Massimo Olivucci

List of Publications by Citations

277 papers	14,945 citations	66 h-index	111 g-index
306 ext. papers	16,256 ext. citations	9 avg, IF	6.26 L-index

#	Paper	IF	Citations
277	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
276	Potential energy surface crossings in organic photochemistry. *Chemical Society Reviews*, **1996**, 25, 321	58.5	677
275	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.5	310
274	Computational evidence in favor of a two-state, two-mode model of the retinal chromophore photoisomerization. *Proceedings of the National Academy of Sciences of the United States of America* , **2000**, 97, 9379-84	11.5	301
273	Ultrafast decay of electronically excited singlet cytosine via a pi,pi* to n(O),pi* state switch. *Journal of the American Chemical Society*, **2002**, 124, 6818-9	16.4	278
272	Origin, nature, and fate of the fluorescent state of the green fluorescent protein chromophore at the CASPT2//CASSCF resolution. *Journal of the American Chemical Society*, **2004**, 126, 5452-64	16.4	270
271	The C5H6NH2+Protonated Shiff Base:□Anab InitioMinimal Model for Retinal Photoisomerization. *Journal of the American Chemical Society*, **1997**, 119, 6891-6901	16.4	259
270	Photoactivation of the photoactive yellow protein: why photon absorption triggers a trans-to-cis Isomerization of the chromophore in the protein. *Journal of the American Chemical Society*, **2004**, 126, 4228-33	16.4	246
269	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
268	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
267	An MC-SCF study of the S1 and S2 photochemical reactions of benzene. *Journal of the American Chemical Society*, **1993**, 115, 673-682	16.4	208
266	Ab Initio Photoisomerization Dynamics of a Simple Retinal Chromophore Model. *Journal of the American Chemical Society*, **1997**, 119, 12687-12688	16.4	172
265	A conical intersection mechanism for the photochemistry of butadiene. A MC-SCF study. *Journal of the American Chemical Society*, **1993**, 115, 3710-3721	16.4	167
264	Ultrafast Radiationless Deactivation of Organic Dyes: Evidence for a Two-State Two-Mode Pathway in Polymethine Cyanines. *Journal of the American Chemical Society*, **2000**, 122, 2911-2924	16.4	164
263	Optimization and characterization of the lowest energy point on a conical intersection using an MC-SCF Lagrangian. *Chemical Physics Letters*, **1992**, 197, 217-223	2.5	164
262	Theory and Simulation of the Ultrafast Double-Bond Isomerization of Biological Chromophores. *Chemical Reviews*, **2017**, 117, 13502-13565	68.1	160
261	Relaxation Paths from a Conical Intersection: The Mechanism of Product Formation in the Cyclohexadiene/Hexatriene Photochemical Interconversion. *Journal of Physical Chemistry A*, **1997**, 101, 2023-2032	2.8	144

260	The Azulene S1State Decays via a Conical Intersection:A CASSCF Study with MMVB Dynamics. *Journal of the American Chemical Society*, **1996**, 118, 169-175	16.4	144
259	Photoisomerization Path for a Realistic Retinal Chromophore Model: The Nonatetraeniminium Cation. *Journal of the American Chemical Society*, **1998**, 120, 1285-1288	16.4	143
258	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
257	Reaction Path of a sub-200 fs Photochemical Electrocyclic Reaction. *Journal of Physical Chemistry A*, **2001**, 105, 4458-4469	2.8	141
256	Conical intersections as a mechanistic feature of organic photochemistry. *Pure and Applied Chemistry*, **1995**, 67, 783-789	2.1	141
255	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
254	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
253	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
252	Potential-energy surfaces for ultrafast photochemistry Static and dynamic aspects. *Faraday Discussions*, **1998**, 110, 51-70	3.6	132
251	What Happens during the Picosecond Lifetime of 2A1 Cyclohexa-1,3-diene? A CAS-SCF Study of the Cyclohexadiene/Hexatriene Photochemical Interconversion. *Journal of the American Chemical Society*, **1994**, 116, 10141-10151	16.4	128
250	Dynamic Electron Correlation Effects on the Ground State Potential Energy Surface of a Retinal Chromophore Model. *Journal of Chemical Theory and Computation*, **2012**, 8, 4069-80	6.4	127
249	Simulation of MC-SCF results on covalent organic multi-bond reactions: molecular mechanics with valence bond (MM-VB). *Journal of the American Chemical Society*, **1992**, 114, 1606-1616	16.4	119
248	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
247	Ground and excited state CASPT2 geometry optimizations of small organic molecules. *Journal of Computational Chemistry*, **2003**, 24, 298-309	3.5	118
246	Excited-State Potential Surface Crossings in Acrolein: A Model for Understanding the Photochemistry and Photophysics of .alpha.,.beta.-Enones. *Journal of the American Chemical Society* , **1994**, 116, 2103-2114	16.4	116
245	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
244	A Computational Strategy for Organic Photochemistry. *Reviews in Computational Chemistry*, **2007**, 87-146		106
243	Relationship between photoisomerization path and intersection space in a retinal chromophore model. *Journal of the American Chemical Society*, **2003**, 125, 2804-8	16.4	103

242	Geometry optimisation on a hypersphere. Application to finding reaction paths from a conical intersection. *Chemical Physics Letters*, **1995**, 243, 1-8	2.5	103
241	The mechanism of ground-state-forbidden photochemical pericyclic reactions: evidence for real conical intersections. *Journal of the American Chemical Society*, **1990**, 112, 1737-1744	16.4	102
240	Assessment of Approximate Coupled-Cluster and Algebraic-Diagrammatic-Construction Methods for Ground- and Excited-State Reaction Paths and the Conical-Intersection Seam of a Retinal-Chromophore Model. *Journal of Chemical Theory and Computation*, **2015**, 11, 5758-81	6.4	99
239	The retinal chromophore/chloride ion pair: structure of the photoisomerization path and interplay of charge transfer and covalent states. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6255-60	11.5	99
238	Initial Excited-State Relaxation of the Isolated 11-cis Protonated Schiff Base of Retinal: Evidence for in-Plane Motion from ab Initio Quantum Chemical Simulation of the Resonance Raman Spectrum. *Journal of the American Chemical Society*, **1999**, 121, 1023-1029	16.4	96
237	Molecular "Trigger" for the Radiationless Deactivation of Photoexcited Conjugated Hydrocarbons. *Journal of the American Chemical Society*, **1995**, 117, 11584-11585	16.4	95
236	Classical wavepacket dynamics through a conical intersection. Application to the S1/S0 photochemistry of benzene. *Chemical Physics Letters*, **1995**, 242, 27-32	2.5	93
235	Coherent ultrafast torsional motion and isomerization of a biomimetic dipolar photoswitch. *Physical Chemistry Chemical Physics*, **2010**, 12, 3178-87	3.6	89
234	Do Photochemical Ring-Openings Occur in the Spectroscopic State? 1B2 Pathways for the Cyclohexadiene/Hexatriene Photochemical Interconversion. *The Journal of Physical Chemistry*, **1996**, 100, 19364-19366		89
233	Cooperating Rings incis-Stilbene Lead to an S0/S1Conical Intersection. *Journal of Physical Chemistry A*, **1997**, 101, 3841-3847	2.8	88
232	The molecular mechanism of thermal noise in rod photoreceptors. *Science*, **2012**, 337, 1225-8	33.3	85
231	Counterion controlled photoisomerization of retinal chromophore models: a computational investigation. *Journal of the American Chemical Society*, **2004**, 126, 16018-37	16.4	84
230	Structure of the conical intersections driving the cis-trans photoisomerization of conjugated molecules. *Photochemistry and Photobiology*, **2002**, 76, 622-33	3.6	82
229	New General Tools for Constrained Geometry Optimizations. *Journal of Chemical Theory and Computation*, **2005**, 1, 1029-37	6.4	81
228	Excited-state reaction pathways for s-cis buta-1,3-diene. *Journal of Chemical Physics*, **1995**, 102, 5733-5742	3.9	81
227	Can Fulvene S1 Decay Be Controlled? A CASSCF Study with MMVB Dynamics. *Journal of the American Chemical Society*, **1996**, 118, 5254-5260	16.4	81
226	Excited-state cis-trans isomerization of cis-hexatriene. A CAS-SCF computational study. *Journal of the American Chemical Society*, **1994**, 116, 1077-1085	16.4	81
225	Mechanism of Carbene Formation from the Excited States of Diazirine and Diazomethane: An MC-SCF Study. *Journal of the American Chemical Society*, **1994**, 116, 2064-2074	16.4	81

224	Conical Intersection Mechanism for Photochemical Ring Opening in Benzospiropyran Compounds. *Journal of the American Chemical Society*, **1997**, 119, 10815-10820	16.4	80
223	Computational Photochemistry. *Theoretical and Computational Chemistry*, **2005**, 1-33		80
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221	CASPT2//CASSCF and TDDFT//CASSCF Mapping of the Excited State Isomerization Path of a Minimal Model of the Retinal Chromophore. *Journal of Physical Chemistry A*, **2004**, 108, 1208-1213	2.8	79
220	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
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218	Probing the Photochemical Funnel of a Retinal Chromophore Model via Zero-Point Energy Sampling Semiclassical Dynamics. *Journal of Physical Chemistry A*, **2004**, 108, 4685-4693	2.8	78
217	Force Fields for Ultrafast Photochemistry: The S2 (1Bu) -> S1 (2Ag) -> S0 (1Ag) Reaction Path for all-trans-Hexa-1,3,5-triene. *Journal of the American Chemical Society*, **1997**, 119, 11487-11494	16.4	77
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214	A fast photoswitch for minimally perturbed peptides: investigation of the trans-->cis photoisomerization of N-methylthioacetamide. *Journal of the American Chemical Society*, **2004**, 126, 8823-34	16.4	72
213	Predicting forbidden and allowed cycloaddition reactions: potential surface topology and its rationalization. *Accounts of Chemical Research*, **1990**, 23, 405-412	24.3	72
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211	On the Validity of the McConnell-I Model of Ferromagnetic Interactions: The [2.2]Paracyclophane Example. *Journal of Physical Chemistry A*, **1998**, 102, 8404-8412	2.8	66
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197	Ab initio MC-SCF study of thermal and photochemical [2 + 2] cycloadditions. *Journal of the Chemical Society, Faraday Transactions*, **1994**, 90, 1617		56
196	An MC-SCF/MP2 Study of the Photochemistry of 2,3-Diazabicyclo[2.2.1]hept-2-ene:□Production and Fate of Diazenyl and Hydrazonyl Biradicals. *Journal of the American Chemical Society*, **1998**, 120, 2391-2407	16.4	55
195	Modelling Photochemical Reactivity of Organic Systems □A New Challenge to Quantum Computational Chemistry. *Israel Journal of Chemistry*, **1993**, 33, 265-276	3.4	55
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180	Comparison of the isomerization mechanisms of human melanopsin and invertebrate and vertebrate rhodopsins. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 1714-9	11.5	47
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178	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
177	Conical Intersection Pathways in the Photocycloaddition of Ethene and Benzene: A CASSCF Study with MMVB Dynamics. *Journal of the American Chemical Society*, **1996**, 118, 7353-7360	16.4	46
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172	An MC-SCF Study of Styrene Singlet-State Photoisomerization. *Journal of the American Chemical Society*, **1995**, 117, 6944-6953	16.4	43
171	Fluorescence of radical ions in liquid solution: Wurster’s blue as a case study. *Angewandte Chemie - International Edition*, **2011**, 50, 4496-8	16.4	42

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167	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
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165	Excited-state singlet manifold and oscillatory features of a nonatetraeniminium retinal chromophore model. *Journal of the American Chemical Society*, **2003**, 125, 12509-19	16.4	39
164	Conical Intersections in Charge-Transfer Induced Quenching This work was supported by the Swiss National Science Foundation (Projects 52489.98, 54108.98, and 58000.99), the Fonds der Chemischen Industrie, the Universit□di Siena (Progetto di Ateneo A.A. 99/00), and NATO (CRG 950748).. *Angewandte Chemie - International Edition*, **2000**, 39, 4582-4586	16.4	39
163	Relaxation Paths and Dynamics of Photoexcited Polyene Chains: Evidence for Creation and Annihilation of Neutral Soliton Pairs. *Journal of the American Chemical Society*, **2000**, 122, 5568-5581	16.4	39
162	Substituent Effects in Buta-1,3-diene Photochemistry: A CAS-SCF Study of 2,3-Dimethylbutadiene and 2-Cyanobutadiene Excited-State Reaction Paths. *Journal of the American Chemical Society*, **1994** , 116, 2034-2048	16.4	39
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