Oliver Weingart

List of Publications by Year
in descending order

59 papers	4,354 citations	186265 28 h-index	149698 56 g-index
61 all docs	61 docs citations	61 times ranked	5083 citing authors

#	Article	IF	Citations
1	<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
2	Conical intersection dynamics of the primary photoisomerization event in vision. Nature, 2010, 467, 440-443.	27.8	779
3	Coordinatively unsaturated metal sites (open metal sites) in metalâ€“organic frameworks: design and applications. Chemical Society Reviews, 2020, 49, 2751-2798.	38.1	449
4	Metalâ€“Organic Frameworks with Potential Application for SO₂ Separation and Flue Gas Desulfurization. ACS Applied Materials & Interfaces, 2019, 11, 17350-17358.	8.0	143
5	Chiral Pathways and Periodic Decay in cis-Azobenzene Photodynamics. Journal of Physical Chemistry Letters, 2011, 2, 1506-1509.	4.6	129
6	Capture and Separation of SO₂ Traces in Metalâ€“Organic Frameworks via Preâ€Synthetic Pore Environment Tailoring by Methyl Groups. Angewandte Chemie - International Edition, 2021, 60, 17998-18005.	13.8	92
7	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.	2.5	81
8	Substrate-induced symmetry reduction of CuPc on Cu(111): An LT-STM study. Surface Science, 2009, 603, L39-L43.	1.9	73
9	Bicycle-Pedal Isomerization in a Rhodopsin Chromophore Model. Journal of the American Chemical Society, 2009, 131, 16-17.	13.7	72
10	Product formation in rhodopsin by fast hydrogen motions. Physical Chemistry Chemical Physics, 2011, 13, 3645.	2.8	70
11	Cooperating Dinitrogen and Phenyl Rotations in trans-Azobenzene Photoisomerization. Journal of Chemical Theory and Computation, 2012, 8, 2352-2358.	5.3	68
12	The Twisted C11C12 Bond of the Rhodopsin ChromophoreA Photochemical Hot Spot. Journal of the American Chemical Society, 2007, 129, 10618-10619.	13.7	59
13	Zirconium and Aluminum MOFs for Low-Pressure SO₂ Adsorption and Potential Separation: Elucidating the Effect of Small Pores and NH₂ Groups. ACS Applied Materials & Interfaces, 2021, 13, 29137-29149.	8.0	59
14	Ground and Excited States of Retinal Schiff Base Chromophores by Multiconfigurational Perturbation Theory. Biophysical Journal, 2006, 91, L07-L09.	0.5	58
15	COBRAMM 2.0 â€” A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations. Journal of Molecular Modeling, 2018, 24, 271.	1.8	55
16	Photochemistry of Visual Pigment Chromophore Models by Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2007, 111, 3782-3788.	2.6	51
17	Interfacial States in Donorâ€“Acceptor Organic Heterojunctions: Computational Insights into Thiophene-Oligomer/Fullerene Junctions. Journal of Chemical Theory and Computation, 2013, 9, 533-542.	5.3	45
18	Wavepacket Splitting and Twoâ€Pathway Deactivation in the Photoexcited Visual Pigment Isorhodopsin. Angewandte Chemie - International Edition, 2014, 53, 2504-2507.	13.8	45

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19	Electron promotion and electronic friction in atomic collision cascades. New Journal of Physics, 2007, 9, 38-38.	2.9	41
20	Nonadiabatic Decay Dynamics of a Benzylidene Malononitrile. Journal of Physical Chemistry A, 2012, 116, 1510-1518.	2.5	38
21	Modelling Time-Resolved Two-Dimensional Electronic Spectroscopy of the Primary Photoisomerization Event in Rhodopsin. Journal of Physical Chemistry B, 2014, 118, 8396-8405.	2.6	35
22	Tracking the primary photoconversion events in rhodopsins by ultrafast optical spectroscopy. Photochemical and Photobiological Sciences, 2015, 14, 213-228.	2.9	35
23	Protein Assistance in the Photoisomerization of Rhodopsin and 9-cis-RhodopsinInsights from Experiment and Theory. Journal of the American Chemical Society, 2007, 129, 1052-1054.	13.7	34
24	Encapsulation of Phosphorescent Pt(II) Complexes in Zn-Based Metalâ€“Organic Frameworks toward Oxygen-Sensing Porous Materials. Inorganic Chemistry, 2020, 59, 7252-7264.	4.0	34
25	Sampling excited state dynamics: influence of HOOP mode excitations in a retinal model. Physical Chemistry Chemical Physics, 2012, 14, 14299.	2.8	32
26	Tracking excited state decay mechanisms of pyrimidine nucleosides in real time. Nature Communications, 2021, 12, 7285.	12.8	32
27	The photoformation of a phthalide: a ketene intermediate traced by FSRS. Physical Chemistry Chemical Physics, 2015, 17, 376-386.	2.8	29
28	Spectral properties and isomerisation path of retinal in C1C2 channelrhodopsin. Physical Chemistry Chemical Physics, 2015, 17, 25142-25150.	2.8	28
29	Relationship between Excited State Lifetime and Isomerization Quantum Yield in Animal Rhodopsins: Beyond the One-Dimensional Landauâ€“Zener Model. Journal of Physical Chemistry Letters, 2018, 9, 3315-3322.	4.6	28
30	Bond torsion affects the product distribution in the photoreaction of retinal model chromophores. Journal of Molecular Modeling, 2006, 12, 713-721.	1.8	27
31	Density-functional theory study of vibrational relaxation of CO stretching excitation on Si(100). Journal of Chemical Physics, 2008, 129, 174702.	3.0	27
32	The role of HOOP-modes in the ultrafast photo-isomerization of retinal models. Chemical Physics, 2008, 349, 348-355.	1.9	26
33	Fast Photoisomerization of a Rhodopsin Modelâ€”An Ab Initio Molecular Dynamics Study. Angewandte Chemie - International Edition, 2000, 39, 2784-2786.	13.8	24
34	Modeling hot-electron generation induced by electron promotion in atomic collision cascades in metals. Physical Review B, 2008, 77, .	3.2	23
35	Excited state molecular dynamics of retinal model chromophores. Phase Transitions, 2005, 78, 17-24.	1.3	22
36	Modelling vibrational coherence in the primary rhodopsin photoproduct. Journal of Chemical Physics, 2012, 137, 22A523.	3.0	22

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37	Combined Quantum and Molecular Mechanics (QM/MM) Approaches to Simulate Ultrafast Photodynamics in Biological Systems. Current Organic Chemistry, 2017, 21, 586-601.	1.6	19
38	Periodic decay in the photoisomerisation of p-aminoazobenzene. Physical Chemistry Chemical Physics, 2013, 15, 11814.	2.8	17
39	Impact of fluorination on the photophysics of the flavin chromophore: a quantum chemical perspective. Physical Chemistry Chemical Physics, 2019, 21, 9912-9923.	2.8	16
40	Dual Photochemical Reaction Pathway in Flavin-Based Photoreceptor LOV Domain: A Combined Quantum-Mechanics/Molecular-Mechanics Investigation. Journal of Physical Chemistry B, 2017, 121, 9583-9596.	2.6	14
41	QM/MM Photodynamics of Retinal in the Channelrhodopsin Chimera C1C2 with OM3/MRCI. ChemPhotoChem, 2019, 3, 107-116.	3.0	11
42	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	2.9	10
43	Cyclic diphenic hydrazide: crystal structure, resolution, absolute configuration, and enantiomerization pathway investigation. Tetrahedron: Asymmetry, 2004, 15, 537-543.	1.8	9
44	Femtosecond Spectroscopy of Calcium Dipicolinateâ€"A Major Component of Bacterial Spores. Journal of Physical Chemistry B, 2016, 120, 9376-9386.	2.6	9
45	Fluorinated azobenzenes as supramolecular halogen-bonding building blocks. Beilstein Journal of Organic Chemistry, 2019, 15, 2013-2019.	2.2	9
46	On the role of electronic friction and electron promotion in kinetic excitation of solids. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 281-285.	1.4	8
47	New Perspectives on an Old Issue: A Comparative MSâ€CASPT2 and OM2â€MRCI Study of Polyenes and Protonated Schiff Bases. Photochemistry and Photobiology, 2017, 93, 1345-1355.	2.5	8
48	The role of electronic friction of low-energy recoils in atomic collision cascades. Nuclear Instruments & Methods in Physics Research B, 2007, 258, 83-86.	1.4	7
49	On the large apparent Stokes shift of phthalimides. Physical Chemistry Chemical Physics, 2019, 21, 4839-4853.	2.8	7
50	Einlagerung und Abtrennung von SO 2 â€Spuren in Metallâ€organischen GerÃ¼stverbindungen durch prÃsynthetische Anpassung der Porenumgebung mit Methylgruppen. Angewandte Chemie, 2021, 133, 18145-18153.	2.0	6
51	Supramolecular networks by imine halogen bonding. Chemical Communications, 2022, , .	4.1	5
52	Solid-State Landscape of 4,4â€²-Azobis(3,5-dimethyl-1H-pyrazole) with the Isolation of Conformer-Dependent Polymorphs. Crystal Growth and Design, 2020, 20, 2721-2733.	3.0	4
53	The Photophysics of Dibenzo[a,j]phenazine. ChemPhotoChem, 2021, 5, 335-347.	3.0	3
54	Structural and Energetic Aspects of Entacapone-Theophylline-Water Cocrystal. Solids, 2022, 3, 66-92.	2.4	3

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55	Excited State Isomerization of Small Polyeneiminium Ions - The Influence of Initial Torsion and Methyl Substitution on Md-Calculated Reaction Dynamics. Phase Transitions, 2002, 75, 19-29.	1.3	2
56	Protein Induced Torsion of the Retinal Chromophore and How it Affects the Photochemistry of Rhopdopsin. AIP Conference Proceedings, 2007, , .	0.4	0
57	Introductionâ€"Festschrift in Honor of Prof. Volker BuÃŸ. Photochemistry and Photobiology, 2017, 93, 1335-1335.	2.5	0
58	The Photophysics of Dibenzo[a,j]phenazine. ChemPhotoChem, 2021, 5, 297-297.	3.0	0
59	Bond torsion affects the product distribution in the photoreaction of retinal model chromophores. , 0, , 713-721.		0