Nicolas Ferr

List of Publications by Citations

97 papers	6,191 citations	37 h-index	78 g-index
100 ext. papers	6,847 ext. citations	6.3 avg, IF	5.5 L-index

#	Paper	IF	Citations
97	MOLCAS 7: the next generation. *Journal of Computational Chemistry*, **2010**, 31, 224-47	3.5	1425
96	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
95	Tracking the excited-state time evolution of the visual pigment with multiconfigurational quantum chemistry. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 7764-9	11.5	239
94	Structure, initial excited-state relaxation, and energy storage of rhodopsin resolved at the multiconfigurational perturbation theory level. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 17908-13	11.5	216
93	Chemi- and Bioluminescence of Cyclic Peroxides. *Chemical Reviews*, **2018**, 118, 6927-6974	68.1	172
92	Probing the rhodopsin cavity with reduced retinal models at the CASPT2//CASSCF/AMBER level of theory. *Journal of the American Chemical Society*, **2003**, 125, 6868-9	16.4	142
91	The ultrafast photoisomerizations of rhodopsin and bathorhodopsin are modulated by bond length alternation and HOOP driven electronic effects. *Journal of the American Chemical Society*, **2011**, 133, 3354-64	16.4	139
90	Properties of the emitting state of the green fluorescent protein resolved at the CASPT2//CASSCF/CHARMM level. *Journal of the American Chemical Society*, **2005**, 127, 11534-5	16.4	133
89	Shape of Multireference, Equation-of-Motion Coupled-Cluster, and Density Functional Theory Potential Energy Surfaces at a Conical Intersection. *Journal of Chemical Theory and Computation*, **2014**, 10, 3074-84	6.4	132
88	The color of rhodopsins at the ab initio multiconfigurational perturbation theory resolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 17154-9	11.5	118
87	Specific force field parameters determination for the hybrid ab initio QM/MM LSCF method. *Journal of Computational Chemistry*, **2002**, 23, 610-24	3.5	115
86	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
85	Color-tuning mechanism of firefly investigated by multi-configurational perturbation method. *Journal of the American Chemical Society*, **2010**, 132, 706-12	16.4	100
84	The chemistry of bioluminescence: an analysis of chemical functionalities. *ChemPhysChem*, **2011**, 12, 3064-76	3.2	93
83	The molecular mechanism of thermal noise in rod photoreceptors. *Science*, **2012**, 337, 1225-8	33.3	85
82	Assignment of the EPR spectrum of 5,5-dimethyl-1-pyrroline N-oxide (DMPO) superoxide spin adduct. *Journal of Organic Chemistry*, **2005**, 70, 1198-203	4.2	81
81	Approximate electrostatic interaction operator for QM/MM calculations. *Chemical Physics Letters*, **2002**, 356, 331-339	2.5	79

80	Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. *Journal of Chemical Theory and Computation*, **2013**, 9, 3917-32	6.4	78
79	An artificial molecular switch that mimics the visual pigment and completes its photocycle in picoseconds. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 17642-7	11.5	78
78	Systematic Theoretical Investigation on the Light Emitter of Firefly. *Journal of Chemical Theory and Computation*, **2011**, 7, 798-803	6.4	71
77	Anabaena sensory rhodopsin is a light-driven unidirectional rotor. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 21322-6	11.5	64
76	Structure of the intersection space associated with ZIE photoisomerization of retinal in rhodopsin proteins. *Faraday Discussions*, **2004**, 127, 179-91	3.6	58
75	Relationship between the excited state relaxation paths of rhodopsin and isorhodopsin. *Journal of the American Chemical Society*, **2008**, 130, 3382-8	16.4	56
74	Quantum chemical modeling of rhodopsin mutants displaying switchable colors. *Physical Chemistry Chemical Physics*, **2012**, 14, 12485-95	3.6	54
73	Complete-active-space self-consistent-field/Amber parameterization of the Lys296□etinal□Glu113 rhodopsin chromophore-counterion system. *Theoretical Chemistry Accounts*, **2004**, 112, 335	1.9	54
72	Quantum chemical modeling and preparation of a biomimetic photochemical switch. *Angewandte Chemie - International Edition*, **2007**, 46, 414-20	16.4	53
71	Unique QM/MM potential energy surface exploration using microiterations. *International Journal of Quantum Chemistry*, **2011**, 111, 3339-3346	2.1	50
70	Application of the local self-consistent-field method to core-ionized and core-excited molecules, polymers, and proteins: True orthogonality between ground and excited states. *Journal of Chemical Physics*, **2002**, 117, 4119-4125	3.9	49
69	Modeling, preparation, and characterization of a dipole moment switch driven by Z/E photoisomerization. *Journal of the American Chemical Society*, **2010**, 132, 9310-9	16.4	46
68	Are the bio- and chemiluminescence states of the firefly oxyluciferin the same as the fluorescence state?. *Photochemistry and Photobiology*, **2013**, 89, 319-25	3.6	45
67	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, 4060-9	6.4	45
66	The amide bond: pitfalls and drawbacks of the link atom scheme. *Computational and Theoretical Chemistry*, **2003**, 632, 71-82		45
65	Toward Automatic Rhodopsin Modeling as a Tool for High-Throughput Computational Photobiology. *Journal of Chemical Theory and Computation*, **2016**, 12, 6020-6034	6.4	39
64	Chemiluminescence of Coelenterazine and Fluorescence of Coelenteramide: A Systematic Theoretical Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 2796-807	6.4	39
63	Characterization of the conical intersection of the visual pigment rhodopsin at the CASPT2//CASSCF/AMBER level of theory. *Molecular Physics*, **2006**, 104, 983-991	1.7	39

62	Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. *Journal of Chemical Theory and Computation*, **2016**, 12, 839-50	6.4	38
61	QM/MM study on the light emitters of aequorin chemiluminescence, bioluminescence, and fluorescence: a general understanding of the bioluminescence of several marine organisms. *Chemistry - A European Journal*, **2013**, 19, 8466-72	4.8	37
60	Spin decontamination of broken-symmetry density functional theory calculations: deeper insight and new formulations. *Physical Chemistry Chemical Physics*, **2015**, 17, 14375-82	3.6	36
59	Understanding bacterial bioluminescence: a theoretical study of the entire process, from reduced flavin to light emission. *Chemistry - A European Journal*, **2014**, 20, 7979-86	4.8	35
58	Prediction of nitroxide hyperfine coupling constants in solution from combined nanosecond scale simulations and quantum computations. *Journal of Chemical Physics*, **2008**, 128, 244504	3.9	35
57	Hybrid QM/MM simulations of the obelin bioluminescence and fluorescence reveal an unexpected light emitter. *Journal of Physical Chemistry B*, **2014**, 118, 2896-903	3.4	28
56	Can the Closed-Shell DFT Methods Describe the Thermolysis of 1,2-Dioxetanone?. *Journal of Chemical Theory and Computation*, **2012**, 8, 4359-63	6.4	26
55	Theoretical study of the photochemical generation of triplet acetophenone. *Physical Chemistry Chemical Physics*, **2013**, 15, 19293-300	3.6	25
54	Simulation and Analysis of the Spectroscopic Properties of Oxyluciferin and Its Analogues in Water. *Journal of Chemical Theory and Computation*, **2018**, 14, 2117-2126	6.4	24
53	Modeling the fluorescence of protein-embedded tryptophans with ab initio multiconfigurational quantum chemistry: the limiting cases of parvalbumin and monellin. *Journal of Physical Chemistry B*, **2009**, 113, 16082-90	3.4	24
52	Additive Decomposition of the Physical Components of the Magnetic Coupling from Broken Symmetry Density Functional Theory Calculations. *Journal of Chemical Theory and Computation*, **2013**, 9, 3429-36	6.4	23
51	Effects of water re-location and cavity trimming on the CASPT2//CASSCF/AMBER excitation energy of Rhodopsin. *Theoretical Chemistry Accounts*, **2007**, 118, 185-191	1.9	23
50	Analysis of the physical contributions to magnetic couplings in broken symmetry density functional theory approach. *Journal of Chemical Physics*, **2012**, 137, 114106	3.9	22
49	An Average Solvent Electrostatic Configuration Protocol for QM/MM Free Energy Optimization: Implementation and Application to Rhodopsin Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 6391-6404	6.4	21
48	DNA nucleobase properties and photoreactivity: Modeling environmental effects. *Pure and Applied Chemistry*, **2009**, 81, 743-754	2.1	21
47	Choosing the right molecular machine learning potential. *Chemical Science*, **2021**, 12, 14396-14413	9.4	21
46	Further insights into the environmental effects on the computed hyperfine coupling constants of nitroxides in aqueous solution. *Journal of Physical Chemistry B*, **2009**, 113, 15047-56	3.4	20
45	Chemical Tuning of Magnetic Exchange Couplings Using Broken-Symmetry Density Functional Theory. *Inorganic Chemistry*, **2018**, 57, 12769-12776	5.1	19

44	UV-visible absorption spectrum of FAD and its reduced forms embedded in a cryptochrome protein. *Physical Chemistry Chemical Physics*, **2020**, 22, 12447-12455	3.6	17
43	Structure and spectromagnetic properties of the superoxide radical adduct of DMPO in water: elucidation by theoretical investigations. *Journal of Physical Chemistry B*, **2010**, 114, 11793-803	3.4	17
42	Photophysics of acetophenone interacting with DNA: why the road to photosensitization is open. *Photochemistry and Photobiology*, **2015**, 91, 323-30	3.6	14
41	Triplet state photochemistry and the three-state crossing of acetophenone within time-dependent density-functional theory. *Journal of Chemical Physics*, **2014**, 140, 134305	3.9	14
40	A new three-layer hybrid method (LSCF/MM/Madelung) devoted to the study of chemical reactivity in zeolites. Preliminary results. *Computational and Theoretical Chemistry*, **2003**, 632, 83-90		14
39	Mechanism of the initial conformational transition of a photomodulable peptide. *Angewandte Chemie - International Edition*, **2005**, 44, 6077-81	16.4	13
38	The Local Self-Consistent Field Principles and Applications to Combined Quantum Mechanical-Molecular Mechanical Computations on Biomacromolecular Systems. *ACS Symposium Series*, **1998**, 234-249	0.4	13
37	Effect of point mutations on the ultrafast photo-isomerization of Anabaena sensory rhodopsin. *Faraday Discussions*, **2018**, 207, 55-75	3.6	13
36	Efficient Analytic Second Derivative of Electrostatic Embedding QM/MM Energy: Normal Mode Analysis of Plant Cryptochrome. *Journal of Chemical Theory and Computation*, **2020**, 16, 3816-3824	6.4	12
35	Theoretical study of the photochemical initiation in nitroxide-mediated photopolymerization. *Journal of Physical Chemistry A*, **2014**, 118, 4464-70	2.8	11
34	What Are the Physical Contents of Hubbard and Heisenberg Hamiltonian Interactions Extracted from Broken Symmetry DFT Calculations in Magnetic Compounds?. *Journal of Chemical Theory and Computation*, **2017**, 13, 6253-6265	6.4	10
33	Toward a computational photobiology. *Pure and Applied Chemistry*, **2005**, 77, 977-993	2.1	10
32	Population of triplet states in acetophenone: A quantum dynamics perspective. *Comptes Rendus Chimie*, **2016**, 19, 50-56	2.7	10
31	An Effective Procedure for Analyzing Molecular Vibrations in Terms of Local Fragment Modes. *Journal of Chemical Theory and Computation*, **2016**, 12, 4768-4777	6.4	10
30	Sampling the protonation states: the pH-dependent UV absorption spectrum of a polypeptide dyad. *Physical Chemistry Chemical Physics*, **2018**, 20, 23252-23261	3.6	10
29	CpHMD-Then-QM/MM Identification of the Amino Acids Responsible for the Anabaena Sensory Rhodopsin pH-Dependent Electronic Absorption Spectrum. *Journal of Chemical Theory and Computation*, **2019**, 15, 4535-4546	6.4	9
28	Magnetic exchange coupling in bis-nitroxides: a theoretical analysis of the solvent effects. *Physical Chemistry Chemical Physics*, **2012**, 14, 5504-11	3.6	9
27	Structural and atoms-in-molecules analysis of hydrogen-bond network around nitroxides in liquid water. *Journal of Chemical Physics*, **2010**, 133, 124508	3.9	9

26	Quantitative evaluation of the aqueous dihydronitroxide nitrogen hyperfine coupling constant from QM/MM//MD computations. *Computational and Theoretical Chemistry*, **2009**, 898, 49-55		9
25	Quantum Chemical Modeling and Preparation of a Biomimetic Photochemical Switch. *Angewandte Chemie*, **2007**, 119, 418-424	3.6	9
24	Mapping the ultrafast vibrational dynamics of all-trans and 13-cis retinal isomerization in Anabaena Sensory Rhodopsin. *Physical Chemistry Chemical Physics*, **2018**, 20, 30159-30173	3.6	9
23	Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021**, 97, 243-269	3.6	8
22	pH-Dependent absorption spectrum of a protein: a minimal electrostatic model of Anabaena sensory rhodopsin. *Physical Chemistry Chemical Physics*, **2017**, 19, 14073-14084	3.6	7
21	Analytic QM/MM atomic charge derivatives avoiding the scaling of coupled perturbed equations with the MM subsystem size. *Journal of Chemical Physics*, **2019**, 151, 041102	3.9	7
20	Electronic basis of the comparable hydrogen bond properties of small H2CO/(H2O)n and H2NO/(H2O)n systems (n = 1, 2). *Journal of Physical Chemistry A*, **2007**, 111, 11673-82	2.8	7
19	Assessing the accuracy of a QM/MM//MD combined protocol to compute spectromagnetic properties of polyfunctional nitroxides in solution. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	6
18	Time-Dependent Density Functional Theory **2020**, 13-46		6
17	Computation of the Isotropic Hyperfine Coupling Constant: Efficiency and Insights from a New Approach Based on Wave Function Theory. *Journal of Chemical Theory and Computation*, **2017**, 13, 475-487	6.4	5
16	pH-Dependent Absorption Spectrum of Oxyluciferin Analogues in the Presence of Adenosine Monophosphate. *ChemPhotoChem*, **2019**, 3, 1219-1230	3.3	5
15	Electrostatic interactions in peptides. Polarisation effects due to an α-helix. *Theoretical Chemistry Accounts*, **2004**, 111, 328-334	1.9	5
14	Analytic Energy, Gradient, and Hessian of Electrostatic Embedding QM/MM Based on Electrostatic Potential-Fitted Atomic Charges Scaling Linearly with the MM Subsystem Size. *Journal of Chemical Theory and Computation*, **2021**, 17, 538-548	6.4	5
13	Magnetic Properties of Conjugated Hydrocarbons from Topological Hamiltonians. *Challenges and Advances in Computational Chemistry and Physics*, **2016**, 361-395	0.7	4
12	Geometrical embedding governs a dramatic variation of electron paramagnetic resonance hyperfine coupling constants of disulfide radical anions. *Journal of Physical Chemistry B*, **2011**, 115, 6776-83	3.4	4
11	Imidazoline-N-oxyl: a DFT study of its protonation reaction. *ChemPhysChem*, **2009**, 10, 2419-28	3.2	2
10	Mechanism of the Initial Conformational Transition of a Photomodulable Peptide. *Angewandte Chemie*, **2005**, 117, 6231-6235	3.6	2
9	Frustration, ring exchange, and the absence of long-range order in EtMe3Sb[Pd(dmit)2]2: From first principles to many-body theory. *Physical Review Materials*, **2020**, 4,	3.2	2

8	Analysis of the Magnetic Exchange Interaction in Halide-Bridged Cu(II) Binuclear Complexes: Deciphering the Paths. *Current Inorganic Chemistry*, **2014**, 3, 235-241		2
7	Improved evaluation of spin-polarization energy contributions using broken-symmetry calculations. *Journal of Chemical Physics*, **2020**, 153, 054120	3.9	2
6	pH-Dependent absorption spectrum of oxyluciferin analogues in the active site of firefly luciferase. *Physical Chemistry Chemical Physics*, **2020**, 22, 21731-21740	3.6	2
5	Infrared spectroscopy from electrostatic embedding QM/MM: local normal mode analysis of infrared spectra of arabidopsis thaliana plant cryptochrome. *Physical Chemistry Chemical Physics*, **2021**, 23, 1666-1674	3.6	2
4	UV Photochemistry of Acetylacetaldehyde Trapped in Cryogenic Matrices. *Journal of Physical Chemistry A*, **2020**, 124, 4916-4928	2.8	1
3	Sub-picosecond C=C bond photo-isomerization: evidence for the role of excited state mixing. *Comptes Rendus Physique*, **2021**, 22, 1-28	1.4	0
2	Anabaena Sensory Rhodopsin: Effect of point mutations on PSBR photo-isomerization speed. *EPJ Web of Conferences*, **2019**, 205, 10004	0.3	
1	Towards an accurate treatment of <- transitions: Moving onto. *Chemical Physics Letters*, **2013**, 580, 14-20	2.5	