Massimo Olivucci

List of Publications by Year in Descending Order

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	Quantum-classical simulations of rhodopsin reveal excited-state population splitting and its effects on quantum efficiency.. *Nature Chemistry*, **2022**,	17.6	4
276	Evolution of the Automatic Rhodopsin Modeling (ARM) Protocol.. *Topics in Current Chemistry*, **2022**, 380, 21	7.2	0
275	Evolution of the Automatic Rhodopsin Modeling (ARM) Protocol. *Topics in Current Chemistry Collections*, **2022**, 105-152	1.8	
274	On the Automatic Construction of QM/MM Models for Biological Photoreceptors: Rhodopsins as Model Systems. *Challenges and Advances in Computational Chemistry and Physics*, **2021**, 1-75	0.7	2
273	Pro219 is an electrostatic color determinant in the light-driven sodium pump KR2. *Communications Biology*, **2021**, 4, 1185	6.7	2
272	On the Transition from a Biomimetic Molecular Switch to a Rotary Molecular Motor. *Journal of Physical Chemistry Letters*, **2021**, 12, 3875-3884	6.4	3
271	Unlocking the Double Bond in Protonated Schiff Bases by Coherent Superposition of S and S. *Journal of Physical Chemistry Letters*, **2021**, 12, 5639-5643	6.4	2
270	QM/MM Investigation of the Spectroscopic Properties of the Fluorophore of Bacterial Luciferase. *Journal of Chemical Theory and Computation*, **2021**, 17, 605-613	6.4	3
269	Effect of charge-transfer enhancement on the efficiency and rotary mechanism of an oxindole-based molecular motor. *Chemical Science*, **2021**, 12, 7486-7497	9.4	5
268	Frontiers in Multiscale Modeling of Photoreceptor Proteins. *Photochemistry and Photobiology*, **2021** , 97, 243-269	3.6	8
267	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
266	Free Energy Computation for an Isomerizing Chromophore in a Molecular Cavity via the Average Solvent Electrostatic Configuration Model: Applications in Rhodopsin and Rhodopsin-Mimicking Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 5885-5895	6.4	2
265	Computational and Spectroscopic Characterization of the Photocycle of an Artificial Rhodopsin. *Journal of Physical Chemistry Letters*, **2020**, 11, 4245-4252	6.4	2
264	Modern quantum chemistry with [Open]Molcas. *Journal of Chemical Physics*, **2020**, 152, 214117	3.9	106
263	Web-ARM: A Web-Based Interface for the Automatic Construction of QM/MM Models of Rhodopsins. *Journal of Chemical Information and Modeling*, **2020**, 60, 1481-1493	6.1	10
262	Excited-State Vibronic Dynamics of Bacteriorhodopsin from Two-Dimensional Electronic Photon Echo Spectroscopy and Multiconfigurational Quantum Chemistry. *Journal of Physical Chemistry Letters*, **2020**, 11, 3889-3896	6.4	4
261	Quantum and Quantum-Classical Studies of the Photoisomerization of a Retinal Chromophore Model. *Journal of Chemical Theory and Computation*, **2020**, 16, 6032-6048	6.4	14

260	Anabaena Sensory Rhodopsin: Effect of point mutations on PSBR photo-isomerization speed. *EPJ Web of Conferences*, **2019**, 205, 10004	0.3	
259	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.4	310
258	Multistate Multiconfiguration Quantum Chemical Computation of the Two-Photon Absorption Spectra of Bovine Rhodopsin. *Journal of Physical Chemistry Letters*, **2019**, 10, 6293-6300	6.4	8
257	Red-shifting mutation of light-driven sodium-pump rhodopsin. *Nature Communications*, **2019**, 10, 1993	17.4	34
256	Bile Acid Binding Protein Functionalization Leads to a Fully Synthetic Rhodopsin Mimic. *Journal of Physical Chemistry Letters*, **2019**, 10, 2235-2243	6.4	7
255	a-ARM: Automatic Rhodopsin Modeling with Chromophore Cavity Generation, Ionization State Selection, and External Counterion Placement. *Journal of Chemical Theory and Computation*, **2019**, 15, 3134-3152	6.4	25
254	Assessment of MC-PDFT Excitation Energies for a Set of QM/MM Models of Rhodopsins. *Journal of Chemical Theory and Computation*, **2019**, 15, 1915-1923	6.4	8
253	Synthesis, spectroscopy and QM/MM simulations of a biomimetic ultrafast light-driven molecular motor. *Photochemical and Photobiological Sciences*, **2019**, 18, 2259-2269	4.2	12
252	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
251	Two-State, Three-Mode Parametrization of the Force Field of a Retinal Chromophore Model. *Journal of Physical Chemistry A*, **2019**, 123, 1710-1719	2.8	10
250	Fluorescence Enhancement of a Microbial Rhodopsin via Electronic Reprogramming. *Journal of the American Chemical Society*, **2019**, 141, 262-271	16.4	23
249	Vibrational coherence and quantum yield of retinal-chromophore-inspired molecular switches. *Faraday Discussions*, **2019**, 221, 299-321	3.6	8
248	Engineering the vibrational coherence of vision into a synthetic molecular device. *Nature Communications*, **2018**, 9, 313	17.4	29
247	Evidence for a vibrational phase-dependent isotope effect on the photochemistry of vision. *Nature Chemistry*, **2018**, 10, 449-455	17.6	56
246	A Comparative Study of Modern Homology Modeling Algorithms for Rhodopsin Structure Prediction. *ACS Omega*, **2018**, 3, 7555-7566	3.9	29
245	Effect of point mutations on the ultrafast photo-isomerization of Anabaena sensory rhodopsin. *Faraday Discussions*, **2018**, 207, 55-75	3.6	13
244	Electronic State Mixing Controls the Photoreactivity of a Rhodopsin with all- trans Chromophore Analogues. *Journal of Physical Chemistry Letters*, **2018**, 9, 6350-6355	6.4	13
243	Systematic Excited State Studies of Reversibly Switchable Fluorescent Proteins. *Journal of Chemical Theory and Computation*, **2018**, 14, 3163-3172	6.4	7

242	Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landau-Zener Model. *Journal of Physical Chemistry Letters*, **2018**, 9, 3315-3322	6.4	20
241	Ab Initio Investigation of Photochemical Reaction Mechanisms: From Isolated Molecules to Complex Environments **2017**, 1943-1994		
240	Optomechanical Control of Quantum Yield in Trans-Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. *Angewandte Chemie - International Edition*, **2017**, 56, 3842-3846	16.4	18
239	Optomechanical Control of Quantum Yield in Trans□Cis Ultrafast Photoisomerization of a Retinal Chromophore Model. *Angewandte Chemie*, **2017**, 129, 3900-3904	3.6	3
238	Theory and Simulation of the Ultrafast Double-Bond Isomerization of Biological Chromophores. *Chemical Reviews*, **2017**, 117, 13502-13565	68.1	160
237	Impact of Electronic State Mixing on the Photoisomerization Time Scale of the Retinal Chromophore. *Journal of Physical Chemistry Letters*, **2017**, 8, 5222-5227	6.4	23
236	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
235	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
234	Mechanism of excited state deactivation of indan-1-ylidene and fluoren-9-ylidene malononitriles. *Physical Chemistry Chemical Physics*, **2016**, 18, 32786-32795	3.6	8
233	Space and Time Evolution of the Electrostatic Potential During the Activation of a Visual Pigment. *Journal of Physical Chemistry Letters*, **2016**, 7, 2563-7	6.4	7
232	Design, Synthesis, and Dynamics of a Green Fluorescent Protein Fluorophore Mimic with an Ultrafast Switching Function. *Journal of the American Chemical Society*, **2016**, 138, 9807-25	16.4	32
231	Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. *Journal of Chemical Theory and Computation*, **2016**, 12, 839-50	6.4	38
230	Ab Initio Investigation of Photochemical Reaction Mechanisms: From Isolated Molecules to Complex Environments **2016**, 1-52		
229	Modulation of thermal noise and spectral sensitivity in Lake Baikal cottoid fish rhodopsins. *Scientific Reports*, **2016**, 6, 38425	4.9	19
228	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. *Journal of Computational Chemistry*, **2016**, 37, 506-41	3.5	1047
227	Role of the Molecular Environment in Flavoprotein Color and Redox Tuning: QM Cluster versus QM/MM Modeling. *Journal of Chemical Theory and Computation*, **2015**, 11, 3878-94	6.4	23
226	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
225	Molecular bases for the selection of the chromophore of animal rhodopsins. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 15297-302	11.5	33

224	A surface hopping algorithm for nonadiabatic minimum energy path calculations. *Journal of Computational Chemistry*, **2015**, 36, 312-20	3.5	6
223	Quantum Monte Carlo Treatment of the Charge Transfer and Diradical Electronic Character in a Retinal Chromophore Minimal Model. *Journal of Chemical Theory and Computation*, **2015**, 11, 992-1005	6.4	35
222	Directionality of Double-Bond Photoisomerization Dynamics Induced by a Single Stereogenic Center. *Journal of Physical Chemistry Letters*, **2015**, 6, 599-604	6.4	46
221	Ultrafast Photoisomerization of Chiral Biomimetic Molecular Switches. *Springer Proceedings in Physics*, **2015**, 517-520	0.2	
220	Initial excited-state dynamics of an N-alkylated indanylidene-pyrroline (NAIP) rhodopsin analog. *Journal of Physical Chemistry B*, **2014**, 118, 12243-50	3.4	9
219	Learning from photobiology how to design molecular devices using a computer. *Chemical Society Reviews*, **2014**, 43, 4019-36	58.5	35
218	A Conical Intersection Controls the Deactivation of the Bacterial Luciferase Fluorophore. *Angewandte Chemie*, **2014**, 126, 10028-10033	3.6	7
217	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
216	Designing conical intersections for light-driven single molecule rotary motors: from precessional to axial motion. *Journal of Organic Chemistry*, **2014**, 79, 3587-600	4.2	53
215	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
214	A conical intersection controls the deactivation of the bacterial luciferase fluorophore. *Angewandte Chemie - International Edition*, **2014**, 53, 9870-5	16.4	19
213	Toward an understanding of the retinal chromophore in rhodopsin mimics. *Journal of Physical Chemistry B*, **2013**, 117, 10053-70	3.4	35
212	Mapping the Excited State Potential Energy Surface of a Retinal Chromophore Model with Multireference and Equation-of-Motion Coupled-Cluster Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 4495-506	6.4	76
211	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
210	Probing vibrationally mediated ultrafast excited-state reaction dynamics with multireference (CASPT2) trajectories. *Journal of Physical Chemistry A*, **2013**, 117, 11271-5	2.8	2
209	Effects of the protein environment on the spectral properties of tryptophan radicals in Pseudomonas aeruginosa azurin. *Journal of the American Chemical Society*, **2013**, 135, 4822-33	16.4	22
208	Influence of the Chemical Design on the Coherent Photoisomerization of Biomimetic Molecular Switches. *EPJ Web of Conferences*, **2013**, 41, 05006	0.3	0
207	Inverse versus Normal Dithienylethenes: Computational Investigation of the Photocyclization Reaction. *Journal of Physical Chemistry Letters*, **2013**, 4, 2190-2196	6.4	35

206	Combined Self-Consistent-Field and Spin-Flip Tamm-Dancoff Density Functional Approach to Potential Energy Surfaces for Photochemistry. *Journal of Physical Chemistry Letters*, **2013**, 4, 253-8	6.4	41
205	Conical Intersection and Potential Energy Surface Features of a Model Retinal Chromophore: Comparison of EOM-CC and Multireference Methods. *Journal of Chemical Theory and Computation*, **2013**, 9, 284-92	6.4	62
204	Isomer-dependent vibrational coherence in ultrafast photoisomerization. *New Journal of Physics*, **2013**, 15, 105022	2.9	14
203	Computational Photochemistry and Photobiology **2012**, 1029-1056		4
202	Toward a stable □-cycloalkyl amino acid with a photoswitchable cationic side chain. *Journal of Organic Chemistry*, **2012**, 77, 1738-48	4.2	16
201	Mechanistic origin of the vibrational coherence accompanying the photoreaction of biomimetic molecular switches. *Chemistry - A European Journal*, **2012**, 18, 15296-304	4.8	43
200	Origin of Fluorescence in 11-cis Locked Bovine Rhodopsin. *Journal of Chemical Theory and Computation*, **2012**, 8, 2559-63	6.4	27
199	Photoisomerization and relaxation dynamics of a structurally modified biomimetic photoswitch. *Journal of Physical Chemistry A*, **2012**, 116, 3527-33	2.8	29
198	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
197	Quantum chemical modeling of rhodopsin mutants displaying switchable colors. *Physical Chemistry Chemical Physics*, **2012**, 14, 12485-95	3.6	54
196	Ab Initio Investigation of Photochemical Reaction Mechanisms: From Isolated Molecules to Complex Environments **2012**, 1359-1404		1
195	The molecular mechanism of thermal noise in rod photoreceptors. *Science*, **2012**, 337, 1225-8	33.3	85
194	Using the computer to understand the chemistry of conical intersections. *Photochemical and Photobiological Sciences*, **2011**, 10, 867-86	4.2	56
193	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
192	Unique QM/MM potential energy surface exploration using microiterations. *International Journal of Quantum Chemistry*, **2011**, 111, 3339-3346	2.1	50
191	Fluoreszenz von Radikalionen in flüssiger Phase: der Fall Wursters Blau. *Angewandte Chemie*, **2011**, 123, 4589-4591	3.6	9
190	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
189	Fast excited-state deactivation in N(5)-ethyl-4a-hydroxyflavin pseudobase. *Journal of Physical Chemistry B*, **2011**, 115, 7136-43	3.4	18

188	Linear dichroism amplification: adapting a long-known technique for ultrasensitive femtosecond IR spectroscopy. *Journal of Chemical Physics*, **2011**, 134, 124516	3.9	10
187	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
186	Computational Photobiology and Beyond. *Australian Journal of Chemistry*, **2010**, 63, 413	1.2	34
185	Coherent ultrafast torsional motion and isomerization of a biomimetic dipolar photoswitch. *Physical Chemistry Chemical Physics*, **2010**, 12, 3178-87	3.6	89
184	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
183	Aborted double bicycle-pedal isomerization with hydrogen bond breaking is the primary event of bacteriorhodopsin proton pumping. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20172-7	11.5	74
182	Matrix isolation and computational studies of the CF2I radical. *Chemical Physics Letters*, **2010**, 496, 68-73	2.5	7
181	How Does the Relocation of Internal Water Affect Resonance Raman Spectra of Rhodopsin? An Insight from CASSCF/Amber Calculations. *Journal of Chemical Theory and Computation*, **2009**, 5, 3096-104	6.4	11
180	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
179	Protein Influence on Electronic Spectra Modeled by Multipoles and Polarizabilities. *Journal of Chemical Theory and Computation*, **2009**, 5, 649-58	6.4	58
178	Structure of the photochemical reaction path populated via promotion of CF(2)I(2) into its first excited state. *Journal of Physical Chemistry A*, **2009**, 113, 10767-71	2.8	17
177	Fluorenylidene-pyrroline biomimetic light-driven molecular switches. *Journal of Organic Chemistry*, **2009**, 74, 4666-74	4.2	33
176	A novel biomimetic photochemical switch at work: design of a photomodulable peptide. *Photochemical and Photobiological Sciences*, **2009**, 8, 1639-49	4.2	12
175	Ultrafast Isomerization Dynamics of Biomimetic Photoswitches. *Springer Series in Chemical Physics*, **2009**, 343-345	0.3	
174	Relationship between the excited state relaxation paths of rhodopsin and isorhodopsin. *Journal of the American Chemical Society*, **2008**, 130, 3382-8	16.4	56
173	Origin of the absorption maxima of the photoactive yellow protein resolved via ab initio multiconfigurational methods. *Journal of Physical Chemistry B*, **2008**, 112, 7153-6	3.4	29
172	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
171	Recent applications of a QM/MM scheme at the CASPT2//CASSCF/AMBER (or CHARMM) level of theory in photochemistry and photobiology. *Journal of Physics: Conference Series*, **2008**, 101, 012001	0.3	5

170	Chemical selectivity through control of excited-state dynamics. *Angewandte Chemie - International Edition*, **2008**, 47, 6322-5	16.4	38
169	Chemische Selektivität durch Kontrolle der Dynamik angeregter Zustände. *Angewandte Chemie*, **2008**, 120, 6420-6424	3.6	8
168	Switching on molecular iodine elimination through isomerization: The F2CI isomer of difluorodiiodomethane. *Chemical Physics Letters*, **2008**, 462, 192-195	2.5	15
167	Effect of opsin on the shape of the potential energy surfaces at the conical intersection of the Rhodopsin chromophore. *Chemical Physics*, **2008**, 347, 483-491	2.3	10
166	Photostability versus photodegradation in the excited-state intramolecular proton transfer of nitro enamines: competing reaction paths and conical intersections. *Journal of the American Chemical Society*, **2007**, 129, 3703-13	16.4	31
165	The role of the intersection space in the photochemistry of tricyclo[3.3.0.0(2,6)]octa-3,7-diene. *Journal of Physical Chemistry A*, **2007**, 111, 2830-8	2.8	6
164	Quantum chemical modeling and preparation of a biomimetic photochemical switch. *Angewandte Chemie - International Edition*, **2007**, 46, 414-20	16.4	53
163	Quantum Chemical Modeling and Preparation of a Biomimetic Photochemical Switch. *Angewandte Chemie*, **2007**, 119, 418-424	3.6	9
162	Synthesis of biomimetic light-driven molecular switches via a cyclopropyl ring-opening/nitrilium ion ring-closing tandem reaction. *Tetrahedron*, **2007**, 63, 4975-4982	2.4	22
161	Structure of the Conical Intersections Driving the cis–trans Photoisomerization of Conjugated Molecules. *Photochemistry and Photobiology*, **2007**, 76, 622-633	3.6	3
160	Complex excited dynamics around a plateau on a retinal-like potential surface: chaos, multi-exponential decays and quantum/classical differences. *Theoretical Chemistry Accounts*, **2007**, 117, 1061-1072	1.9	14
159	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
158	A Computational Strategy for Organic Photochemistry. *Reviews in Computational Chemistry*, **2007**, 87-146		106
157	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
156	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
155	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
154	Toward a computational photobiology. *Pure and Applied Chemistry*, **2005**, 77, 977-993	2.1	10
153	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

152	The ring-opening reaction of chromenes: a photochemical mode-dependent transformation. *Journal of Physical Chemistry A*, **2005**, 109, 8684-92	2.8	38
151	Mechanism of the N-cyclopropylimine-1-pyrroline photorearrangement. *Journal of the American Chemical Society*, **2005**, 127, 441-8	16.4	30
150	Structure, spectroscopy, and spectral tuning of the gas-phase retinal chromophore: the beta-ionone "handle" and alkyl group effect. *Journal of Physical Chemistry A*, **2005**, 109, 6597-605	2.8	79
149	Photoisomerization mechanism of 11-cis-locked artificial retinal chromophores: acceleration and primary photoproduct assignment. *Journal of the American Chemical Society*, **2005**, 127, 2433-42	16.4	25
148	Toward accurate computations in photobiology **2005**, 269-289		1
147	New General Tools for Constrained Geometry Optimizations. *Journal of Chemical Theory and Computation*, **2005**, 1, 1029-37	6.4	81
146	Mechanism of the Norrish-Yang photocyclization reaction of an alanine derivative in the singlet state: origin of the chiral-memory effect. *Angewandte Chemie - International Edition*, **2005**, 44, 2390-3	16.4	32
145	Mechanism of the initial conformational transition of a photomodulable peptide. *Angewandte Chemie - International Edition*, **2005**, 44, 6077-81	16.4	13
144	A tiny excited-state barrier can induce a multiexponential decay of the retinal chromophore: a quantum dynamics investigation. *Angewandte Chemie - International Edition*, **2005**, 44, 5118-21	16.4	48
143	Mechanism of the Norrish□Yang Photocyclization Reaction of an Alanine Derivative in the Singlet State: Origin of the Chiral-Memory Effect. *Angewandte Chemie*, **2005**, 117, 2442-2445	3.6	8
142	Mechanism of the Initial Conformational Transition of a Photomodulable Peptide. *Angewandte Chemie*, **2005**, 117, 6231-6235	3.6	2
141	A Tiny Excited-State Barrier Can Induce a Multiexponential Decay of the Retinal Chromophore: A Quantum Dynamics Investigation. *Angewandte Chemie*, **2005**, 117, 5248-5251	3.6	10
140	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
139	Computational Photochemistry. *Theoretical and Computational Chemistry*, **2005**, 1-33		80
138	Computational Investigation of Photochemical Reaction Mechanisms. *Molecular and Supramolecular Photochemistry*, **2005**, 31-110		2
137	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
136	CONICAL INTERSECTIONS AND ORGANIC REACTION MECHANISMS. *Advanced Series in Physical Chemistry*, **2004**, 271-320		45
135	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

134	An innovative approach to the design of plastic antibodies: molecular imprinting via a non-polar transition state analogue. *Journal of Molecular Catalysis A*, **2004**, 217, 31-36		22
133	Structure of the intersection space associated with ZIE photoisomerization of retinal in rhodopsin proteins. *Faraday Discussions*, **2004**, 127, 179-91	3.6	58
132	Counterion controlled photoisomerization of retinal chromophore models: a computational investigation. *Journal of the American Chemical Society*, **2004**, 126, 16018-37	16.4	84
131	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
130	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
129	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
128	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
127	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
126	Design and photochemical characterization of a biomimetic light-driven Z/E switcher. *Journal of the American Chemical Society*, **2004**, 126, 9349-59	16.4	53
125	Ground and excited state CASPT2 geometry optimizations of small organic molecules. *Journal of Computational Chemistry*, **2003**, 24, 298-309	3.5	118
124	A simple approach for improving the hybrid MMVB force field: application to the photoisomerization of s-cis butadiene. *Journal of Computational Chemistry*, **2003**, 24, 1357-63	3.5	28
123	The amide bond: pitfalls and drawbacks of the link atom scheme. *Computational and Theoretical Chemistry*, **2003**, 632, 71-82		45
122	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
121	Computational study on the origin of the stereoselectivity for the photochemical denitrogenation of diazabicycloheptene. *Journal of the American Chemical Society*, **2003**, 125, 10947-59	16.4	36
120	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
119	Photoisomerization acceleration in retinal protonated Schiff-base models. *Photochemical and Photobiological Sciences*, **2003**, 2, 1250-5	4.2	25
118	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
117	Computer simulation of photoinduced molecular motion and reactivity. *International Journal of Photoenergy*, **2002**, 4, 57-68	2.1	14

116	Retinal chromophore photoinduced molecular motion and reactivity: isolated conditions and counterion effects. *Journal of Computational Methods in Sciences and Engineering*, **2002**, 2, 431-439	0.3	
115	Cyclooctatetraene computational photo- and thermal chemistry: a reactivity model for conjugated hydrocarbons. *Journal of the American Chemical Society*, **2002**, 124, 13770-89	16.4	60
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