Markus Oppel

List of Publications by Year
in descending order

30	1,276	840776 11	477307 29
papers	citations	h-index	g-index

34	34	34	1555
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Oxygenâ€Doped PAH Electrochromes: Difurano, Dipyrano, and Furanoâ€Pyrano Containing Naphthaleneâ€Cored Molecules. European Journal of Organic Chemistry, 2022, 2022, .	2.4	7
2	GÃ–CHâ€Arbeitsgruppen stellen sich vor: AG â€žComputational Chemistryâ€œ. Nachrichten Aus Der Chemie, 2022, 70, 82-83.	0.0	0
3	A Density Matrix Renormalization Group Study of the Lowâ€Lying Excited States of a Molybdenum Carbonylâ€Nitrosyl Complex. ChemPhysChem, 2021, 22, 2371-2377.	2.1	2
4	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
5	OpenMolcas: From Source Code to Insight. Journal of Chemical Theory and Computation, 2019, 15, 5925-5964.	5.3	661
6	Discrimination of 1,1-difluoroethylene nuclear spin isomers in the presence of non-adiabatic coupling terms. Chemical Physics Letters, 2017, 683, 205-210.	2.6	3
7	Controlling the Excited-State Dynamics of Nuclear Spin Isomers Using the Dynamic Stark Effect. Journal of Physical Chemistry A, 2016, 120, 4907-4914.	2.5	4
8	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. Journal of Chemical Theory and Computation, 2016, 12, 1207-1219.	5.3	145
9	Enhancing Intersystem Crossing in Phenotiazinium Dyes by Intercalation into DNA. Angewandte Chemie - International Edition, 2015, 54, 4375-4378.	13.8	56
10	Separating nuclear spin isomers using a pumpâ€“dump laser scheme. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	4
11	Discrimination of nuclear spin isomers exploiting the excited state dynamics of a quinodimethane derivative. Journal of Chemical Physics, 2014, 141, 164323.	3.0	7
12	Nuclear Spin Selective Torsional States: Implications of Molecular Symmetry. Zeitschrift Fur Physikalische Chemie, 2013, 227, 1021-1048.	2.8	9
13	Theory of ultrafast nonresonant multiphoton transitions in polyatomic molecules: Basics and application to optimal control theory. Journal of Chemical Physics, 2007, 127, 144102.	3.0	5
14	Application of optimal control theory to ultrafast nonresonant multiphoton transitions in polyatomic molecules. Optics Communications, 2006, 264, 502-510.	2.1	8
15	Control of breaking strong versus weak bonds of BaFCH3 by femtosecond IR + VIS laser pulses: theory and experiment. Physical Chemistry Chemical Physics, 2004, 6, 4283.	2.8	11
16	IRâ€‰+â€‰UV laser pulse control of momenta directed to specific products: Quantum model simulations for HOD*â€‰â†’â€‰Hâ€‰+â€‰OD versus HOâ€‰+â€‰D. Physical Chemistry Chemical Physics, 2003, 5, 4806-4813.	2.8	58
17	Theory of ultrafast non-resonant multi-photon transitions: basics and application to CpMn(CO)3. Chemical Physics Letters, 2003, 380, 536-541.	2.6	10
18	Hydrogen adsorption on the tetragonal ZrO2(101) surface: a theoretical study of an important catalytic reactantElectronic supplementary information (ESI) available: data for geometrical and charge differences in detail. See http://www.rsc.org/suppdata/cp/b2/b202330j/. Physical Chemistry Chemical Physics, 2002, 4, 3500-3508.	2.8	77

#	Article	IF	Citations
19	Absorption and Fluorescence Excitation Spectra of 9-(N-carbazolyl)-anthracene:Â Effects of Intramolecular Vibrational Redistribution and Diabatic Transitions Involving Electron Transferâ€. Journal of Physical Chemistry A, 2001, 105, 2911-2924.	2.5	17
20	Analysis and control of laser induced fragmentation processes in CpMn(CO)3. Chemical Physics, 2001, 267, 247-260.	1.9	77
21	Optimal control of rotational motion of dissociation fragments by infrared laser pulses: application to a three-dimensional model of HONO2 in the gas phase at temperatures below 1 K. Chemical Physics Letters, 2001, 339, 243-254.	2.6	3
22	Excited state photoelectron spectroscopy on molecular aggregates containing aromatic molecules. Journal of Electron Spectroscopy and Related Phenomena, 2000, 108, 141-151.	1.7	9
23	Infrared-laser-pulse control of bond- and state-selective excitation, dissociation and space quantization: application to a three-dimensional model of HONO2 in the ground electronic state. Applied Physics B: Lasers and Optics, 2000, 71, 319-329.	2.2	7
24	Fluorescence lifetimes of 9-(N-carbazolyl)-anthracene: Effects of intramolecular vibrational redistribution and electronic transitions in coupled bright and dark states. Journal of Chemical Physics, 2000, 112, 8819-8829.	3.0	7
25	Chemical Reactions in Ionic Molecular Aggregates. An ab initio and R2PI-Study of the Halogenbenzene/Ammonia System. Zeitschrift Fur Physikalische Chemie, 2000, 214, .	2.8	1
26	Infrared-laser control of vibrational state redistribution during molecular dissociation: The time-dependent flux method in model simulations forHONO2in the excited electronic state. Physical Review A, 1999, 60, 3663-3666.	2.5	6
27	Picosecond laser control of bond-selective dissociation and clockwise and anticlockwise rotation of the dissociation fragments: applications to a three-dimensional model of HONO2 in the ground electronic state. Chemical Physics, 1999, 250, 131-143.	1.9	6
28	Selective vibronic excitation and bond breaking by picosecond UV and IR laser pulses: application to a two-dimensional model of HONO2. Chemical Physics Letters, 1999, 313, 332-340.	2.6	7
29	Ultrafast laser control of vibrational dynamics for a two-dimensional model of HONO2 in the ground electronic state: separation of conformers, control of the bond length, selective preparation of the discrete and the continuum states. Chemical Physics, 1998, 232, 111-130.	1.9	12
30	Quasi-Coherent Molecular Vibrations with Energies above the Dissociation Threshold in the Ground Electronic State. Journal of Physical Chemistry A, 1998, 102, 4271-4276.	2.5	11