Samer Gozem

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

45 papers	1,571 citations	21 h-index	39 g-index
56 ext. papers	1,810 ext. citations	10 avg, IF	4.75 L-index

#	Paper	IF	Citations
45	OS100: A Benchmark Set of 100 Digitized UV-Visible Spectra and Derived Experimental Oscillator Strengths.. *Journal of Physical Chemistry A*, **2022**,	2.8	1
44	Quantum-classical simulations of rhodopsin reveal excited-state population splitting and its effects on quantum efficiency.. *Nature Chemistry*, **2022**,	17.6	4
43	Cyclopropenone (c-C3H2O) as a Tracer of the Nonequilibrium Chemistry Mediated by Galactic Cosmic Rays in Interstellar Ices. *Astrophysical Journal*, **2021**, 911, 24	4.7	3
42	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
41	A Single-Point Mutation in d-Arginine Dehydrogenase Unlocks a Transient Conformational State Resulting in Altered Cofactor Reactivity. *Biochemistry*, **2021**, 60, 711-724	3.2	4
40	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
39	Ionic Atmosphere Effect on the Absorption Spectrum of a Flavoprotein: A Reminder to Consider Solution Ions. *Journal of Physical Chemistry Letters*, **2021**, 12, 8384-8396	6.4	1
38	Tuning Protein Dynamics to Sense Rapid Endoplasmic-Reticulum Calcium Dynamics. *Angewandte Chemie - International Edition*, **2021**, 60, 23289-23298	16.4	0
37	Tuning Protein Dynamics to Sense Rapid Endoplasmic-Reticulum Calcium Dynamics. *Angewandte Chemie*, **2021**, 133, 23477	3.6	0
36	The effect of hydrogen-bonding on flavin's infrared absorption spectrum. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 262, 120110	4.4	3
35	Probing the Electronic Structure of Bulk Water at the Molecular Length Scale with Angle-Resolved Photoelectron Spectroscopy. *Journal of Physical Chemistry Letters*, **2020**, 11, 5162-5170	6.4	14
34	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
33	Electrostatic Spectral Tuning Maps for Biological Chromophores. *Journal of Physical Chemistry B*, **2019**, 123, 4813-4824	3.4	14
32	Fluorescence Properties of Flavin Semiquinone Radicals in Nitronate Monooxygenase. *ChemBioChem*, **2019**, 20, 1646-1652	3.8	13
31	Electronic spectra of flavin in different redox and protonation states: a computational perspective on the effect of the electrostatic environment. *Physical Chemistry Chemical Physics*, **2019**, 21, 16526-16537	3.6	21
30	Vacuum ultraviolet photoionization cross section of the hydroxyl radical. *Journal of Chemical Physics*, **2018**, 148, 184302	3.9	15
29	Fluorescence-Based Assay for Carbonic Anhydrase Inhibitors. *CheM*, **2017**, 2, 271-282	16.2	14

28	Theory and Simulation of the Ultrafast Double-Bond Isomerization of Biological Chromophores. *Chemical Reviews*, **2017**, 117, 13502-13565	68.1	160
27	Photoelectron Spectroscopy Study of Quinonimides. *Journal of the American Chemical Society*, **2017**, 139, 11138-11148	16.4	14
26	Supramolecular Sensors for Opiates and Their Metabolites. *Journal of the American Chemical Society*, **2017**, 139, 14954-14960	16.4	53
25	Electronic Spectra of Tris(2,2Sbipyridine)-M(II) Complex Ions in Vacuo (M = Fe and Os). *Inorganic Chemistry*, **2017**, 56, 7029-7037	5.1	12
24	Probing the Photodynamics of Rhodopsins with Reduced Retinal Chromophores. *Journal of Chemical Theory and Computation*, **2016**, 12, 839-50	6.4	38
23	A study of interstellar aldehydes and enols as tracers of a cosmic ray-driven nonequilibrium synthesis of complex organic molecules. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 7727-32	11.5	77
22	Photoelectron wave function in photoionization: plane wave or Coulomb wave?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4532-40	6.4	97
21	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
20	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
19	Ligand influence on the electronic spectra of monocationic copper-bipyridine complexes. *Physical Chemistry Chemical Physics*, **2015**, 17, 31938-46	3.6	29
18	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
17	Learning from photobiology how to design molecular devices using a computer. *Chemical Society Reviews*, **2014**, 43, 4019-36	58.5	35
16	A Conical Intersection Controls the Deactivation of the Bacterial Luciferase Fluorophore. *Angewandte Chemie*, **2014**, 126, 10028-10033	3.6	7
15	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
14	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
13	A conical intersection controls the deactivation of the bacterial luciferase fluorophore. *Angewandte Chemie - International Edition*, **2014**, 53, 9870-5	16.4	19
12	Toward an understanding of the retinal chromophore in rhodopsin mimics. *Journal of Physical Chemistry B*, **2013**, 117, 10053-70	3.4	35
11	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

10	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
9	Probing vibrationally mediated ultrafast excited-state reaction dynamics with multireference (CASPT2) trajectories. *Journal of Physical Chemistry A*, **2013**, 117, 11271-5	2.8	2
8	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
7	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
6	Computational Photochemistry and Photobiology **2012**, 1029-1056		4
5	Origin of Fluorescence in 11-cis Locked Bovine Rhodopsin. *Journal of Chemical Theory and Computation*, **2012**, 8, 2559-63	6.4	27
4	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
3	The molecular mechanism of thermal noise in rod photoreceptors. *Science*, **2012**, 337, 1225-8	33.3	85
2	Calculations on the Kinetics, Thermodynamics, and Selectivity of Methyl Radical Addition to Olefins Coordinated to d8 and d0 Transition-Metal Fragments: Two Distinct and Opposite anti-EvansPolanyi Effects with Potential Practical Implications. *Organometallics*, **2008**, 27, 5426-5429	3.8	9
1	The ezSpectra suite: An easy-to-use toolkit for spectroscopy modeling. *Wiley Interdisciplinary Reviews: Computational Molecular Science*,e1546	7.9	21