-index

#	Paper	IF	Citations
34	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
33	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
32	Multiconfiguration Pair-Density Functional Theory. *Journal of Chemical Theory and Computation*, **2014**, 10, 3669-80	6.4	246
31	The generalized active space concept in multiconfigurational self-consistent field methods. *Journal of Chemical Physics*, **2011**, 135, 044128	3.9	178
30	Multiconfiguration Pair-Density Functional Theory: A New Way To Treat Strongly Correlated Systems. *Accounts of Chemical Research*, **2017**, 50, 66-73	24.3	175
29	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, 1245-58	6.4	134
28	On the analysis of the Cr-Cr multiple bond in several classes of dichromium compounds. *Inorganic Chemistry*, **2010**, 49, 5216-22	5.1	87
27	SplitGAS Method for Strong Correlation and the Challenging Case of Cr2. *Journal of Chemical Theory and Computation*, **2013**, 9, 3375-84	6.4	86
26	Understanding the Mechanism Stabilizing Intermediate Spin States in Fe(II)-Porphyrin. *Journal of Physical Chemistry A*, **2018**, 122, 4935-4947	2.8	53
25	A two-coordinate manganese(0) complex with an unsupported Mn-Mg bond: allowing access to low coordinate homo- and heterobimetallic compounds. *Journal of the American Chemical Society*, **2014**, 136, 5283-6	16.4	52
24	Strong correlation treated via effective hamiltonians and perturbation theory. *Journal of Chemical Physics*, **2011**, 134, 034114	3.9	52
23	Assessing metal-metal multiple bonds in Cr-Cr, Mo-Mo, and W-W compounds and a hypothetical U-U compound: a quantum chemical study comparing DFT and multireference methods. *Chemistry - A European Journal*, **2012**, 18, 1737-49	4.8	49
22	Multiconfiguration pair-density functional theory: barrier heights and main group and transition metal energetics. *Journal of Chemical Theory and Computation*, **2015**, 11, 82-90	6.4	44
21	Systematic Expansion of Active Spaces beyond the CASSCF Limit: A GASSCF/SplitGAS Benchmark Study. *Journal of Chemical Theory and Computation*, **2015**, 11, 3010-21	6.4	41
20	Second-Order Perturbation Theory for Generalized Active Space Self-Consistent-Field Wave Functions. *Journal of Chemical Theory and Computation*, **2016**, 12, 3208-13	6.4	39
19	Separated-pair approximation and separated-pair pair-density functional theory. *Chemical Science*, **2016**, 7, 2399-2413	9.4	37
18	Role of Valence and Semicore Electron Correlation on Spin Gaps in Fe(II)-Porphyrins. *Journal of Chemical Theory and Computation*, **2019**, 15, 1492-1497	6.4	32

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17	Oxidative stretching of metal-metal bonds to their limits. *Inorganic Chemistry*, **2014**, 53, 4777-90	5.1	30
16	NECI: N-Electron Configuration Interaction with an emphasis on state-of-the-art stochastic methods. *Journal of Chemical Physics*, **2020**, 153, 034107	3.9	28
15	Computational insights into uranium complexes supported by redox-active diimine ligands. *Inorganic Chemistry*, **2012**, 51, 2058-64	5.1	22
14	Compression of Spin-Adapted Multiconfigurational Wave Functions in Exchange-Coupled Polynuclear Spin Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 2202-2215	6.4	16
13	Controversial electronic structures and energies of Fe2, Fe 2 (+), and Fe 2 (-) resolved by RASPT2 calculations. *Journal of Chemical Physics*, **2014**, 141, 204309	3.9	16
12	Chemical insights into the electronic structure of Fe(II) porphyrin using FCIQMC, DMRG, and generalized active spaces. *International Journal of Quantum Chemistry*, **2021**, 121, e26454	2.1	11
11	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. *Topics in Catalysis*, **2009**, 52, 444-455	2.3	10
10	Resolution of Low-Energy States in Spin-Exchange Transition-Metal Clusters: Case Study of Singlet States in [Fe(III)S] Cubanes. *Journal of Physical Chemistry A*, **2021**, 125, 4727-4740	2.8	10
9	Spin-Pure Stochastic-CASSCF via GUGA-FCIQMC Applied to Iron-Sulfur Clusters. *Journal of Chemical Theory and Computation*, **2021**, 17, 5684-5703	6.4	9
8	Hydrogenolysis of hydroxymatairesinol on Y derived catalysts: A computational study. *Journal of Molecular Catalysis A*, **2010**, 333, 136-144		7
7	Systematic conformational search analysis of the SRR and RRR epimers of 7-hydroxymatairesinol. *Journal of Physical Organic Chemistry*, **2010**, 23, 141-147	2.1	5
6	Molecular-Level Characterization of Heterogeneous Catalytic Systems by Algorithmic Time Dependent Monte Carlo. *Topics in Catalysis*, **2009**, 52, 431-443	2.3	3
5	Foundation of Multi-Configurational Quantum Chemistry **2020**, 133-203		3
4	Modeling magnetic interactions in high-valent trinuclear [MnO] complexes through highly compressed multi-configurational wave functions. *Physical Chemistry Chemical Physics*, **2021**, 23, 19766-19780	3.6	2
3	Quenched Lewis Acidity: Studies on the Medium Dependent Fluorescence of Zinc(II) Complexes. *Chemistry - A European Journal*, **2021**, 27, 15158-15170	4.8	2
2	Comment on "Fe2: As simple as a Herculean labour. Neutral (Fe2), cationic (Fe2(+)), and anionic (Fe2(-)) species" [J. Chem. Phys. 142, 244304 (2015)]. *Journal of Chemical Physics*, **2016**, 144, 027101	3.9	1
1	Enhancement of superexchange due to synergetic breathing and hopping in corner-sharing cuprates. *Nature Physics*, **2022**, 18, 190-195	16.2	1