MickaÃ«l G Delcey

List of Publications by Year
in descending order

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	Soft X-ray signatures of cationic manganeseâ€“oxo systems, including a high-spin manganese(<scp>v</scp>) complex. Physical Chemistry Chemical Physics, 2022, 24, 3598-3610.	2.8	10
2	Approaching the Attosecond Frontier of Dynamics in Matter with the Concept of X-ray Chronoscopy. Applied Sciences (Switzerland), 2022, 12, 1721.	2.5	2
3	Unravelling the mechanism of pH-regulation in dinoflagellate luciferase. International Journal of Biological Macromolecules, 2020, 164, 2671-2680.	7.5	0
4	Origin of core-to-core x-ray emission spectroscopy sensitivity to structural dynamics. Structural Dynamics, 2020, 7, 044102.	2.3	14
5	Toward a Computational Ecotoxicity Assay. Journal of Chemical Information and Modeling, 2020, 60, 3792-3803.	5.4	5
6	Exact semi-classical lightâ€“matter interaction operator applied to two-photon processes with strong relativistic effects. Journal of Chemical Physics, 2020, 153, 024114.	3.0	5
7	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
8	Simulations of valence excited states in coordination complexes reached through hard X-ray scattering. Physical Chemistry Chemical Physics, 2020, 22, 8325-8335.	2.8	7
9	Vibrational wavepacket dynamics in Fe carbene photosensitizer determined with femtosecond X-ray emission and scattering. Nature Communications, 2020, 11, 634.	12.8	75
10	Quantifying similarity for spectra with a large number of overlapping transitions: Examples from soft X-ray spectroscopy. Chemical Physics, 2020, 535, 110786.	1.9	6
11	Spectroscopy of linear and circular polarized light with the exact semiclassical lightâ€“matter interaction. Annual Reports in Computational Chemistry, 2019, 15, 39-76.	1.7	6
12	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
13	Tracing the 267 nm-Induced Radical Formation in Dimethyl Disulfide Using Time-Resolved X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2019, 10, 1382-1387.	4.6	24
14	Multiconfigurational Approach to X-ray Spectroscopy of Transition Metal Complexes. Challenges and Advances in Computational Chemistry and Physics, 2019, , 185-217.	0.6	13
15	Efficient calculations of a large number of highly excited states for multiconfigurational wavefunctions. Journal of Computational Chemistry, 2019, 40, 1789-1799.	3.3	47
16	Core-level nonlinear spectroscopy triggered by stochastic X-ray pulses. Nature Communications, 2019, 10, 4761.	12.8	23
17	Inner projection techniques for the low-cost handling of two-electron integrals in quantum chemistry. Molecular Physics, 2017, 115, 2052-2064.	1.7	11
18	Cost and sensitivity of restricted activeâ€space calculations of metal Lâ€edge Xâ€ray absorption spectra. Journal of Computational Chemistry, 2016, 37, 477-486.	3.3	59

#	Article	IF	Citations
19	<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
20	Simulations of iron K pre-edge X-ray absorption spectra using the restricted active space method. Physical Chemistry Chemical Physics, 2016, 18, 3250-3259.	2.8	67
21	Molecular Orbital Simulations of Metal 1s2p Resonant Inelastic X-ray Scattering. Journal of Physical Chemistry A, 2016, 120, 5848-5855.	2.5	31
22	Viewing the Valence Electronic Structure of Ferric and Ferrous Hexacyanide in Solution from the Fe and Cyanide Perspectives. Journal of Physical Chemistry B, 2016, 120, 7182-7194.	2.6	76
23	Analytical State-Average Complete-Active-Space Self-Consistent Field Nonadiabatic Coupling Vectors: Implementation with Density-Fitted Two-Electron Integrals and Application to Conical Intersections. Journal of Chemical Theory and Computation, 2016, 12, 3636-3653.	5.3	112
24	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	4.6	89
25	Analytical gradients of the state-average complete active space self-consistent field method with density fitting. Journal of Chemical Physics, 2015, 143, 044110.	3.0	31
26	Orbital entanglement and CASSCF analysis of the Ruâ€“NO bond in a Ruthenium nitrosyl complex. Physical Chemistry Chemical Physics, 2015, 17, 14383-14392.	2.8	58
27	Restricted active space calculations of L-edge X-ray absorption spectra: From molecular orbitals to multiplet states. Journal of Chemical Physics, 2014, 141, 124116.	3.0	109
28	Analytical gradients of complete active space self-consistent field energies using Cholesky decomposition: Geometry optimization and spin-state energetics of a ruthenium nitrosyl complex. Journal of Chemical Physics, 2014, 140, 174103.	3.0	48
29	Revisiting H₂O Nucleation around Au⁺ and Hg²⁺: The Peculiar â€œPseudo-Softâ€•Character of the Gold Cation. Journal of Chemical Theory and Computation, 2014, 10, 1900-1909.	5.3	7
30	Accurate calculations of geometries and singletâ€“triplet energy differences for active-site models of [NiFe] hydrogenase. Physical Chemistry Chemical Physics, 2014, 16, 7927-7938.	2.8	58
31	Parallelization of a multiconfigurational perturbation theory. Journal of Computational Chemistry, 2013, 34, 1937-1948.	3.3	35
32	Communication: Theoretical prediction of the structure and spectroscopic properties of the $ilde{mathrm{X}}$Xlf and $ilde{mathrm{A}}$Alf states of hydroxymethyl peroxy (HOCH2OO) radical. Journal of Chemical Physics, 2013, 138, 021105.	3.0	5
33	Chemiluminescence and Fluorescence States of a Small Model for Coelenteramide and Cypridina Oxyluciferin: A CASSCF/CASPT2 Study. Journal of Chemical Theory and Computation, 2011, 7, 4060-4069.	5.3	49
34	Calibration of Cholesky Auxiliary Basis Sets for Multiconfigurational Perturbation Theory Calculations of Excitation Energies. Journal of Chemical Theory and Computation, 2010, 6, 747-754.	5.3	79