

# Mickaël G Delcey

## List of Publications by Year in descending order

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34  
papers

3,442  
citations

331670

21  
h-index

345221

36  
g-index

42  
all docs

42  
docs citations

42  
times ranked

3702  
citing authors

#	ARTICLE	IF	CITATIONS
1	<sc>Molcas</sc> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
2	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
3	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020, 152, 214117.	3.0	281
4	Analytical State-Average Complete-Active-Space Self-Consistent Field Nonadiabatic Coupling Vectors: Implementation with Density-Fitted Two-Electron Integrals and Application to Conical Intersections. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3636-3653.	5.3	112
5	Restricted active space calculations of L-edge X-ray absorption spectra: From molecular orbitals to multiplet states. <i>Journal of Chemical Physics</i> , 2014, 141, 124116.	3.0	109
6	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 622-626.	4.6	89
7	Calibration of Cholesky Auxiliary Basis Sets for Multiconfigurational Perturbation Theory Calculations of Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 747-754.	5.3	79
8	Viewing the Valence Electronic Structure of Ferric and Ferrous Hexacyanide in Solution from the Fe and Cyanide Perspectives. <i>Journal of Physical Chemistry B</i> , 2016, 120, 7182-7194.	2.6	76
9	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. <i>Nature Communications</i> , 2020, 11, 634.	12.8	75
10	Simulations of iron K pre-edge X-ray absorption spectra using the restricted active space method. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3250-3259.	2.8	67
11	Cost and sensitivity of restricted active space calculations of metal L-edge X-ray absorption spectra. <i>Journal of Computational Chemistry</i> , 2016, 37, 477-486.	3.3	59
12	Accurate calculations of geometries and singlet-triplet energy differences for active-site models of [NiFe] hydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 7927-7938.	2.8	58
13	Orbital entanglement and CASSCF analysis of the Ru-NO bond in a Ruthenium nitrosyl complex. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 14383-14392.	2.8	58
14	Chemiluminescence and Fluorescence States of a Small Model for Coelenteramide and Cypridina Oxyluciferin: A CASSCF/CASPT2 Study. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 4060-4069.	5.3	49
15	Analytical gradients of complete active space self-consistent field energies using Cholesky decomposition: Geometry optimization and spin-state energetics of a ruthenium nitrosyl complex. <i>Journal of Chemical Physics</i> , 2014, 140, 174103.	3.0	48
16	Efficient calculations of a large number of highly excited states for multiconfigurational wavefunctions. <i>Journal of Computational Chemistry</i> , 2019, 40, 1789-1799.	3.3	47
17	Parallelization of a multiconfigurational perturbation theory. <i>Journal of Computational Chemistry</i> , 2013, 34, 1937-1948.	3.3	35
18	Analytical gradients of the state-average complete active space self-consistent field method with density fitting. <i>Journal of Chemical Physics</i> , 2015, 143, 044110.	3.0	31

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19	Molecular Orbital Simulations of Metal 1s2p Resonant Inelastic X-ray Scattering. <i>Journal of Physical Chemistry A</i> , 2016, 120, 5848-5855.	2.5	31
20	Tracing the 267 nm-Induced Radical Formation in Dimethyl Disulfide Using Time-Resolved X-ray Absorption Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1382-1387.	4.6	24
21	Core-level nonlinear spectroscopy triggered by stochastic X-ray pulses. <i>Nature Communications</i> , 2019, 10, 4761.	12.8	23
22	Origin of core-to-core x-ray emission spectroscopy sensitivity to structural dynamics. <i>Structural Dynamics</i> , 2020, 7, 044102.	2.3	14
23	Multiconfigurational Approach to X-ray Spectroscopy of Transition Metal Complexes. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 185-217.	0.6	13
24	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. <i>Molecular Physics</i> , 2017, 115, 2052-2064.	1.7	11
25	Soft X-ray signatures of cationic manganese-oxo systems, including a high-spin manganese( $\nu$ ) complex. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3598-3610.	2.8	10
26	Revisiting $H_2O$ Nucleation around $Au^{+}$ and $Hg^{2+}$ : The Peculiar "Pseudo-Soft" Character of the Gold Cation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1900-1909.	5.3	7
27	Simulations of valence excited states in coordination complexes reached through hard X-ray scattering. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8325-8335.	2.8	7
28	Spectroscopy of linear and circular polarized light with the exact semiclassical light-matter interaction. <i>Annual Reports in Computational Chemistry</i> , 2019, 15, 39-76.	1.7	6
29	Quantifying similarity for spectra with a large number of overlapping transitions: Examples from soft X-ray spectroscopy. <i>Chemical Physics</i> , 2020, 535, 110786.	1.9	6
30	Communication: Theoretical prediction of the structure and spectroscopic properties of the $\text{X}^{\cdot}$ and $\text{A}^{\cdot}$ states of hydroxymethyl peroxy (HOCH <sub>2</sub> OO) radical. <i>Journal of Chemical Physics</i> , 2013, 138, 021105.	3.0	5
31	Toward a Computational Ecotoxicity Assay. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3792-3803.	5.4	5
32	Exact semi-classical light-matter interaction operator applied to two-photon processes with strong relativistic effects. <i>Journal of Chemical Physics</i> , 2020, 153, 024114.	3.0	5
33	Approaching the Attosecond Frontier of Dynamics in Matter with the Concept of X-ray Chronoscopy. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 1721.	2.5	2
34	Unravelling the mechanism of pH-regulation in dinoflagellate luciferase. <i>International Journal of Biological Macromolecules</i> , 2020, 164, 2671-2680.	7.5	0